БЪЛГАРСКА АКАДЕМИЯ НА НАУКИТЕ
НАЦИОНАЛЕН ИНСТИТУТ ПО ГЕОФИЗИКА, ГЕОДЕЗИЯ И ГЕОГРАФИЯ

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МУЛТИМАЩАБНО МОДЕЛИРАНЕ НА ПРЕНОС НА ЗАМЪРСИТЕЛИ В АТМОСФЕРАТА

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УВОД

Качеството на въздуха е ключов фактор както за комфорта и качеството на живот на хората, така и за състоянието на екосистемите, така че голямата обществена значимост на проблемите на атмосферното замърсяване едва ли буди съмнение у някого.

Численото моделиране на атмосферното замърсяване у нас има вече доста дълга история. Началото е поставено в края на 70-те - началото на 80-те години на миналия век (Yordanov et al., 1979a,b, Djolov, Syrakov, 1979, Syrakov, Djolov, 1979, Сираков Д. et al. 1982, Джолов et al. 1983, Syrakov D. 1997a,b).

Скоро след това работа по тази тематика започва и в тогавашния Геофизичен институт на БАН (Ганев, Лазаров, 1979, Ganev and Yordanov, 1981, Syrakov et al., 1983a,b,c, 1987a, 1987b, 1988a, 1988b, 1989a, 1989b, Syrakov and Ganev, 1983, 1989a, 1989b)

В началото на този век в рамките на проекта BULAIR от 5РП на ЕК беше усвоена и адаптирана US EPA Models-3 system. С помощта на тези модели бяха решени следните задачи в рамките на проектите BULAIR (5РП), ACCENT и QUANTIFY (6РП), CECILIA и SEE-Grid-sci, (7РП) и др.

С методите на численото моделиране у нас са решавани най-разнообразни задачи, например:

Изучаване на локалния и регионален пренос над Балканския полуостров, включително обмен на замърсяване между държавите: Dimitrova et al. (2001), Ganev et al. (2008a-d), Prodanova et al. (2005a,b, 2006a,b, 2008b), Syrakov and Prodanova (1997), Syrakov et al. (2001, 2002), Zerefos et al. (2000)

Регионално и локално моделиране на отделни епизоди с цел изучаване на определено явление, разкриване на взаимодействията между процесите и взаимното влияние на различни мащаби: Ganev et al (2003, 2009, 2011), Prodanova (2006c,d, 2007, 2008a), Syrakov E. et al. (1989a,b), Todorova et al. (2009, 2011), Zrefos et al. (1998, 2000, 2004a,b,)

Анализ на риска при аварийно отделяне на отровни вещества в атмосферата: Brandiyska et al. (2011a-c, 2012), Todorova et al. (2010, 2012)

Изследване влиянието на измененията в локалния климат върху замърсяването в България: Syrakov et al. (2009b, 2010, 2011, 2012)

Беше създадена и българска **национална система за прогноза на химическото време:** Etropolska et al. (2010, 2011), Syrakov et al. (2009a)

Вижда се, че въпреки многообразието от решени задачи и многобройните получени резултати, достатъчно мащабни, изчерпателни и детайлни симулации, които да дадат представа за климата на замърсяване на страната **у нас до сега не бяха правени**.

Изброените по-горе работи са основата и в голяма степен мотивацията на настоящия дисертационен труд.

Не пряко, но съществено влияние върху изложената по-нататък работа има обстоятелството, че тя е извършена в една професионално среда с високи научни критерии и съществени постижения в областта на моделиране на замърсяването – например Zlatev, 1995, Zlatev Z. and I. Dimov, 2006, Zlatev, Batchvarova, 2007, Dimov et al., 1996, 1998, 2004 a,b, 2005, Dimov, Zlatev, 2002, Georgiev, Zlatev, 1998, 1999, 2000, 2001, 2006, Georgiev, Donev, 2006, Ebel et al. 2007.

Настоящото изследване има следните цели:

1.) Със средствата на численото моделиране да генерира на статистически **представителен** ансамбъл от достатъчно **надеждни** и **детайлни** симулации на състава на атмосферата в страната. Така дефинираната цел съдържа три ключови думи, които следва да бъдат пояснени:

- Изискването за **представителност** на ансамбъла означава, че той трябва да отразява "почти изчерпателно" възможното многообразие на метеорологични условия, така че получените резултати в съвкупност наистина да характеризират "климата на замърсяване на атмосферата" в страната;
- Изискването за **надеждност** на симулациите означава, че резултатите трябва да бъдат надлежно проверени чрез сравнение с данни от измерванията и да удовлетворяват изискванията за качество на симулациите, дефинирани от националната и европейска нормативна база (European Parliament, 2002 и Приложение №4 към чл.15, т.2 от Наредба №4 от 5.07.2004);
- Изискването за **детайлност** на симулациите означава, че получените полета на различни характеристики на замърсяването трябва да бъдат с достатъчно висока пространствена и времева разрешаваща способност, така че да отразяват конфигурации и да отчитат двустранните взаимодействия от различни (градски-локални-регионални) мащаби;

2.) Изясняване, на основата на получения ансамбъл от симулации, на основните характеристики на климата на замърсяване на страната – типични и екстремни стойности стойности с характерните им денонощен ход, годишна и сезонна повтаряемост.

3.) Изясняване на произхода на замърсяването и проследяване и характеризиране на основните процеси и механизми, водещи до формиране състава на атмосферата в страната;

От практическа гледна точка на настоящия труд следва да се гледа като на разработване на методика за получаване на научно обосновани, надеждни и представителни оценки на състава на атмосферата и неговия произход – основа за формулиране на стратегии за редуциране на замърсяването на въздуха.

Дисертационният труд се състои от четири глави.

В Глава I е направен кратък преглед на различни модели, използвани при моделиране състава на атмосферата и н методиките за инвентаризация на емисиите, накратко са описани числените експерименти и са приведени сравнени на моделните резултати с данни от измерванията.

В Глава II са приведени и коментирани някои от основните резултати относно климата на приземното замърсяване в страната.

Глава III е посветена на изследване приноса на различни категории източници към общата картина на замърсяването в страната.

Глава IV е посветена на изследване на различните процеси на пренос и трансформация и на оценка на приноса им към формиране на общата картина на замърсяването в страната.

Авторът дължи благодарност за плодотворното сътрудничество и постоянния интерес към работата по настоящият дисертационен труд на колегите си К. Ганев (научен ръководител), Д. Сираков, Н. Милошев, М. Проданова, А. Тодорова и Г. Йорданов.

Изключително полезни и крайно необходими бяха консултациите с Е. Атанасов и М. Дурчова от ИИКТ относно работа с компютърни клъстери и grid.

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ГЛАВА I МЕТОДИКА НА ИЗСЛЕДВАНЕТО

В Глава I е представена методиката, с която е проведено настоящото изследване.

В I.2. е направен кратък преглед на съществуващите числени модели и инвентаризации на емисиите и наличните в страната данни от измерванията на качеството на въздуха.

В I.3. накратко е описана методиката на изследване – модели, входни данни, емисионно моделиране, области на интегриране и телескопизация (nesting), организация на числените експерименти.

В I.4. е разгледана верификация на компютърните симулации – сравнение на моделните концентрации с данни от измерванията.

В автореферата ще бъдат накратко предадено само съдържанието на I.3. и I.4.

Методиката на изследване – модели, входни данни, емисионно моделиране, области на интегриране и телескопизация (nesting), организация на числените експерименти.

Изследванията са проведени на базата на препоръчваната и развивана от Американската агенция по околна среда (ААОС) моделна система **Models-3**, която се състои от 3 подсистеми от модели, а именно:

- **CMAQ** (Denis et al.,1996, Byun and Ching, 1999, Byun and Schere, 2006) - **C**ommunity **M**ulti-scale **A**ir **Q**uality model (http://www.cmaq-model.org/), който е съвкупност от подходящо свързани модули за пресмятане на дисперсията на замърсителите (транспорт, дифузия, суха и мокра депозиция) и техните химични трансформации.

- **MM5** (Dudhia, 1993, Grell et al., 1994) - the **5**th generation PSU/NCAR **M**eso-meteorological **M**odel (http://box.mmm.ucar.edu/mm5/) се използва като метеорологичен пре-процесор.
- **SMOKE** (Coats and Houyoux, 1996, Houyoux and Vukovich, 1999, CEP, 2003) - **S**parse **M**atrix **O**perator **K**ernel **E**missions Modelling System (http://www.smoke-model.org/) - е емисионният пре-процесор на системата **Models-3**. Той подготвя емисионния вход за **CMAQ** и, както всеки друг елемент на системата е многокомпонентен – състои се множество модули, които в различните случаи се комбинират по подходящ начин.

Крупномащабните (фонови) метеорологични данни, използвани в изследването са взети от 'NCEP Global Analysis Data' с хоризонтална разрешаваща способност $1^{o}\times1^{o}$. При използване възможностите за 'nesting' на моделите MM5 и CMAQ беше постигната разрешаваща способност от 3 km за територията на България, чрез последователно решаване на задачата в няколко последователни, вместени една в друга области. Най-външната област (D1) е с хоризонтална разрешаваща способност 81 km, областта D2, която обхваща на практика цяла Европа е с хоризонтална разрешаваща способност 27 km, областта D3, като обхваща на Балканския полуостров е с хоризонтална разрешаваща способност 9 km, а най-вътрешната област, обхващаща България е с хоризонтална разрешаваща способност 9 km.

Беше използвана детайлната инвентаризация на емисиите, направена от TNO, Нидерландия (A. Visschedijk et all., 2007). Инвентаризацията на емисиите е направена на годишна база. Замърсителите са изчислени в групи като CH4, CO, NH3, NMVOC (No Methan VOC, VOC - Volatile Organic Compounds), NOx, SOx, PM10 и PM2.5. Тази инвентаризация е направена чрез де-агрегация на емисиите от инвентаризацията на EMEP (Vestreng, 2001, Vestreng et al, 2005).

За интерполация на емисиите в различните мрежи беше използвана GIS технология, чрез която бяха получени съответните площни и точкови източници за различните области на интегриране. Инвентаризацията на емисиите на TNO са дадени за 10 SNAP категории, което, както ще бъде демонстрирано в Глава III, позволява оценката на приноса на различни човешки дейности към общата картина на замърсяване на страната.

CMAQ, както и другите химически транспортни модели, изисква входа му с емисиите да бъде в определен формат отразяващ еволюцията във времето на всички замърсители, включени в използвания химичен механизъм. При подготовката на файла с емисии за **CMAQ**, трябва да се направят известен брой допълнителни процедури:

- Първо, цялата първична информация трябва да бъде интерполирана в съответната избрана мрежа/ мрежи (гридиране от grid – мрежа);
- Второ, трябва да бъдат наложени времеви профили които да модифицират годишните стойности, така че да се отчетат сезонните, седмичните и дневните вариации на работата на източниците.
- Накрая, емисиите от "фамилиите" органични газове и в по-малка степен SO_x, NO_x и PM2.5 трябва да бъдат разцепени или „преобразувани" в по-голям брой компоненти, съгласно изискванията за емисионен вход на **CMAQ**, които пък зависят от избрания химически механизъм – процедура, наречена "speciation".

При това всеки от различните типове източници: площни (AS), големи точкови (LPS) и биогенни (BgS) следва да се третира по специфичен начин. (емисиите от транспорта също са отделна категория, но поради начина на инвентаризирането им у нас те се обединяват с площните източници). Очевидно, емисионните модели са необходими пре-процесори за моделите на химичните трансформации и пренос на замърсители. Такъв компонент в **Models-3** системата е **SMOKE**. За съжаление, както вече беше отбелязано, той е много силно адаптиран към условията в САЩ – инвентаризации на емисиите, административно деление, категоризации, горивни процеси и т.н..

За целите на настоящото изследване времевите вариации на емисиите са изчислени на базата на дневни, седмични и месечни профили предоставени в (Builtjes et al., 2003, Schaap et al., 2008). Тези времеви профили са специфични за държава, замърсител и относно SNAP (Selected Nomenclature for Air Pollution).

Процедурата по "speciation" е зависима от използвания химичен механизъм. **CMAQ** поддържа различни химични механизми. За целите на озоновото моделиране най-често се използва Carbon Bond v.4 **- CB4** (Gery et al., 1989). Основата на **CB4** механизма е това че реактивността на органичните компоненти в атмосферата може да бъде симулирана добре от различни механизми представящи различни типове въглеродни връзки. От времето на публикуването **CB4**, са направени няколко промени. По-специално, добавена е химия на **PM**. Във версия 4.6 на **CMAQ CB4** е обновен с версия 1.7 на ISORROPIA aerosol model (Nenes ej al., 1998). Според този комбиниран механизъм (CB4-aero3) 10 органични и 5 PM2.5 съставки са добавени към входа с другите неорганични газове.

Разработен беше специфичен подход за осъществяване на това разцепване (speciation). Предлага се за целите на прогноза нивата на озона в нашата страна да се следва технологията разработена от US EPA Emission Factor and Inventory Group (Ryan, R., 2002). Всичката необходима информация може да бъде свалена от съответния уеб сайт (виж цитираната работа в Литературата към този отчет). На същото място може да се намерят профилите на спесиация както на VOC, така и на PM2.5, NOx и SOx и съответните справочни таблици. Много удобно е това че профилите са специфични за химичния механизъм давайки директно разделяне на коефициентите от количеството на VOC в [g/s] към блоковите замърсители в [moles/s], което е изискваният вход на емисиите за CMAQ.

Директното използване на тези доста детайлни данни не е възможно извън Северна Америка защото US EPA SCC (Source Category Code) съдържа около 10000 типа източника, докато CORINAIR съдържа по-малко от 300 типа източника и само 11 SNAP категории. За преодоляване на тази трудност, на основата на експертно проучване бяха открити редица съвпадения между главни Български източници за всеки SNAP и подобни на тях SCC източници. Тегловните (теглата са приноса в проценти на всеки тип източник съгласно US EPA SCC към съответната обща Българска емисия за съответния SNAP) средни за съответните профили на разцепване (speciation) от US EPA SCC са приети като разделящи фактори, специфични за съответния SNAP.

Входната информация, необходима за изчисляване на емисиите са мрежови данни за площните източници (Area Sources – AS), за мощните точкови източници (Large Point Sources – LPS) и данни за характера на земната повърхност (LandUse), необходими за моделиране на естествените (или биогенни) източници (BgS). Последните емитират органика, CO и NO и стойностите им зависят силно от метеорологичните условия, включително слънчевото греене.

SMOKE се използва и за направата на файл с третия вид емисии - биогенните емисии. **SMOKE** в момента поддържа механизма BEIS (Biogenic Emissions Inventory System), версии 2 и 3 (Pierce et al., 1998, Guenther et al., 2000). BEIS2 и BEIS3 се захранват с пространственото разпределение на вида подложна повърхност за първата стъпка от процеса – пресмятане на нормализираните емисии за всяка клетка от мрежата и за всяка категория подложна повърхност (това са емисиите при фиксирани стандартни метеорологични параметри). Финалната стъпка е привеждането на нормализираните емисии към актуални емисии на базата на гридирана, почасова метеорологична информация. В сегашната версия на **SMOKE** е вграден механизма BEIS3.13 (Schwede et al., 2005).

Метеорологичния пре-процесор MM5 беше форсиран с глобалните метеорологични данни 'NCEP Global Analysis Data' с хоризонтална разрешаваща способност $1^{o}\times1^{o}$. В областта D1 моделът е конфигуриран така, че се захранва с крупномащабните данни за температура, влажност и вятър посредством процедура на четиримерна асимилация (FDDA - Stauffer and Seaman, 1990). За всички области (D1, D2, D3, D4) MM5 работи едновременно в режим на "two-way nesting" – решенията в по-вътрешните области влияят на решението в по-външните. Вертикалната резолюция за всички области е 23 σ-нива до височина 100 hPa. MM5 симулациите са направени на периоди от по 3 дни.. Всеки от периодите има начален 12-часов период на "spin-up", който се препокрива с последните 12 часа на предходния период.

Метеорологичния вход за CMAQ се генерира от изхода на MM5 с помощта на метеорологично-химичния интерфейс MCIP, v2.3. Симулациите със CMAQ са проведени само в области D2, D3 и D4. За начални условия в началния момент на симулациите са използвани стандартни за CMAQ (default) профили на концентрациите, които са получени от глобални модели. Граничните условия за по-вътрешните области се генерират от решението в съответната външна. Химическият механизъм CB-4 с хетерогенна (Aqueous-Phase) химия и MEBI (Modified Eulerian Backward Iterative) метод за решаване уравненията на химични трансформации бяха използвани във всички области на интегриране. Симулациите със CMAQ бяха направени с вертикална резолюция от 15 σ-нива. Проведени бяха паралелни пресмятания с пет емисионни сценария:

Сценарий 1: емисионни данни за Европа и България, съгласно инвентаризацията направена от TNO, Нидерландия (A. Visschedijk et all., 2007).

Сценарий 2: Биогенните емисии в България редуцирани с фактора 0.8

Сценарий 3: Емисиите от SNAP категория 1 (енергетика) в България редуцирани с фактора 0.8

Сценарий 4: Емисиите от SNAP категория 7 (пътен транспорт) в България редуцирани с фактора 0.8

Сценарий 5: Емисиите от SNAP категория 2 (не индустриални изгаряния) в България редуцирани с фактора 0.8

Пресмятанията с MM5/CMAQ бяха направени за 8 години - от 2000 до 2007.

Верификация на компютърните симулации – сравнение на моделните концентрации с данни от измерванията.

Симулационните качества на моделите от **Models-3 system** са многократно проверявани и не подлежат на съмнение. Това, обаче, не гарантира автоматично и добро качество на компютърните симулации. Те зависят не само от използваните модели, но също така и от входните данни (качество, пространствено-времева разрешаваща способност) от емисионното моделиране, от правилно подбрани и комбинирани опции на моделите.

Ето защо беше направена проверка на получените моделни резултати посредством сравнение с измерени концентрации в станциите от националната система за контрол качеството на атмосферния въздух (НАСЕМ) са МОСВ.

Данните от измерванията имат задоволително качество. По друг начин стои въпросът с една друга много важна характеристика на данните - тяхната ***представителност***. КАВ се наблюдава в по-големи градове и в места, в които съществува вероятност от влошаване здравето на населението в следствие замърсяване на атмосферата. С други думи мрежата на НАСЕМ е конфигурирана така, че да контролира потенциално най-опасните нива на замърсяване и за това измерванията в станциите и са представителни най-вече само за точките в които се правят измерванията. Например, автоматичната станция разположена на Орлов мост е представителна само за Орлов мост и едва ли за район с размери 3×3 км, каквато е изчислителната мрежа.

В НАСЕМ има само една фонова станция – тази на в. Рожен.

Бяха направени графики на разпръскването (Scatter diagrams) на данните от измерването и моделирането за SO_2, NO_2 и Озон. Един кратък съвместен преглед на всички графики води до следните обобщени изводи:

1.) Картината е доста различна за различните станции и за различните замърсители.

2.) Като правило симулациите подценяват нивата на SO_2 и NO_2. Това е лесно обяснимо, като се има пред вид, че станциите са разположени така, че да контролират потенциално най-опасните нива на замърсяване и за това измерванията в станциите и са представителни най-вече само за точките в които се правят измерванията, докато симулациите дават концентрации пространствено осреднени в клетки с размери 3×3 км.

3.) Съвпадението при озона е, като че ли по-добро. Това вероятно се дължи на факта, че озонът е вторичен замърсител, чиито концентрации не са толкова тясно свързани с детайлната конфигурация и времеви ход на емисиите (входни данни, изчислени със съществена неопределеност). Следва, също така, да се отбележи, че практически за всички станции се наблюдава известно надценяване от модела на по-ниските озонови концентрации, а това означава, че моделните оценки за евентуални опасни озонови концентрации могат да бъдат по-силни от тези, направени на базата на измервания.

4.) За доста от станциите голямата част от отклоненията на измерванията от данните са в границите ± 50%, а това означава, че в доста голяма степен е удовлетворено изискването за не повече от 50% неопределеност за едночасовите дневни средни стойности, дефинирано в съответните европейски директиви (European Parliament, 2002) и Приложение №4 към чл.15, т.2 от Наредба №4 от 5.07.2004.

Направено е сравнение и на пълзящите 8-часови средни (важна характеристика при определяне на озоновия индекс NOD60, измерващ отражението на озоновите концентрации върху човешкото здраве) на симулираните и измерени нива на озона. Резултатите за някои от станциите са показани на **Фиг. I.1.**

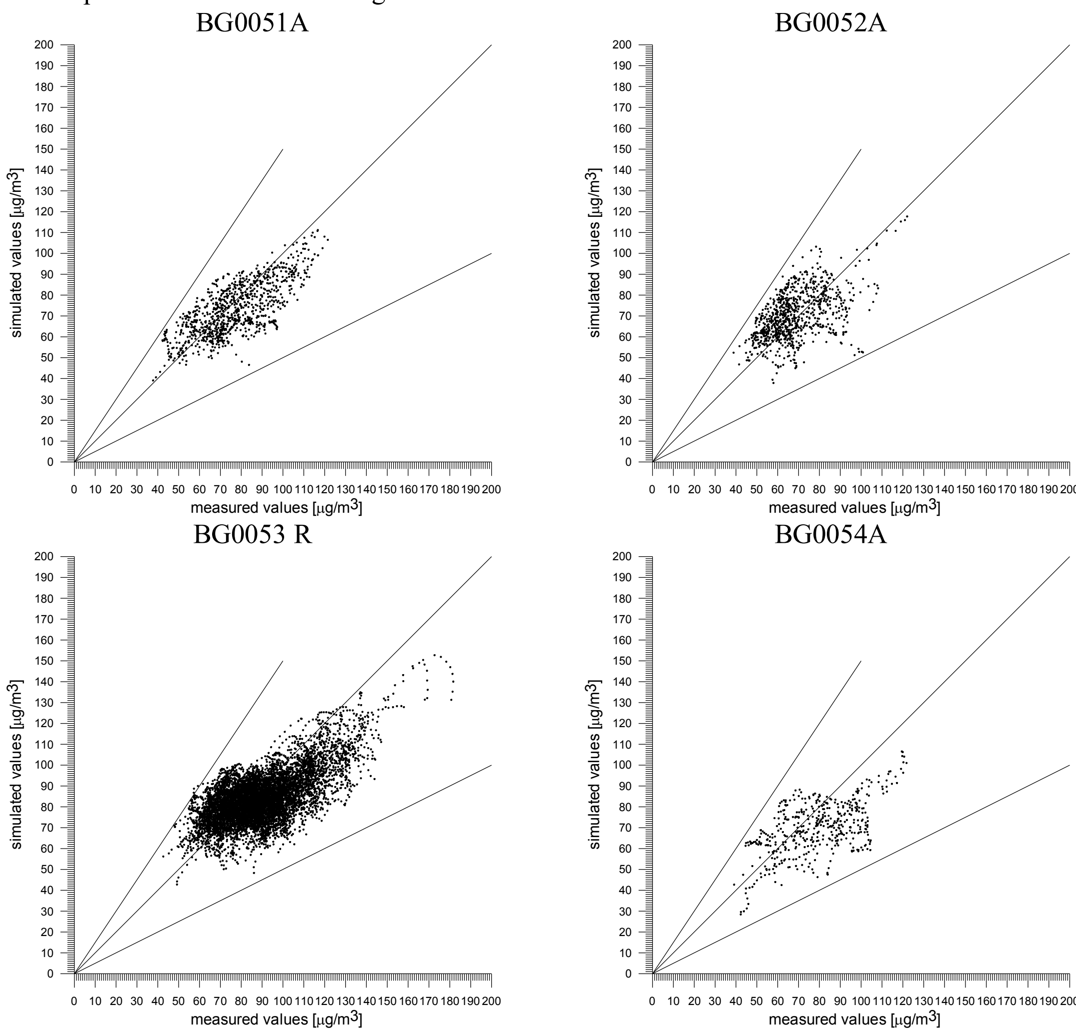
Веднага се забелязва, че съвпадението между симулирани и измерени стойности при 8-часовите пълзящи средни е много по-добро, отколкото при часовите стойности. Очевидно е по-малкото разсейване на точките около линията на идеално съвпадение, както и по-добрата корелация между симулирани и измерени стойности.

Категорично е удовлетворено цитираното по-горе изискване за не повече от 50% неопределеност.

Показаните Scatter diagrams дават много нагледна оценка за степента на съвпадение на моделните резултати с данните от измерванията. Наред с тях са изчислени и някои характеристики (статистически оценки), обективно оценяващи състоятелността на генерирания ансамбъл от компютърни симулации.

Стойностите на съответните статистически характеристики за различни замърсители в станциите на НАСЕМ са показани в дисертацията. Заедно с тях е показан и процентът случаи, когато отклоненията на симулациите от измерванията са в границите ± 50%.

Изводите, които могат да бъдат направени от таблицата по същество съвпадат с тези, направени при анализа на Scatter diagrams.



Фиг. I.1. Сравнение на осреднените с 8-часово пълзящо средно приземни концентрации на озон пресметнатите при **емисионен сценарий 1** със съответно осреднените данни от измерванията в съответните станции на НАСЕМ

Като се има пред вид съществената неопределеност на емисионните входни данни и само частичната представителност на станциите от НАСЕМ, може да се направи заключението, че съвпадението на симулираните резултати с данните от измервания е достатъчно добро (отклоненията са в разумни граници). Това показва, че ансамбълът компютърни симулации като цяло е достатъчно надеждна основа, на която да се правят изводи относно климата на замърсяване на страната, така че разглежданията и изводите в следващите глави имат смисъл.

ГЛАВА II НЯКОИ ОСНОВНИ ФАКТИ ОТНОСНО КЛИМАТА НА АТМОСФЕРНОТО ЗАМЪРСЯВАНЕ В БЪЛГАРИЯ

В резултат на проведените числени симулации беше генериран ансамбъл, достатъчно обемен и изчерпателен, за да може на негова основа да се направи надеждна оценка на климата на атмосферно замърсяване на страната – да се очертаят типични и екстремни характеристики на замърсяването с тяхната повторяемост, пространствена и времева (денонощна, сезонна) изменчивост.

В настоящата ГЛАВА II са показани някои от основните факти относно климата на атмосферно замърсяване в България, изведени от резултатите от компютърните симулации. В този смисъл в параграф II.2. са представени някои осреднени по ансамбъла приземни концентрации на замърсители за територията на България и за отделни точки, а също така и абсолютните максимални, получени при анализ на целия ансамбъл, концентрации за съответния замърсител. В II.3. са представени някои статистически характеристики на осреднените приземни концентрации на различни емисии за територията на България и за отделни точки. В същият параграф са показани и примери за плътността на вероятностно разпределение за някои от основните замърсители с тяхната сезонна и географска изменчивост. И най-накрая в II.5. са представени някои от най-използваните и важни индекси на озоново замърсяване, които са важни не само за човешкото здраве, но също така, горското и селското стопанство.

В автореферата по-подробно ще бъдат коментирани само годишно осреднените двумерни полета на концентрациите, някои статистически характеристики на приземните концентрации на различни замърсители за територията на България и за отделни точки и индексите на замърсяване

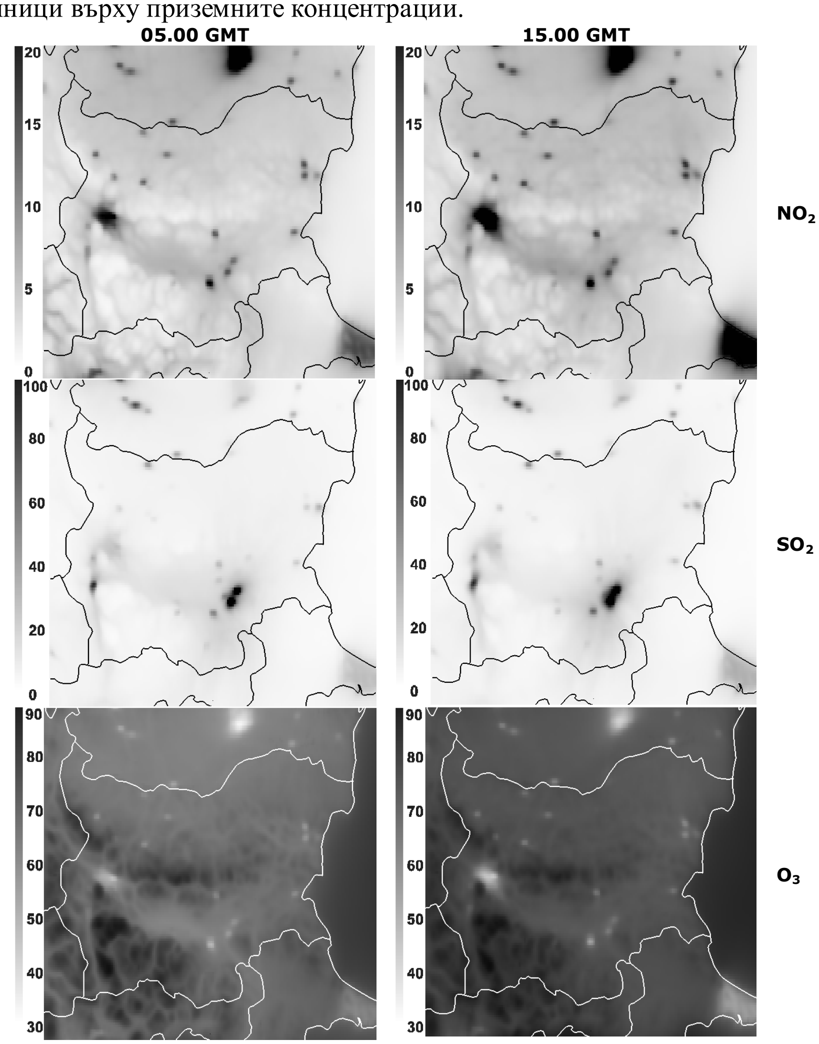
Двумерни осреднени полета на приземните концентрации

Чрез осредняване по 8 годишният ансамбъл на получените чрез числени експерименти полета за различните замърсители могат да бъдат получени средните годишни и сезонни приземни концентрации. Те могат да бъдат разглеждани като "типични" годишни или съответно сезонни денонощни концентрации. От ансамбъла могат да се изведат и абсолютните максимални годишни и сезонни концентрации, също със своя денонощен ход.

Карти за тези "типични" средни и максимални, годишни и по сезони приземни концентрации за отделните замърсители са представени и описани в приложение **II.1.**. Най-известните замърсители, за които тези характеристики са коментирани в самата дисертация са – азотен диоксид (NO_2), озон (O_3), изопрен (ISOP), серен диоксид (SO_2), амония/ амоняк (NH_3), амоний/ амониум (PNH_4), първични органични аерозоли (POA), вторични органични антропогенни аерозоли (SOAA), вторични органични биогенни аерозоли (SOAB), едри прахови частици (CPRM) и фини прахови частици (FPRM), за 05:00, 11:00, 17:00 и 23:00 GMT.

Пример за някои двумерни осреднени полета на приземните концентрации е даден на **Фиг. II.1.**

От картите на средно годишните приземни концентрации на NO_2 се вижда, концентрациите не са много високи и имат добре изразен денонощен ход. В 05:00 часа добре се открояват големите градове с най-високи стойности, като на определени места в тях те достигат около 25μg/m^3. Основната пътна мрежа се характеризира със стойности около 10μg/m^3, като за някои промишлени предприятия и топло електрически централи те са около 20μg/m^3, а типичните стойности за областта са около 5μg/m^3. В 11:00 часа средните стойности в цялата област намаляват и клонят към нулата, влиянието на почти всички източници също намалява, като само София и някои от ТЕЦ-овете оставят леки следи от по-високи стойности върху картата, това не е никак странно имайки в предвид, че по това време на деня е най-активното формиране на озон. По-голямата неустойчивост на атмосферата в обедните часове, която обуславя по-интензивен вертикален пренос, също води до намаляване на приземните концентрации от предимно наземните източници на NO_2. В 17:00 приземните концентрации на NO_2 са най-високи, като над големите градове те достигат максимални стойности от 30μg/m^3, като това най-вероятно е свързано с факта, че именно тогава е най-интензивен автомобилният транспорт (виж Глава **III.**). Стойностите над основната пътна мрежа са около 12μg/m^3, а над предприятията и ТЕЦ-овете до около 20μg/m^3. Типичните стойности за областта са около 7μg/m^3, а планините се открояват като места с нулеви стойности. В 23:00 часа типичните средни стойности за областта се запазват, като над планините те отново те са най-ниски. Влиянието на предприятията, ТЕЦ-овете и големите градове силно намаля и концентрациите им стават почти колкото тези на основната пътна мрежа които са около 10-15μg/m^3. Отново се проявява ефектът на атмосферната стратификация – предимно устойчива през тази част на денонощието, което обуславя по-малко интензивен вертикален обмен и съответно по-голямо влияние на приземните и по-малко на високите източници върху приземните концентрации.



Фиг. II.1. Приземни годишно осреднени концентрации на NO_2, SO_2 and O_3 [μg/m^3] в 05.00 и 17.00 GMT

Топло електрическите централи и големите градове са водещият фактор за високите абсолютни максимални осреднени за целият ансамбъл концентрации на NO_2. Като в 05:00 часа се открояват само ТЕЦ-овете Марица Изток, София и доста обширни области около тях със стойности до около 70μg/m^3, като средно за страната те са около 10μg/m^3, а над планините клонят към нулата. В 11:00 часа максималните концентрации над областта леко нарастват, като над планините си остават нулеви, областите около ТЕЦ-овете Марица Изток и София намаляват, а също така и самите максимални концентрации намалят до около 60μg/m^3. Именно тогава започват да се открояват и ТЕЦ-овете Варна и Бургас със стойности от около 30μg/m^3. В 17:00 и 23:00 часа влиянието на всички ТЕЦ-ове е добре изразено, като то се разпростира на обширни територии около тях и най-вече това на Марица Изток и София, чиито стойности са около 90μg/m^3.

От полетата за средните годишни приземни концентрации на NO_2 и нормите за ПДК, може да се заключи, че СГН се превишава в 17:00 часа само в София, а СЧН не се превишава.

От картите на средно годишните приземни концентрации на озон (O_3) се вижда, че по всяко време на денонощието неговите минимални стойности са 30 - 50μg/m^3. Едно интересно нещо, което се забелязва на картите, е че местата, които се явяват като консуматори на озон са именно местата, на които са високи средните стойности на NO_2, като големите градове, основната пътна мрежа, някои промишлени предприятия и топло електрически централи.

Освен това над морето средните стойности са доста високи около 75μg/m^3, дължащо се най-вероятно на липсата на естествени консуматори на озон какъвто е NO_2, както и на обстоятелството, че озонът не се поглъща от водни повърхности. По планините и най-вече по високите им части, той е с максимални или близки до максималните средни стойности около 85μg/m^3. Това най-вероятно се дължи на факта че това са места, които са далеч от източници на NO_2, които са основни консуматори на озон.

На тези карти също така се вижда, че в 05:00 часа стойностите му са най-ниските, като типичните концентрации за района са около 75μg/m^3. Добре се открояват големите градове, някои предприятия и ТЕЦ-ове с концентрации около 40μg/m^3, също така пътната мрежа със стойности около 60μg/m^3, а високите части на планините Рила, Пирин, Родопите и Стара планина са със стойности до около 85μg/m^3. В 17:00 часа е почти както в 05:00 часа, както концентрациите над основната пътна мрежа нарастват и се изравняват с типичните за страната и почти навсякъде стават около 70μg/m^3, а големите градове, някои предприятия и ТЕЦ-ове се открояват със същите концентрации от около 40μg/m^3. Стойностите над високите части на планините се запазват около 85μg/m^3, като в останалите техни части и над морето те нарастват и стават около 80μg/m^3. В 23:00 часа е почти същото както в 05:00 и 17:00 часа, като почти навсякъде средните стойности се изравняват и стават около 70μg/m^3, като само района на София се откроява, като място с по-ниски стойности от около 50μg/m^3.

За високите части на планините и над морето концентрациите си остават същите около 80-85μg/m^3. В 11:00 часа приземните концентрации на O_3 са най-високи, като почти навсякъде те са около 80μg/m^3, като над планините те са до около 90μg/m^3, а само над ТЕЦ-овете София, Варна, Бургас и Марица Изток те са около 70μg/m^3. Доказателство за изказаното по-горе твърдение, че в 11:00 часа ниските приземни годишно осреднени концентрации на NO_2 най-вероятно се дължат на активното формиране на озон се потвърждава точно на тези карти в 11:00 часа за средните концентрации на озона. Защото именно тогава се наблюдават високите средни стойности на O_3.

Абсолютните максимални осреднени за целият ансамбъл годишни приземни концентрации на озон (O_3) са максимални само по планините и са около 115μg/m^3, като в 05:00 часа над останалата част от областта те са около 100μg/m^3. В 11:00 часа максималните концентрации в областта са най-високи и са около 110μg/m^3, като те са по-високи в северозападна България около 115μg/m^3, като над София и ТЕЦ Марица Изток те са около 120μg/m^3. Също така покрай морския бряг максималните концентрации са доста високи и са около 120μg/m^3. В 17:00 часа стойностите на максималните концентрации навсякъде намаляват. София и някои предприятия се открояват като места с най-ниски стойности около 100μg/m^3, а районите около някои от тях като места с по-високи от средните за страната, това най-вероятно се дължи на времето за реакция на фотохимичните процеси и метеорологичните условия. Отново тогава покрай морския бряг максималните концентрации са по-високи от типичните за страната, като за района на Варна те са най-високи и са около 130μg/m^3. В 23:00 часа стойностите още намаляват навсякъде, и докато по крайбрежието и над планините те са около 115μg/m^3, то над останалата част от страната те са около 100μg/m^3

От разгледаните полета за средните концентрации на O_3 и нормите за ПДК може да се заключи, че средностатистически няма места на които тя да се превишава

На картите за изопрен (ISOP) се вижда, че през цялото време най-ниските стойности са над планините, северозападната част на Дунавската равнина и най-вече през нощта. В останалата част от страната стойностите са по-високи около 0,4μg/m^3, най-вече в Дунавската равнина, като в 05:00 часа най-високите концентрации именно там и са около 0,6μg/m^3. В 11:00 часа стойностите нарастват навсякъде с изключение по планините, като на места в южната част на Дунавската равнина те стават около 0,9μg/m^3. В 17:00 часа концентрациите на изопрен още нарастват и се обособяват загладени зони в северна България с високи стойности около 0,8μg/m^3. В 23:00 часа концентрациите на изопрен в цялата област са много малки почти нулеви, което най-вероятно е свързано с липсата на производство му от растенията и производството на озон.

Абсолютните максимални осреднени за целият ансамбъл годишни приземни концентрации на изопрена са най-ниските стойности за по високите части на планините, северозападната част на Дунавската равнина и най-вече през нощта. В 05:00 и 11:00 часа стойностите са най-високи и са около 8-9$\mu g/m^3$ на отделни но и обширни зони в Дунавската равнина, а в останалата част от страната те са около 3$\mu g/m^3$. В 17:00 часа е времето, когато максималните концентрации са най-високи, като над почти цяла северна и на места в западна България стойностите са най-високи и са около 10$\mu g/m^{3,}$ а над планините те са най-ниски и достигат до 1$\mu g/m^3$. В 23:00 часа концентрациите са най-ниски и над почти цялата област те клонят към нулата, като само на отделни места се забелязват леко по-високи стойности от около 1$\mu g/m^3$, които най-вероятно се дължат на високите му стойности от по-предните часове, метеорологичните условия, а също така и на ниските стойности на NO_2, който спира образуването на озон и съответно консумацията на изопрен.

На картите за средните приземни концентрации на серен диоксид добре се открояват местоположенията и областите на влиянието на ТЕЦ-овете, като цяло над планините, а също така и в северна България концентрациите са най-ниски и са около 5$\mu g/m^3$. Избран е точно този обхват на скалата, а не стойностите на п.д.к., за да може да се илюстрират местоположението и на какво разстояние може да се усети влиянието на източниците на SO_2. В 05:00 и 17:00 часа местоположение на всички ТЕЦ-ове се вижда добре, като над тези зони средните концентрациите са около 70$\mu g/m^3$, с изключение на комплекса Марица Изток където стойностите са максимални и са над 125$\mu g/m^3$. В 11:00 часа се виждат само два от ТЕЦ-овете, първият е ТЕЦ Бобов дол със стойности около 50$\mu g/m^3$, чийто емисии на SO_2 се разпростират по почти цялото дефиле на река Струма. Вторият е комплексът Марица Изток със стойности над 100$\mu g/m^3$, като концентрациите над останалата част от страната са почти около нулата. В 23:00 часа е почти както в 11:00 часа отново се виждат само двата ТЕЦ-а, но концентрациите от ТЕЦ Марица Изток са почти колкото тези от ТЕЦ Бобов дол около 50$\mu g/m^3$, като тогава емисиите на SO_2 от тези два ТЕЦ-а се разпростират над почти цяла южна България, с изключение над планините в нея.

Топло електрическите централи най-вече ТЕЦ Бобовдол и комплекса Марица Изток, чиито емисии се разпространяват над почти цяла източна България и са водещият фактор за високите абсолютни максимални осреднени за целият ансамбъл концентрации на серният диоксид (SO_2).

От разгледаните полета за средните концентрации на SO_2 и нормите за ПДК може да се заключи, че места на които СДН може да се превиши са само под комините на ТЕЦ Марица Изток.

От разгледаните полета за максималните концентрации на SO_2 и нормите за ПДК може да се заключи, че местата на които СЧН може да се превиши са над и около ТЕЦ Бобовдол и

На картите за средните приземни концентрации на амоняк/ амониа (NH_3) добре се открояват местоположенията и областите на влиянието на местата свързани с неговото производство, като места с максимални или завишени средни стойности, а планините и ТЕЦ-овете като места с почти нулеви концентрации. В 05:00 и 17:00 часа в България най-високите концентрации над 2,5$\mu g/m^3$ са около местата свързани с неговото производство, а именно Враца, Девня, Стара Загора и Димитровград. Най-ниските концентрации са над планините и над ТЕЦ-овете в София, Перник и Марица Изток, което е свързано с процеса на десулфуризация, като средно за страната те са около 1$\mu g/m^3$. В 11:00 часа концентрациите са най-ниски и само Димитровград, Стара Загора и Враца се открояват, като места с леко по-високи концентрации около 1,5$\mu g/m^3$, докато над останалата част от областта те са около 0,5$\mu g/m^3$. В 23:00 часа е почти както в 11:00 часа, но почти над цяла България концентрациите са по-високи и са около 1$\mu g/m^3$, само София се откроява с леко по-високи стойности от около 1,5$\mu g/m^3$, а концентрациите са най-ниски само по планините.

Водещият фактор за високите абсолютни максимални осреднени за целият ансамбъл концентрации на амоняк/ амония (от над 20$\mu g/m^3$) са предприятията свързани с неговото производство. За България това са само Враца, Стара Загора и Димитровград, а за Румъния Слобозия, Турну Мъгуреле и Крайова. Типичните максимални концентрации за областта са около 4$\mu g/m^3$, а над планините клонят към нула.

От разгледаните полета за средните и максималните концентрации на NH_3 и нормите за ПДК може да се заключи, че няма места на които тя да се превишава в смисъл на средно по ансамбъла.

Полетата на средните приземни концентрации на амоний/ амониум, доста наподобяват тези за амонякът, като при него ТЕЦ-овете вече не се явяват като места, където той е с минимални средни стойности, а като места в които той се образува и е с максимални средни стойности.

Водещият фактор за високите абсолютни максимални осреднени за целият ансамбъл концентрации на амоний/ амониум (PNH_4) са предприятията свързани с неговото производство, като за България това са София, Враца, Девня, Стара Загора и Димитровград. Високите стойности над Румъния и северна България най-вероятно се дължат на източниците в Девня, Букурещ, Турну Мъгуреле, Крайова и Слобозия. Максималните годишни приземни концентрации на PNH4 остават най-ниски единствено над планините, като места с най-високи максимални концентрации.

Прахът е основен атмосферен замърсител на въздуха. Вредният му здравен ефект зависи главно от размера и химичния състав на суспендираните прахови частици, от адсорбираните на повърхността им други химични съединения, в това число мутагени, ДНК - модулатори и др., както и от участъка на респираторната система, в която те се отлагат. Основни източници на прах са промишлеността, транспорта и енергетиката.

Влиянието им върху човешкото здраве се изразява, когато прахът постъпва в организма предимно чрез дихателната система, при което по- едрите частици се задържат в горните дихателни пътища, а по- фините частици (под 10 μm - ПЧ10) достигат до по-ниските отдели на дихателната система, като водят до увреждане на тъканите в белия дроб. Деца, възрастни и хора с хронични белодробни заболявания, грип или астма са особено чувствителни към високи стойности на ПЧ10.

Наред с това се различават и ПЧ2.5 (фини прахови частици), които са с размери по 2.5 μm. частиците с размери между 10 и 2.5 μm в настоящия труд са наречени едри прахови частици (CPRM).

Вредният ефект на замърсяването с прах е по-силно изразен при едновременно присъствие на серен диоксид в атмосферния въздух. Установено е тяхното синергично действие по отношение на дихателните органи и откритите лигавици. То се проявява с дразнещо действие и зависи от продължителността на експозицията. Кратковременната експозиция на 500μg/m^3 прах и серен диоксид увеличава общата смъртност при населението, а при концентрации наполовина по-ниски се наблюдава повишаване на заболяемостта и нарушаване на белодробната функция. Продължителната експозиция на серен диоксид и прах се проявява с повишаване на неспецифичните белодробни заболявания, предимно респираторни инфекции на горните дихателни пътища и бронхитни - при значително по-ниски концентрации от (30 - 150μg/m^3), което е особено силно проявено при деца. Най-уязвими на комбинираното въздействие на праха и серния диоксид са хронично болните от бронхиална астма и от сърдечносъдови заболявания.

С Наредба № 9 (ДВ, бр. 46/1999 г.), (изм. и доп. ДВ, бр. 86/2005 г.) са приети норми за пределно допустими концентрации (ПДК) за фини прахови частици. Въведените ПДК целят предпазване от техния вреден ефект върху здравето на хората и околната среда. Регламентирани са следните ПДК за фини прахови частици:

От полетата на средните приземни концентрации на едрите прахови частици (CPRM) се вижда, че типичните за страната концентрации са около 1μg/m^3, като през цялото денонощие те са най-ниски над планините. В 05:00 и 17:00 часа местата с максимални средни концентрации от 5μg/m^3, са над някои от техните основни източници най-вече над ТЕЦ-овете Марица Изток, София, Перник и Бобов дол. Другият основен източник на CPRM са предприятия, които също се открояват на картите за тези два часа със стойности от около 2,5μg/m^3. Средните концентрации в 11:00 часа са най-ниски около 0,5μg/m^3, като максимални концентрации се наблюдават само над и около ТЕЦ-овете Марица Изток и София. В 23:00 типичните за страната концентрации са по-високи и се разпределят по-равномерно над цялата страна, като емисиите от ТЕЦ Марица Изток намаляват до около 3μg/m^3, а тези от ТЕЦ София растат и покриват по-обширна територия. около източникът тях.

От разгледаните полета за средните концентрации на CPRM и нормите за ПДК може да се заключи, че места на които тя може да се превиши са над ТЕЦ София, ТЕЦ Перник, ТЕЦ Бобов дол и ТЕЦ Марица Изток.

Водещият фактор за високите абсолютни максимални осреднени за целият ансамбъл концентрации на едрите прахови частици (CPRM) са само около някои от техните източници, а това са ТЕЦ-овете - София, Перник, Варна, Бобов дол и Марица Изток. Планините Рила, Пирин и Родопи се открояват през цялото денонощие, като места с най-ниски максимални стойности.

От полетата на средните приземни концентрации на фините прахови частици (FPRM, или

ПЧ2.5) се вижда, че типичните за страната концентрации са около 0,5μg/m^3, като през цялото денонощие те са най-ниски над планините. В 05:00 и 17:00 часа местата с максимални средни концентрации от 5μg/m^3, са над някои от техните основни източници най-вече над ТЕЦ-овете Марица Изток и София. Другите ТЕЦ-ове и предприятия също се открояват на картите за тези два часа със стойности от около 2,5μg/m^3. Средните концентрации в 11:00 часа са най-ниски под 0,5μg/m^3, като се открояват само ТЕЦ-овете Марица Изток, Бобов дол и София със стойности от около 2μg/m^3. В 23:00 типичните за страната концентрации са по-високи около 1μg/m^3 и се разпределят по-равномерно над цялата страна, като емисиите от ТЕЦ Марица Изток и ТЕЦ София покриват по-обширна територия. около източникът тях.

Водещият фактор за високите абсолютни максимални осреднени за целият ансамбъл концентрации на фините прахови частици (FPRM са само около ТЕЦ Марица Изток. ТЕЦ-овете София и Бобов дол също се открояват на картите за максималните годишни концентрации на FPRM, но с по-ниски стойности от около 15μg/m^3. Планините Рила, Пирин и Родопи се открояват през цялото денонощие, като места с най-ниски максимални стойности.

От разгледаните полета за средните концентрации на FPRM и нормите за ПДК може да се заключи, че места на които тя може да се превиши са над ТЕЦ София, ТЕЦ Перник, ТЕЦ Бобов дол и ТЕЦ Марица Изток.

Статистически характеристики на приземните концентрации на различни замърсители за територията на България и за отделни точки.

Показаните по-горе средногодишни и максимални концентрации на някои съединения не изчерпват информацията, която може да бъде извлечена от компютърно симулирания осем годишен ансамбъл. Той е достатъчно голям и изчерпателен за да позволява разнообразни статистически обработки.

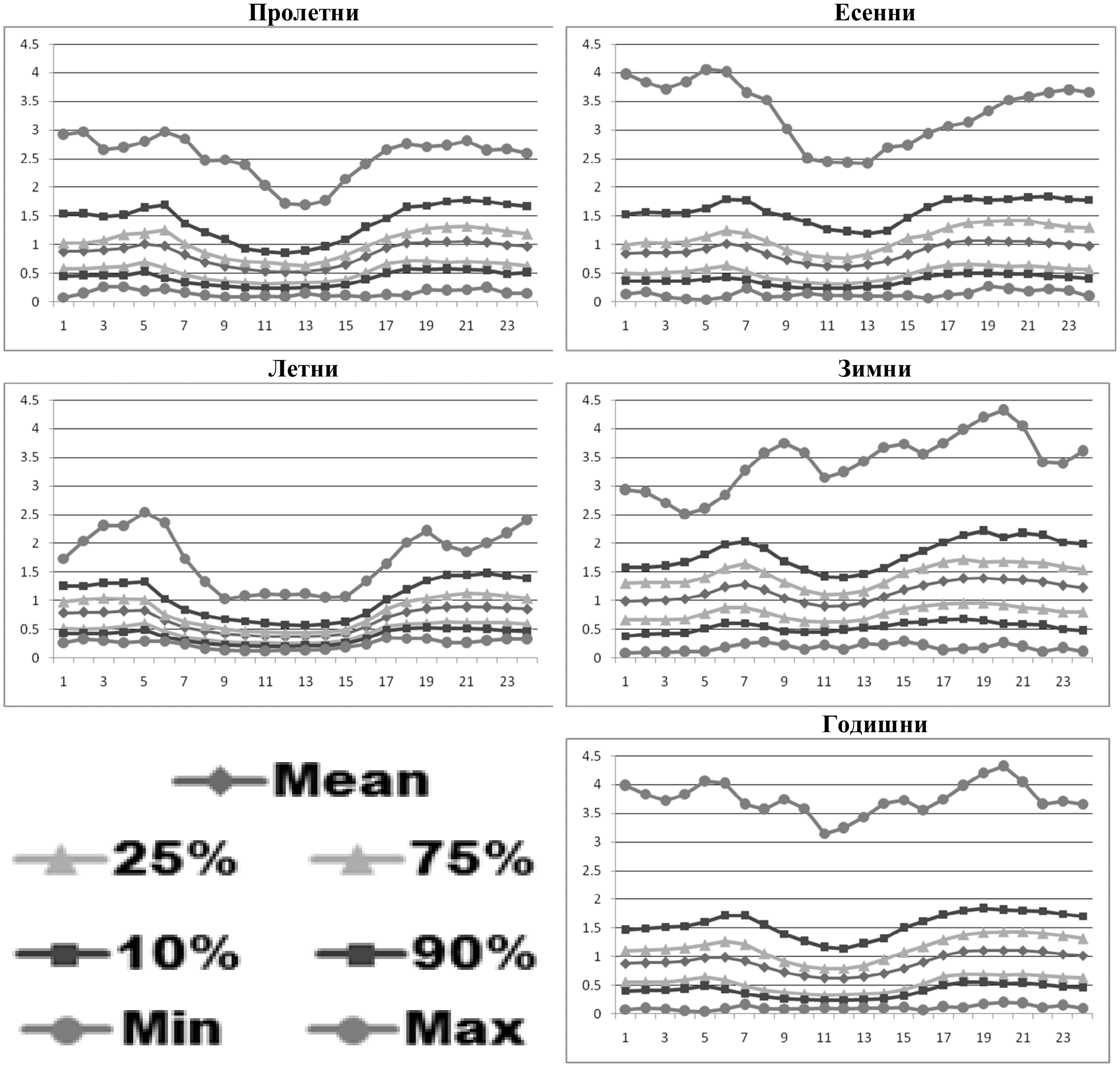
В параграфи II.3.1- II.3.4 от дисертацията са представени графики, които нагледно и лесно разбираемо показват основни ансамблови характеристики на замърсяването. На всички графики са изобразени следните сезонни и годишни характеристики за различни замърсители, осреднени за страната или в отделни нейни точки: средни, минимални и максимални по ансамбъл концентрации, както и кривите, обозначени с 10%, 25%, 75%, 90%. Последните криви изобразяват тези мислени концентрации, за които в съответно 10%, 25%, 75%, 90% от случаите са били симулирани по-ниски концентрации.

По този начин в ивицата 25%-75% попадат 50% от случаите, а в ивицата 10%-90% - 80% от случаите.

Така, показаните в дисертацията криви дават достатъчно добра представа за статистическите характеристики на ансамбъла – средни, дисперсия, асиметрия, ексцес, без последните три характеристики да бъдат показани явно. Тези криви ще бъдат накратко коментирани тук, като ще бъде демонстриран един пример **- Фиг. II.2.**

От графиките за годишно и по сезонно осреднените концентрации на озон (O_3) за България се вижда, че средните концентрациите са с добре изразени денонощен и сезонен ход, като също така те имат и добре изразен максимум през деня, който е свързан с ниските стойности на NO_2 и ускорените фотохимични реакции през този интервал на денонощието. Освен това средните концентрации се разпределят в отрязъка съдържащ 50% случаи. Средните концентрации са доста симетрично разположени не само в различните отрязъци от броя случаи, но също така и спрямо абсолютните минимални и максимални концентрации през различните сезони. Също така средните и абсолютните максимални концентрации на озон са най-високи през пролетта и лятото, което се дължи усиленото влияние фотохимичните трансформации и на метеорологичните (неустойчивата стратификация и съответно спускането от височина на озон към приземния слой).

От графиките за годишно и по сезонно осреднените концентрации на NO_2, NH_3, SO_2, CPRM, и FPRM за България се вижда, че всички концентрации имат добре изразени денонощен и сезонен ход, като денонощният им ход има два добре изразени максимума един рано сутрин и един късно следобед. Освен това средните концентрации се разпределят в отрязъка съдържащ 50% случаи, като те най-вече следват 75% крива. Също така средните концентрации са асиметрично разположени спрямо ивиците, съдържащи различен брой случаи, и то не само през различните части на денонощието, но също така и през различните сезони. Абсолютните максимуми за NO_2 са най-високи през есента, докато за NH_3 се вижда, че комбинацията от пролетният и есенният максимум определят годишният. За SO_2, CPRM, и FPRM (**Фиг. II.2.**) абсолютните им максимуми са най-високи през зимата, което не е странно имайки предвид, че именно тогава са най-големите емисии от енергетиката и отоплението, а също така и от метеорологичните условия (устойчивата стратификация).



Фиг. II.2. Някои статистически характеристики на осреднените приземни концентрации на Фини Прахови Частици (FPRM) μg/m^3 за България

Изследването на замърсяването на въздуха за град София е от голямо значение, не само поради факта, че тук е столицата на страната и е съсредоточена голяма част от населението на страната (1291591 души спрямо преброяване 2011, което представлява 16,4% от населението на България), но също така тя се явява в голяма степен туристически и производствен център, а също така и мястото с най-интензивен автомобилен транспорт. Днес София е най-големият промишлен център на България, като има около 800 големи предприятия. Именно тук са съсредоточени 75% от черната металургия, 50% от полиграфическата, 15% от електротехническата и електронната промишленост, 14% от кожухарската и обувната промишленост на страната. Произвежда се химическа, текстилна и хранително-вкусова продукция. Площта на София е 492 $км^2$ и се разполага от части в Софийската котловина и Витоша, като климатът и е умерено континентален. На юг тя е заобиколена от планините

Витоша, на запад Люлин и на север Стара планина.

Проблем за замърсяването на въздуха на София е нейното разположение в Софийската котловина, която е заобиколена с планини и които намаляват възможността за самопочистване на атмосферата. Въздухът в столицата се замърсява предимно от фини прахови частици и азотните оксиди. След спирането на работа на "Кремиковци", те се генерират основно от автомобилния транспорт, отоплението с твърди и течни горива, замърсените пътни настилки и някои ТЕЦ-ове. Така столичните квартали Дружба, Надежда и Павлово са с най-замърсен въздух, като за първите два освен автомобилния транспорт, важен фактор за мръсния въздух са големите ТЕЦ-ове там.

От графиките за годишно и по сезонно осреднените концентрации на озон (O_3) за София се вижда, че средните концентрациите са с добре изразени денонощен и сезонен ход, като също така те имат и добре изразен максимум през деня, който е свързан с ниските стойности на NO_2 и ускорените фотохимични реакции през този интервал на денонощието. Освен това се вижда, че средните концентрации се разпределят в отрязъка съдържащ 50% случаи. Те са симетрично разположени не само в различните отрязъци от броя случаи, но също така и спрямо абсолютните минимални и максимални концентрации през различните сезони. Както се вижда средните и абсолютните максимални концентрации на озон са най-високи през лятото, което се дължи усиленото влияние фотохимичните трансформации и на метеорологичните условия (неустойчивата стратификация и съответно спускането от височина на стратосферен озон).

От графиките за годишно и по сезонно осреднените концентрации на NO_2, NH_3, SO_2, CPRM, и FPRM за София се вижда, че за всички средните им концентрации имат добре изразени денонощен и сезонен ход, като денонощният им ход има два добре изразени максимума един рано сутрин и един късно следобед. Освен това се вижда, че средните концентрации се разпределят в отрязъка съдържащ 50% случаи, като те най-вече следват 75% крива. Също така асиметричността на разпределението и то не само през различните части на денонощието, но също така и през различните сезони. На графиките също така се вижда, че абсолютните максимуми за NO_2 са най-високи през есента и зимата, докато за NH_3 се вижда, есенният максимум определя годишният. За SO_2, CPRM, и FPRM се вижда, че техните абсолютни максимуми са най-високи през зимата, което не е странно имайки в предвид, че именно тогава е най-голямо производството на емисиите от енергетиката и отоплението, а също така и метеорологичните условия (устойчивата стратификация).

Изследването на замърсяването на въздуха за град Стара Загора е от голямо значение поради факта, че тук е един от икономическите центрове на България. С от население (138 272 души спрямо преброяване 2011, което го прави 6-ят по население град в България). В област Стара Загора се намира най-големият промишлено енергиен комплекс ТЕЦ "Марица Изток" в България, който произвежда около 30% от електроенергията в България, а мини Марица Изток са най-големият производител и преработвател на въглища за страната около 83%. В момента „Марица Изток" се модернизира, като се подменят остарелите инсталации, увеличава се капацитетът на произведената електроенергия и се изграждат пречиствателни мощности, които да редуцират до минимум вредните емисии, изхвърляни в атмосферата. Редом с енергетиката леката и хранително-вкусовата промишленост са също добре застъпени в региона. Градът е разположен в източната част на Горнотракийската низина със средна надморска височина от 196 метра, като климатът е преходно континентален с полъх от Средиземно море. Проблемът със замърсяването на въздуха на Стара Загора е нейното близко разположение до комплексът Марица Изток, който се явява основен замърсител с фини прахови частици и серен диоксид, и то не само за района на града но също така и за целия Балкански полуостров.

Годишно и по сезонно осреднените концентрации на озон (O_3) за Стара Загора доста приличат на тези за София и България, като средните и абсолютните максимални концентрации са най-високи през пролетта, което се дължи най-вероятно на преносът му от други места.

Годишно и по сезонно осреднените концентрации на NO_2 за Стара Загора се вижда, че доста приличат на тези за София и България, като абсолютните максимуми за NO_2 са най-високи през зимата, което най-вероятно се дължи на високото производството на емисиите от енергетиката и отоплението, а също така и метеорологичните условия (устойчивата стратификация). Докато за NH_3 се вижда, че денонощният ход на средните и максималните концентрации е силно изменчив, като това най-добре проявява през есента и зимата, и най-вероятно се дължи на процесите десулфуризация в ТЕЦ Марица Изток. При SO_2 абсолютни максимални концентрации са с два порядъка по-големи от средните и през всички сезони абсолютните максимални концентрации превишават ПДК за SO_2. Едрите и фините прахови частици доста наподобяват тези за SO_2, като средните концентрации са от 5 до 10 пъти по-малки от максималните. От разгледаните замърсители може да се заключи, че ТЕЦ Марица Изток е основният замърсител за района на Стара Загора.

Изследването на замърсяването на въздуха за Рожен е интересно, тъй като това е типично планинска точка, която се намира в централни Родопи с надморска височина 1745 метра, далече от всякакъв вид индустриални замърсители.

От графиките за годишно и по сезонно осреднените концентрации на озон (O_3) за Рожен се вижда, че те доста приличат на тези за София и България, като средните концентрации са най-високи през пролетта, докато абсолютните максимални концентрации са най-високи през зимата, което най-вероятно се дължи на пренос, евентуално на спускането на стратосферен озон и слабите му фотохимични трансформации през този сезон, което води до неговото натрупване.

Графиките за годишно и по сезонно осреднените концентрации на NO_2, NH_3, SO_2, CPRM, и FPRM за Рожен доста наподобяват тези за Стара Загора, като се различават с по-ниски средни и максимални концентрации. Абсолютните максимуми за NO_2 са най-високи през зимата, което най-вероятно се дължи на преносът на емисиите от производството на електроенергия и отопление, а също така и метеорологичните условия (устойчивата стратификация), което води до неговото натрупване. Като това най-добре се вижда през есента и зимата, и най-вероятно се дължи на процесите десулфуризация в ТЕЦ Марица Изток. Абсолютни максимални концентрации на NH_3 и SO_2, са на един порядък по-големи от средните, с изключение през пролетта и лятото при NH_3. При едрите и фините прахови частици имат добре изразени денонощен и сезонен ход, като денонощният им ход има два добре изразени максимума един рано сутрин и един късно следобед. Освен това абсолютните максимуми за CPRM, и FPRM са най-високи през есента и зимата, което най-вероятно се дължи на преносът на емисиите от производството на електроенергия и отопление, а също така и метеорологичните условия (устойчивата стратификация), което води до неговото натрупване.

Индекси на замърсяване

Високите концентрации на озон могат да нанесат поражения на растенията, животните и на човешкото здраве. Всъщност когато се изследват ефектите от високите концентрации на озон, трябва да се взимат пред вид не самите концентрации на озона, а някои свързани величини. Следните четири величини са важни: (виж Amann et al., 1999, European Parliament, 2002):

AOT40C стойности (Accumulated Over Threshold) – акумулирано количество над граница от 40 ppb в часовете на деня през периода от 1 май до 31 юли), което е вредно за посевите когато стойностите надхвърлят 3000 ppb.ч.

AOT40F стойности (AOT40 пресметнато за период от 1 април до 30 септември), което вреди на горите, когато стойностите са над 10000 ppb.ч.

NOD60 (Number Of Days – брой дни, в които 8 – часовите пълзящи средни на озона за всеки час на деня надхвърлят критична стойност от 60 ppb (120 μgm^{-3}). Ако поне веднъж пред деня се надхвърли границата от 60 ppb, денят се отчита като “лош”. Хора с астматични болести имат проблеми в “лошите” дни, затова е желателно да няма такива дни. Премахването на всички такива дни е прекалено амбициозна задача. Изискването обикновено се свежда до максимум 25 “лоши” дни през периода април- септември. Оказва се че на много места е трудно да се изпълни дори и това изискване.

Това, което е общо за всички от симулираните полета на горните три характеристики за годините 2000-2007 е голямата разлика в конфигурацията на полетата през различните години, което е очевидно отражение на влиянието на метеорологичните условия.

В полетата на AOT40C за всички години най-високите стойности са главно в планинските райони. Областите, където са надвишени праговите стойности от 3000 ppb.ч са сравнително малки, освен в години 2000 и донякъде 2003.

В полетата на AOT40 F областите, където са надвишени праговите стойности от 10000 ppb.ч са малки през всички години.

От полетата на NOD60 за повечето години в по-голямата част на страната стойностите на NOD60 не надхвърлят 10 дни. Съществени превишения на стойностите на NOD60 над 20-25 дни в годината се наблюдават през 2000, 2003 и особено през 2007 година, когато и районите с превишения над 20 дни са доста обширни.

ГЛАВА III ОЦЕНКА НА ПРИНОСА НА ЕМИСИИТЕ ОТ ОТДЕЛНИ КАТЕГОРИИ ИЗТОЧНИЦИ (SNAP КАТЕГОРИИ) КЪМ ОБЩАТА КАРТИНА НА ЗАМЪРСЯВАНЕ В СТРАНАТА

Замърсяването на въздуха силно зависи от емисиите на примеси. Ето защо изследването на приноса на емисиите от отделни категории източници (SNAP категории) към общата картина на замърсяване в страната е очевидно задача с голямо практическо значение, чиито резултати могат да бъдат пряко използвани при формулирането на краткосрочни (текущи) решения и дългосрочни стратегии за намаляване на замърсяването на въздуха.

Резултатите в настоящата глава са получени на основата на петте емисионни сценария (всеки един за годините 2000-2007):

Изборът на тези сценарии не е случаен. Източниците от SNAP категория 1 (енергетика) имат най-голям дял в сумарните за страната емисии на SOx, а тези от SNAP категория 7 (пътен транспорт) в сумарните за страната емисии на NOx. Източниците от SNAP категория 2 (не индустриални изгаряния) имат относително малък дял в сумарните за страната емисии на повечето замърсители с изключение на CO, но както ще се види по-долу локално (в големите градове) техния принос може да бъде значителен.

Биогенните източници са значителен емитер на ЛОС, които са важен озонов прекурсор.

Всички оценки, които ще бъдат представени по-долу се отнасят до приземните концентрации.

В параграф III.2. на дисертацията са представени някои осреднени по ансамбъл приноси на източници от споменатите по-горе категории към замърсяването на територията на България. В III.3. са представени съответните оценки, осреднените за територията на България и за отделни нейни точки. Тук тези резултати ще бъдат накратко описани.

Полета на ансамблово осреднените приноси на отделните категории източници към приземните концентрации

Годишни полетата на средните относителни приноси на емисиите от SNAP_01, SNAP_02, SNAP_07 и биогенните емисии водещи до образуването на азотен диоксид (NO_2): Приносът на всички Български източници е изцяло положителен, като приносът от енергетиката е около 50%, но само покрай самите ТЕЦ-ове докато над останалата част от страната се мени между 0 и 10%.

Приносът на източниците от не индустриалното изгаряне е най-малък в сравнение с останалите източници, разпределен е почти равномерно над цялата страна и средно той е около 2%, като само София се откроява с леко по-висок принос от около 5%.

Приносът на източниците от автомобилният транспорт е най-голям, сравнен с останалите източници и е разпределен равномерно над цялата страна. При него през цялото денонощие се открояват някои от пътните артерии в страната и град София, като места с по-високи приноси от типичните за страната в съответният час. Средният принос е около 30%, като в 17:00 часа той е най-голям, а над София и пътната мрежа той става над 70%.

Приносът на биогенните емисии средно за страната е около 20%, като през цялото денонощие той е най-нисък над морският бряг, а над планините и София през деня той става дори нулев. Освен това през нощта приносът на биогенните емисии е по-голям от колкото през деня, което най-вероятно е в следствие на липсата на фотохимични трансформации на NO_2 и превръщането му в O_3 през нощта.

Годишни полетата на средните относителни приноси на емисиите от SNAP_01, SNAP_02, SNAP_07 и биогенните емисии водещи до образуването на озон (O_3):Приносът от енергетиката над цялата страна е малък и е предимно отрицателен около -5%, и то не само над ТЕЦ-ове но и на доста голямо разстояние около тях. Над останалата част от страната той е между 0 и -1%, като само през деня над планините той е положителен но много малък до около 0,5%.

Приносът на източниците от не индустриалното изгаряне също е малък и е разпределен почти равномерно над цялата страна. През нощта средно той е около -05%, като само София се откроява с леко по-висок отрицателен принос около -1%. В 11:00 часа над почти цялата страна той е положителен и е около 0,5% с изключение на София където е леко отрицателен дори нулев. В 17:00 часа приносът на източниците от SNAP_02 за образуването на озон в България е най-силно отрицателен над София около -3%, докато над останалата част от страната той е различен и се мени в интервала от -0,5% до 0,5%

Приносът на източниците от автомобилният транспорт е по-голям, сравнен с източниците от SNAP_01 и SNAP_02. През цялото денонощие почти навсякъде той е отрицателен около -2% с изключение на планините, където е положителен и е около 1%. Освен това се открояват пътните артерии в страната и град София, като места с най-големи отрицателни приноси от около -10%. В 11:00 часа приносът над планините достига до 2%, като средно за страната той става леко отрицателен и почти нулев, а само София се откроява като място с най-голям отрицателен принос от -5%%. В 17:00 часа отрицателният приносът от автомобилният транспорт в страната е най-голям, като София и цялата пътната мрежа силно се открояват с приноси от над -10%.

Приносът на биогенните емисии е най-голям и почти изцяло положителен с изключение на първите часове от денонощието когато той е леко отрицателен. В 05:00 часа приносът над цялата страна е отрицателен около -2%, с изключение над Витоша, Пирин, Рила, Родопите и Стара планина, където той е около 1%. В 11:00 приносът в цялата област е положителен около 3%, като над горе посочените планини е по-малък и е около 1%. В 17:00 часа е обратното над планините той става 3%, а над останалата част от областта около 1%. В 23:00 приносът над страната е положителен и най-висок над планините, като по поречието на река Марица и в северната част на областта той е отрицателен и е около -2%.

Годишни полетата на средните относителни приноси на емисиите от SNAP_01, SNAP_02, SNAP_07 и биогенните емисии водещи до образуването на серен диоксид (SO_2): Приносът на всички Български източници е изцяло положителен, като приносът от енергетиката достига 100% но само покрай самите ТЕЦ-ове, като над южната част от страната е около 40%, с изключение на планините, където е около 20%, а над северната част от страната средният принос е около 20%.

Приносът на източниците от не индустриалното изгаряне е по-малък в сравнение с източниците от енергетиката, като почти през цялото денонощие е разпределен равномерно над цялата страна и средно е около 10%, като в 17:00 часа над цялата страна и над София през цялото денонощие той е леко по-висок около 20%.

Приносът на източниците от автомобилният транспорт е равномерно разпределен над цялата страна и е около 2%, като отново през деня само София се леко се откроява с по-висок принос от около 4%. В 17:00 часа приносът на SNAP_07 нараства, като за югозападната част от страната той е около 4%, а над останалата е около 6%

Приносът на биогенните емисии е най-малък, като средно за страната през цялото денонощие е под 1%, като в 11:00 часа той нараства и е най-голям в северна България около 2%.

Годишни полетата на средните относителни приноси на емисиите от SNAP_01, SNAP_02, SNAP_07 и биогенните емисии водещи до образуването на изопрен (ISOP): Приносът на източниците от енергетиката през цялото денонощие е почти нулев над планините и северна България, докато над останалата част от страната е около 5%. Единствените места които се открояват със значително по-голям принос от около 15% са Бургас в 05:00 часа и Стара Загора в 11:00 часа.

Приносът на източниците от не индустриалното изгаряне е най-малък в сравнение с останалите източници. Разпределението му е почти равномерно над цялата страна, като през нощта приносът на източниците от не индустриалното изгаряне е по-голям отколкото през деня. Също така на картите се вижда, че през цялото денонощие над планините той се запазва и е около 1%.

При приносът на източниците от автомобилният транспорт през цялото денонощие добре изпъкват София и морския бряг с по-високи приноси от типичните за страната в дадения час. В 05:00 часа той е най-голям около 50% и е равномерно разпределен над цялата страна. В 11:00 часа приносът е предимно отрицателен, като той бива положителен над северозападната част от Дунавската равнина и Горнотракийската низина. В 17:00 часа той отново е положителен около 15% и равномерно разпределен над цялата страната. В 23:00 часа приносът на места нараства и средно за страната е около 30%, като в източна България става около 70%, а в централна намаля и става около -10%.

Приносът на биогенните емисии е най-голям и равномерно разпределен, като над Рила, Пирин и София е по-малък в сравнение с приноса над останалата част от областта. През нощта той е по-малък около 50%, в сравнение през деня когато той е около 90-100%.

Годишни полетата на средните относителни приноси на емисиите от SNAP_01, SNAP_02, SNAP_07 и биогенните емисии водещи до образуването на амоняк/ амония (NH_3): Приносът на антропогенните източници в България е изцяло отрицателен, като само приносът на биогенните емисии е положителен. Приносът на емисиите от енергетиката е около -50% но само покрай самите ТЕЦ-ове, и постепенно отслабващ с отдалечаването им от тях. За планините и северозападна България той е между -10% и 0%. Приносът на източниците от не индустриалното изгаряне е най-малък в сравнение с останалите източници, разпределен е почти равномерно над цялата страна и около -10%, като само над високите части на планините и в отделни часове северна и/ или източна България се открояват с по-малък принос от около -3%. Източниците от автомобилният транспорт почти през цялото денонощие е отрицателен принос от -5 до -10%. Местата с положителен но близък до 0% принос са над морето и на места в долният ляв квадрант на областта. Приносът на биогенните емисии е с добре изразен денонощен ход и е изцяло положителен по планините. През нощта над почти цялата област той е около -5%, докато през деня в 11:00 часа е най-голям и е около 5% над цялата област, а в 17:00 часа той намалява, като става отново отрицателен северна и източна България.

Годишни полетата на средните относителни приноси на емисиите от SNAP_01, SNAP_02, SNAP_07 и биогенните емисии водещи до образуването на амоний/ амониум (NH_4): Приносът на антропогенните източници в България е изцяло положителен, докато приносът на биогенните емисии варира през денонощието. Приносът на емисиите от енергетиката е около 20% но само покрай самите ТЕЦ-ове, и постепенно отслабващ с отдалечаването им от тях. За планините и северозападна България той е между 0% и 5%. Приносът на източниците от не индустриалното изгаряне е равномерно разпределен над почти цялата страна и е около 2%, като само високите части на планините той е нулев. Приносът е най-висок в 17:00 и 23:00 часа около 6%. И тук само София се откроява като място с най-висок принос от около 10%. Приносът на източниците от автомобилният транспорт през цялото денонощие е положителен, най-нисък над планините под 1% и най-висок в централна България от около 3% до 4%. Приносът на биогенните емисии е с добре изразен денонощен ход и е изцяло отрицателен по планините. През деня над почти цялата област той е около -1%, докато през нощта в 05:00 часа е най-голям и е около 2% в северната част на областта. В 23:00 часа в източна България приносът е положителен а в западна отрицателен.

Годишни полетата на средните относителни приноси на емисиите от SNAP_01, SNAP_02, SNAP_07 и биогенните емисии водещи до образуването на първични органични аерозоли (POA): Приносът на антропогенните източници от България е изцяло положителен. Приносът от енергетиката е около 20% но само над някои от ТЕЦ-овете (Бобов Дол, Варна и Марица Изток), като той е почти нулев над планините и в северна България. Приносът на източниците от не индустриалното изгаряне през цялото денонощие над цялата страна е еднакъв и е около 10%. Приносът на източниците от автомобилният е разпределен равномерно над цялата страна и варира през денонощието. Той бива най-голям в 17:00 около 4%, като тогава се открояват София и пътната мрежа с по-висок принос. Приносът на биогенните емисии е изцяло отрицателен и много малък до -0,1%, като хаотичното разпределение на максималните приноси показани на картите с червени точки се дължат най-вече от пресмятането на произведенията на много малки стойности.

Годишни полетата на средните относителни приноси на емисиите от SNAP_01, SNAP_02, SNAP_07 и биогенните емисии водещи до образуването на вторични органични антропогенни аерозоли (SOAA): Приносът от енергетиката е най-малък и изцяло отрицателен, като само над някои от ТЕЦ-овете (Бобов Дол, Варна и Марица Изток) той е около 3% докато над ТЕЦ-овете в Пловдив и Бобов дол той е около -4%. Приносът на източниците от не индустриалното изгаряне и биогенните емисии (фиг. **III.2.8.2.** и фиг. **III.2.8.4**) е изцяло положителен, почти равномерно разпределен по време и пространство и е най-голям от около 20% до 30%. Приносът на източниците от автомобилният транспорт през цялото денонощие е най-голям над планините от 3% до 5% и най-нисък в централна България. В 05:00 и 17:00 часа приносът в цялата страна е положителен, разпределен е почти равномерно и е най-голям около 2% докато приносът на автомобилният транспорт за страната в 11:00 и 23:00 часа е по-малък и е отрицателен в западна и централна България.

Годишни полетата на средните относителни приноси на емисиите от SNAP_01, SNAP_02, SNAP_07 и биогенните емисии водещи до образуването на вторични органични биогенни аерозоли (SOAB): Приносът от енергетиката е най-малък и изцяло положителен около 1%, като само над някои от ТЕЦ-овете (Бобов Дол, Варна и Марица Изток) той е около 4%. Приносът на източниците от не индустриалното изгаряне е положителен около 5% и почти равномерно разпределен, като над планините и през нощта е по-малък отколкото през деня и над останалата територия от страната. Приносът на източниците от автомобилният транспорт над София е отрицателен през цялото денонощие до -5% и е най-висок над планините и централна България. В 17:00 часа се наблюдава най-голям принос на автомобилният транспорт за страната, като на места в централна България той е около 5%. През почти цялото денонощие той има равномерно разпределение над цялата страна. Приносът на биогенните емисии е най-голям над 90% и почти равномерно разпределен. като той е най-нисък над високите части на планините и източна България.

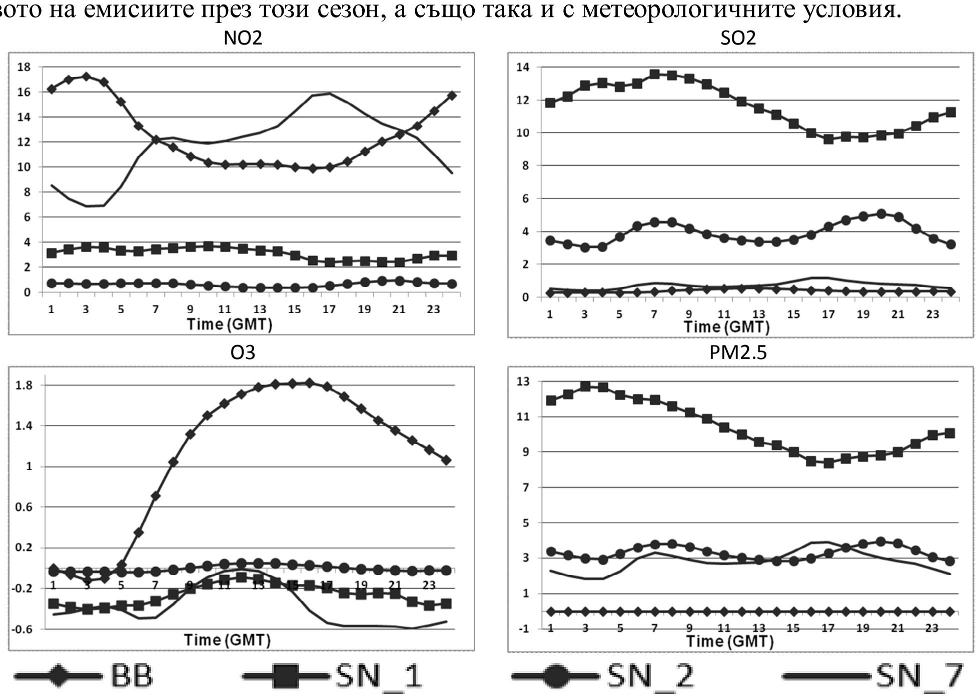
Годишни полетата на средните относителни приноси на емисиите от SNAP_01, SNAP_02, SNAP_07 и биогенните емисии водещи до образуването на едри прахови частици (CPRM): Приносът на всички Български източници е изцяло положителен. Като приносът от енергетиката е над 50% но само покрай самите ТЕЦ-ове, а над останалата част от страната е около 20%. Приносът на източниците от не индустриалното изгаряне през цялото денонощие е разпределен равномерно над цялата страна и средно той е около 15%, като само София се откроява с леко по-нисък принос от около 10%. Приносът на източниците от автомобилният транспорт е разпределен равномерно над цялата страна но се мени през различните часове. Почти през цялото денонощие София се откроява с по-висок принос (до 20%) от типичния принос за страната, като в 17:00 часа приносът на всякъде е най-голям и дори могат да се видят части от основната пътна мрежа. Приносът на биогенните емисии е изцяло отрицателен и много малък до -0,1%, като хаотичното разпределение на максималните приноси показани на картите с червени точки се дължат най-вече от пресмятането на много малки произведения.

Годишни полетата на средните относителни приноси на емисиите от SNAP_01, SNAP_02, SNAP_07 и биогенните емисии водещи до образуването на фини прахови частици (FPRM): Приносът на всички Български източници е изцяло положителен. Приносът от енергетиката е над 50% но само покрай самите ТЕЦ-ове, като тяхното влияние се усеща над почти цялата територия на страната с принос от около 25%. Приносът на източниците от не индустриалното изгаряне през цялото денонощие е разпределен равномерно над цялата страна и средно той е около 8%, като само София се откроява с леко по-нисък принос от около 5%. Приносът на източниците от автомобилният транспорт е разпределен равномерно над цялата страна но се мени през различните часове. Почти през цялото денонощие София се откроява с по-висок принос (до над 20%) от типичния принос за страната, като в 17:00 часа приносът на всякъде е най-голям и дори могат да се видят части от основната пътна мрежа. Приносът на биогенните емисии е изцяло отрицателен и много малък до -0,1%, като хаотичното разпределение на максималните приноси показани на картите с червени точки се дължат най-вече от пресмятането на много малки произведения.

Оценки на годишно и сезонно осреднените приземни приноси (в %) на различните източници за територията на България и за отделни точки.

Резултатите за приземният относителен принос на различните източници осреднени по осем годишният ансамбъл получени чрез компютърно симулиране, могат да бъдат използвани за да се определят, както относителните приноси на отделните източници за определен замърсител за страната, но също така и за, която и да е точка от областта. Това би могло да бъде ценна информация на основа на която регулаторните органи да формулират някои дългосрочни или краткосрочни стратегии за намаляване на емисиите от които и да е източник, за да се предпази съответната област от превишаване на ПДК.

Оценки на годишно и по сезонно осреднените приземни приноси (в %) на емисиите от SNAP_01, SNAP_02, SNAP_07 и биогенните емисии водещи до образуването на различни замърсители осреднени за територията на България: Приземните относителни приноси на отделните източници водещи до образуването на азотен диоксид (NO_2) за България показват, че всички източници са с положителен принос и с добре изразени сезонен и денонощен ход, който е различен за различните източници. Приносът на биогенните емисии е най-голям през нощта, като минимумът му е следобед, освен това приносът на биогенните емисии е най-голям през лятото и най-малък през зимата, което най-вероятно се дължи на фотохимичните процеси на трансформация на NO_2. Разглеждайки приносът на източниците от SNAP_07 се вижда, че той е в противофаза с този на биогенните емисии, като лятото през деня двата приноса са почти равни и са по около 15%. Това не е странно като се знае, че азотния диоксид и летливите органични съединения са основните прекурсори на озона. Приносът на енергетиката е около четири пъти по-малък от този на горните два, като през зимата той нараства до около 5%, а през лятото е най-малък. Приносът на източниците от SNAP_02 е най-малък и клонящ към 0%, като само през зимата той нараства до около 2%. Повишеният принос на източниците от SNAP_01 и SNAP_02 през зимата най-вероятно е свързано с повишеното количеството на емисиите през този сезон, а също така и с метеорологичните условия.



Фиг. **III.1.** Графики на “типичния” годишно осреднен денонощен ход на осреднените за територията на България приноси [%] на биогенните емисии и тези от SNAP_01, SNAP_02 и SNAP_07 водещи до образуването на NO_2, SO_2, O_3 и PM2.5.

Приземните относителни приноси на отделните източници водещи до образуването на озон (O_3) за България показват, че всички източници са с добре изразени сезонен и денонощен ход, който е почти еднакъв за всички източници. През пролетта и есента се вижда, че приносът на биогенните емисии е основно положителен и е най-голям, като той е отрицателен само в началото на деня. Приносът на всички останали източници тогава е основно отрицателен с изключение на тези от SNAP_02 и на SNAP_07 през пролетта по обяд. През лятото приносът на биогенните емисии е изцяло положителен и е около пет пъти по-голям от приносът на всички останали, които достигат до 1% само по обяд. През зимата приносът на всички източници е най-малък, положителен принос около 0,05% имат само източниците от SNAP_02 по обяд, докато приносът на всички останали източници е изцяло отрицателен. Най-голям отрицателен принос имат източниците от SNAP_07 около -1,25%, а този на биогенните и от SNAP_01 е почти равен и е около -0,6%.

Приземните относителни приноси на отделните източници водещи до образуването на изопрен (ISOP) за България показват, че приносът на биогенните емисии е най-голям, с добре изразени денонощен и сезонен ход, който се мени от 65% до 85% в зависимост от сезона. Разглеждайки приносът на източниците от SNAP_07 се вижда, че той е по-малък и в противофаза с този на биогенните емисии. През лятото приносът на SNAP_07 достига едва 10%, докато през останалите сезони през нощта той е по-голям от този на биогенните. Приносите на емисиите от енергетиката и

SNAP_02 са почти нулеви и леко отрицателни през различните сезони.

Всички типове източници водещи до образуването на амоняк имат добре изразени денонощен и сезонен ход, като отрицателният принос на SNAP_01, който е водещ през всички сезони, през зимата става положителен. Следващият по големина е приносът на емисиите от SNAP_02, който винаги е отрицателен и е най-голям през зимата около -10%. Приносът на SNAP_07 е най-малък и през всички сезони е отрицателен. Приносът на биогенните емисии през всеки сезон се мени, като по обяд той е най-голям. През зимата е много малък и изцяло отрицателен , през лятото е изцяло положителен и много голям, а през пролетта и есента е положителен само по обяд но много малък.

Всички типове източници водещи до образуването на серен диоксид са с положителен принос и с добре изразени сезонен и денонощен ход, който е различен за различните източници. На всички фигури се вижда, че най-голям принос има енергетиката, докато приносите на биогенните емисии и SNAP_07 са почти нулеви. Приносът на източниците от SNAP_02 е втори по големина, като през зимата е най-голям, а през лятото най-малък и е почти колкото приносът на SNAP_07.

През всички сезони антропогенните източници водещи до образуването на едри прахови частици имат положителен принос, с добре изразени сезонен и денонощен ход, който е различен за различните източници. Приносът на биогенните емисии е много малък дори нулев и може да бъде отрицателен. През лятото и есента енергетиката има най-голям принос до 10%, следван от този на SNAP_02, които през лятото е колкото приносът на емисиите от SNAP_07 около 2%, а през есента е около два пъти повече от него. През пролетта и средно за годината в началото е водещ приносът на енергетиката, след което почти се изравнява с този на SNAP_02 и в те си разменят местата. През зимата приносът от SNAP_01 е водещ само през нощта, докато през деня е този на SNAP_02.

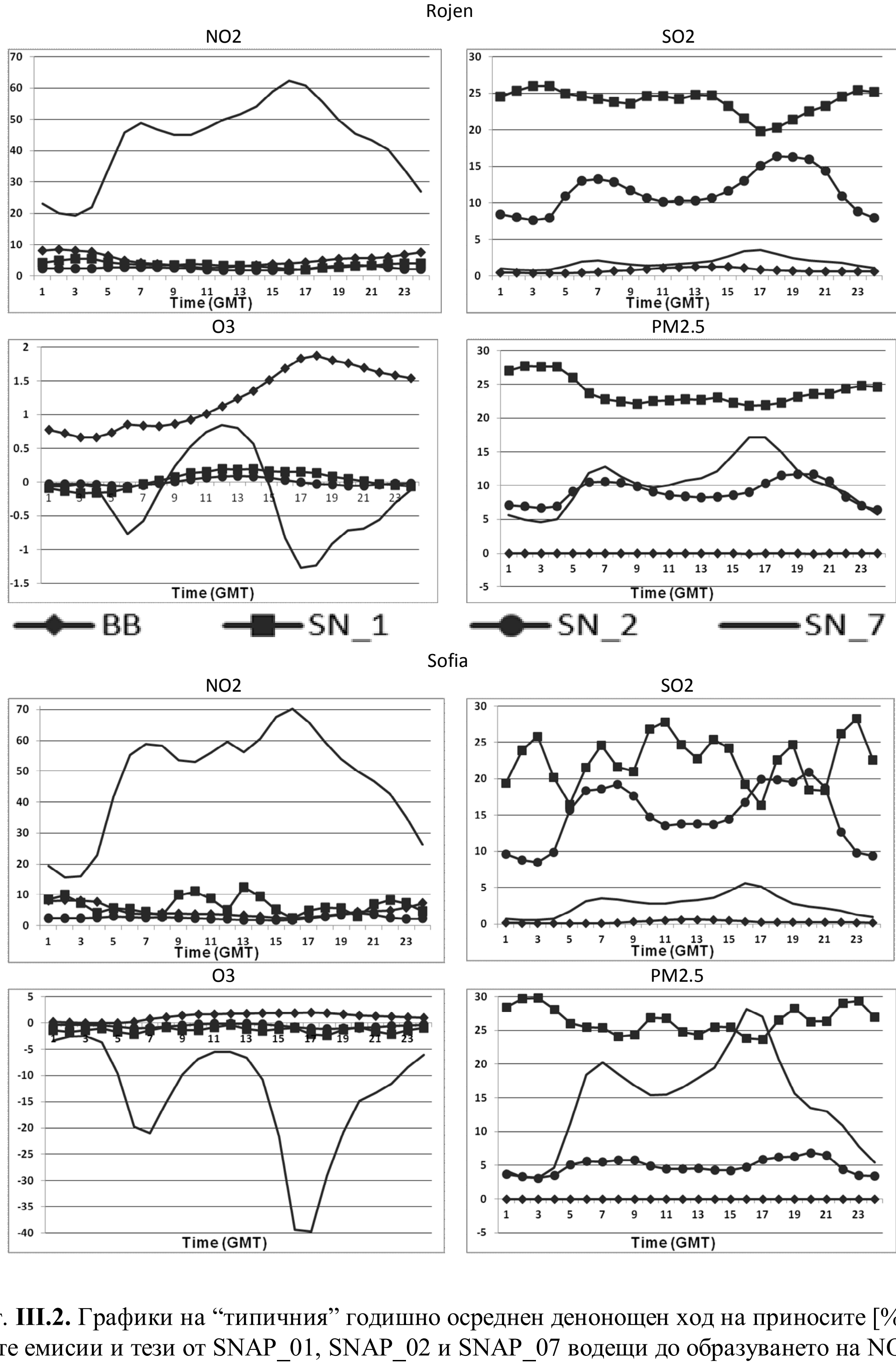
През всички сезони антропогенните източници водещи до образуването на фини прахови частици имат положителен принос, с добре изразени сезонен и денонощен ход, който е различен за различните източници. Приносът на биогенните емисии е много малък дори нулев и може да бъде отрицателен. Както се вижда навсякъде доминиращият принос е този на източниците от енергетиката около 12%. През пролетта и зимата приносът на SNAP_02 е вторият по големина следван от източниците от автомобилният транспорт, като през есента и лятото е обратното, а средно за годината двата приноса са почти равни.

Оценки на годишно и по сезонно осреднените приземни приноси (в %) на емисиите от SNAP_01, SNAP_02, SNAP_07 и биогенните емисии водещи до образуването на различни замърсители осреднени за територията на София: Приземните относителни приноси на отделните източници водещи до образуването на азотен диоксид (NO_2) за София са с положителен принос и с добре изразени сезонен и денонощен ход, който е различен за различните източници. На всички фигури се вижда, че приносът на емисиите от автомобилният транспорт е най-голям през деня, като през лятото достига до 80%, а през зимата 60%. През нощта отново той е доминиращ но с принос от около 10 до 20% в зависимост от сезона. Приносите на останалите източници е сравнително малък спрямо този от SNAP_07, като само този от енергетика леко изпъква над останалите с принос от около10%.

Приземните относителни приноси на отделните източници водещи до образуването на озон за София през различните сезони за отделните източници е различен но с почти еднакъв денонощен ход. Приносът на биогенните емисии навсякъде е положителен, а този на източниците от автомобилният транспорт е най-голям и навсякъде е отрицателен с изключение на следобедните часове през лятото. Приносът на източниците от SNAP_01 и SNAP_02 е много малък и варира около нулата

Приземните относителни приноси на отделните източници водещи до образуването на изопрен (ISOP) за София показват, че те са с добре изразени денонощен и сезонен ход, като приносът на биогенните емисии е най-голям и през деня достига 100%, а през нощта в зависимост от сезона се мени между 0 и 10%. Приносът на автомобилният транспорт, е най-голям през деня вариращ между 80% до 100%. През деня силно намаля, като в привечерните часове през лятото дори става леко отрицателен. Приносът на източниците от SNAP_01 и SNAP_02 е много малък в сравнение с другите два приноса, клонящ и вариращ около нулата.

Всички типове източници водещи до образуването на амоняк имат добре изразен сезонен ход, като доминира отрицателният приносът на SNAP_01 до -20%, с изключение през зимата, но тогава той е по-голям и достига -35%. Следващият по големина е приносът на SNAP_02, който също винаги е отрицателен и става доминиращ през зимата достигайки -85%. Приносът на SNAP_07 е най-малък, клонящ към нулата и през повечето време е отрицателен, само в сутрешните летни часове става леко положителен. Приносът на биогенните емисии през всеки сезон се мени, като по обяд той е най-голям. През зимата е много малък и изцяло отрицателен , през лятото е изцяло положителен и достига до 5%, а през пролетта и есента е положителен само по обед но е много малък.



Фиг. **III.2.** Графики на "типичния" годишно осреднен денонощен ход на приносите [%] на биогенните емисии и тези от SNAP_01, SNAP_02 и SNAP_07 водещи до образуването на NO_2, SO_2, O_3 и PM2.5 в Рожен и София.

Всички типове източници водещи до образуването на серен диоксид са с положителен принос и с добре изразен сезонен ход, който е различен за различните източници. На всички фигури се вижда, че най-голям принос има енергетиката, докато приносът на биогенните емисии е почти нулев. Приносът на SNAP_07 силно се мени през сезоните, като през пролетта и зимата той е почти нулев. През есента достига до 5% но е три пъти по малък от този на SNAP_02, а през лятото двата приноса се изравняват и следват един друг. Приносът на източниците от SNAP_02 е втори по големина, като е през зимата той е доминиращ, а през лятото става почти колкото приносът на SNAP_07.

През всички сезони антропогенните източници водещи до образуването на едри прахови частици имат положителен принос, с добре изразени сезонен и денонощен ход, който е различен за различните източници. Приносът на биогенните емисии е много малък дори нулев и може да бъде отрицателен. През всички сезони енергетиката има почти през цялото денонощие постоянен принос около 20%. През пролетта приносите на SNAP_02 и SNAP_07 са почти равни и са около 10%, докато през лятото и есента този от SNAP_07 става значително по-голям, като през деня е колкото приносът на SNAP_01, а в следобедните часове дори по-голям от него. Приносът на SNAP_02 е около 25% и е доминиращ през зимата, като по обед леко намаля и се изравнява с приноса на енергетиката, а приносът на SNAP_07 е на половина колкото него.

През всички сезони антропогенните източници водещи до образуването на фини прахови частици имат положителен принос, с добре изразени сезонен и денонощен ход, който е различен за различните източници. Приносът на биогенните емисии е много малък дори нулев и може да бъде отрицателен. Почти през цялото денонощие енергетиката има постоянен принос, който се мени през различните сезони, но почти постоянно е доминиращ. Вторият по големина е приносът на автомобилният транспорт, като през пролетта и лятото през деня става по-голям от този на SNAP_01. Приносът на SNAP_02 е значително по-малък, като през зимата неговото влияние се усилва и става колкото това на SNAP_07.

Оценки на годишно и по сезонно осреднените приземни приноси (в %) на емисиите от SNAP_01, SNAP_02, SNAP_07 и биогенните емисии водещи до образуването на различни замърсители осреднени за територията на Стара Загора: Приземните относителни приноси на отделните източници водещи до образуването на азотен диоксид (NO_2) за Стара Загора показват, че всички източници са с положителен принос и с добре изразени сезонен и денонощен ход, който е различен за различните източници. На фигурите се вижда, че приносът на биогенните емисии е най-голям през нощта, с изключение на зимата, като минимумът му е следобед, освен това приносът на биогенните емисии е най-голям през лятото и най-малък през зимата, което най-вероятно се дължи на фотохимичните процеси на трансформация на NO_2. Разглеждайки приносът на източниците от SNAP_07 се вижда, че той е има най-голям принос и е в противофаза с този на биогенните емисии. Приносът на енергетиката е около четири пъти по-малък от този на горните два, като през зимата той нараства до около 5%, а през лятото е най-малък. Приносът на източниците от SNAP_02 е най-малък и клонящ към 0%, като само през зимата той нараства до около 5%. Повишеният принос на източниците от SNAP_01 и SNAP_02 през зимата най-вероятно е свързано с повишеното количеството на емисиите през този сезон, а също така и с метеорологичните условия.

Приземните относителни приноси на отделните източници водещи до образуването на озон (O_3) за Стара Загора се вижда, че всички източници са с добре изразени сезонен и денонощен ход, който е почти еднакъв за всички източници. Приносът на биогенните емисии е основно положителен и най-голям, като само в първите часове на денонощието и през зимата той е отрицателен. Приносът на SNAP_02, като цяло е най-малкият и е леко положителен само по обяд, а през останалото време е отрицателен. SNAP_07 през повечето време има най-голям отрицателен принос, като само по обед през пролетта и целият ден на лятото той става положителен, като се доближава до приносът на биогенните емисии. Приносът от енергетиката е изцяло отрицателен с изключение през деня на лятото когато става положителен но в сравнение с другите приноси той е нищожно малък както и този на SNAP_02.

Приземните относителни приноси на отделните източници водещи до образуването на изопрен (ISOP) за Стара Загора се вижда, че приносът на биогенните емисии е най-голям, с добре изразени денонощен и сезонен ход, който се мени от 30% до 110% (принос надвишаващ 100% е интуитивно неприемлив, но той е възможен, като се имат пред вид сложните и нелинейни взаимодействия между примесите) в зависимост от сезона. Разглеждайки приносът на източниците от SNAP_07 се вижда, че той е по-малък и в противофаза с този на биогенните емисии. През лятото приносът на SNAP_07 е предимно отрицателен, като достига до -40%, докато през останалите сезони през нощта той е по-голям от този на биогенните. Приносите на емисиите от енергетиката и SNAP_02 са почти нулеви и променят знака си през различните сезони.

Всички типове източници водещи до образуването на амоняк имат добре изразен сезонен ход, като само при биогенните емисии може да се види лек денонощен ход и положителен принос през деня. Приносът на SNAP_01, е водещ през всички сезони, като с изключение на зимата леко се откроява неговият денонощен ход. Следващият по големина е приносът на емисиите от SNAP_02, който през зимата е равен или по голям от този на SNAP_01, а през лятото е нулев. Приносът на SNAP_07 е най-малък и през всички сезони е отрицателен и близък до нулата.

Всички типове източници водещи до образуването на серен диоксид са с положителен принос и с добре изразени сезонен и денонощен ход, който е различен за различните източници. На всички фигури се вижда, че най-голям принос има енергетиката, докато приносите на биогенните емисии и SNAP_07 са почти нулеви. Приносът на източниците от SNAP_02 е втори по големина, като през зимата е най-голям, а през лятото най-малък и е почти колкото приносът на SNAP_07.

Всички типове източници водещи до образуването на едри прахови частици имат положителен принос, с добре изразени сезонен и денонощен ход, който е различен за различните източници. Приносът на биогенните емисии е много малък дори нулев и може да бъде отрицателен. През лятото и есента енергетиката има най-голям принос до 30%, следван от този на SNAP_02, които през есента е колкото приносът на емисиите от SNAP_07 около 10%, а през пролетта е около три пъти повече от него. През зимата приносите на SNAP_01 и SNAP_02 са почти равни и са по около 30% всеки. Приносът на SNAP_07 е около 5% до 10%, като е втори по големина през лятото и в следобедните часове тогава се изравнява с приноса на SNAP_01.

Всички типове източници водещи до образуването на фини прахови частици имат положителен принос, с добре изразени сезонен и денонощен ход, който е различен за различните източници. Приносът на биогенните емисии е много малък дори нулев и може да бъде отрицателен. Както се вижда навсякъде доминиращият принос е този на източниците от енергетиката около 35%. През зимата приносът на SNAP_02 е вторият по големина следван от източниците от автомобилният транспорт, като през пролетта двата приноса се изравняват, а през лятото и есента приносът на SNAP_07 е втори по големина и дори става равен на този от енергетиката в летните следобедни часове.

Оценки на годишно и по сезонно осреднените приземни приноси (в %) на емисиите от SNAP_01, SNAP_02, SNAP_07 и биогенните емисии водещи до образуването на различни замърсители осреднени за територията на Рожен: Приземните относителни приноси на отделните източници водещи до образуването на азотен диоксид (NO_2) за Рожен показват, че всички антропогенни източници, почти винаги са с положителен принос и с добре изразени сезонни и денонощни ходове, които са различен за различните източници. На всички фигури се вижда, че приносът на автомобилният транспорт е най-голям, като през лятото достига до 75%. Приносът на всички останали източници е пренебрежимо малък спрямо него, като дори биогенните емисии имат отрицателен принос през лятото и зимата, както и тези от SNAP_01.

Всички източници водещи до образуването на озон са с добре изразени сезонен и денонощен ход, който е различен за всички източници. Приносите на SNAP_01 и SNAP_02 са най-малки и са положителни само през деня, като този от енергетиката е изцяло положителен през лятото и изцяло отрицателен през зимата. Най-голям положителен принос имат биогенните емисии до 5% като през зимата той става отрицателен и клонящ към нулата. Приносът на автомобилният транспорт е отрицателен през зимата, есента и през нощта на пролетта, като през лятото е изцяло положителен и дори през деня става по-голям от този на биогенните емисии, а през пролетта по обед се изравнява с тях.

Приземните относителни приноси на отделните източници водещи до образуването на изопрен (ISOP) за Рожен показват, че приносът на биогенните емисии е най-голям, с добре изразени денонощен и сезонен ход, който се мени от 10% до 100% в зависимост от сезона. Разглеждайки приносът на източниците от SNAP_07 се вижда, че той е по-малък и в противофаза с този на биогенните емисии. През лятото приносът на SNAP_07 в 03:00 часа достига едва 10%, докато през останалото време и по обед през пролетта той е отрицателен и може да стане -60%. През останалите сезони през нощта той е по-голям от този на биогенните. Приносите на SNAP_01 и SNAP_02 са почти нулеви и леко отрицателни през различните сезони.

Всички антропогенни източници водещи до образуването на амоняк имат отрицателен принос, добре изразени денонощен и сезонен ход. Приносът на SNAP_01 е най-голям до -26% и доминиращ през почти всички сезони. Като само през зимата доминиращ става вторият по големина приносът на SNAP_02, но с огромен отрицателен принос до -55%, поради което в годишно осреднените приноси той е с по-голям принос от този на енергетиката. Приносът на биогенните емисии е положителен през всеки сезон, като само на пролет рано сутрин той е леко отрицателен. SNAP_07 има най-малък отрицателен принос през всички сезони до -5%.

Всички източници водещи до образуването на серен диоксид са с положителен принос и с добре изразени сезонен и денонощен ход, който е различен за различните източници. На всички фигури се вижда, че най-голям принос има енергетиката около 25%, докато приносите на биогенните емисии и SNAP_07 са почти нулеви. Приносът на източниците от SNAP_02 е втори по големина и е около 10%, като през зимата той е най-голям, а през лятото приносът от не индустриалното изгаряне силно намаля и е почти колкото приносите на SNAP_07 и биогенните емисии.

През всички сезони антропогенните източници имат положителен принос водещи до образуването на едри прахови частици, с добре изразени сезонен и денонощен ход, който е различен за различните източници. Приносът на биогенните емисии е много малък дори нулев и може да бъде отрицателен. През всички сезонни енергетиката има принос около 20%, като той е доминиращ през лятото и есента. Втори по големина е този на SNAP_02, които през зимата и пролетта е по-голям от този на SNAP_01, а през есента е през деня е много близо до него. Приносът на емисиите от SNAP_07 е около 12%, като в 16:00 часа на лятото и есента е най-голям около 18% и е по-голям от този на енергетиката. През лятото втори по значимост е приносът на автомобилният транспорт.

През всички сезони антропогенните източници имат положителен принос водещи до образуването на фини прахови частици, с добре изразени сезонен и денонощен ход, който е различен за различните източници. Приносът на биогенните емисии е много малък дори нулев и може да бъде отрицателен. Както се вижда навсякъде доминиращият принос е този на източниците от енергетиката около 25%. През зимата приносът на SNAP_02 е вторият по големина следван от източниците от автомобилният транспорт, като през пролетта тези два приноса са почти равни. Приносът на SNAP_07 е втори по големина през лятото и есента, като през есента в 17:00 часа става по-голям от този на енергетиката.

За произхода и механизмите за образуване на приземния озон в България

Впечатление прави малкият относителен принос на биогенните емисии към формирането на приземния озон. На пръв поглед това изглежда странно, като се има пред вид, че биогенните емисии са голям източник на ЛОС, такива като изопрен, терпен, а ЛОС от своя страна са един от основните прекурсори на озона.

Приносите на основните източници на NOx също е малък. За да се обясни този факт трябва по-подробно да се разгледат реакциите на озоновата фотохимия (Finlayson-Pitts and Pitts, 1986, Seinfeld and Pandis, 1998, Staehelin, Prévôt and Barnes, 2000) и по специално чрез системата верижни реакции на ROx/HOx радикалите.

OH радикалите могат да реагират:

(i) с органични съединения, водещи до формиране на пероксирадикал, което води до образуване на озон чрез окисляване на NO до NO_2, или

(ii) OH може да реагира с NO_2, формирайки HNO_3 което е крайна реакция, потискаща образуването на O_3.

Доминирането на механизъм (i) над (ii) зависи от съотношението на концентрациите на NO_2 и сумарната концентрация на не метанови ЛОС (взети с тегла пропорционални на скоростите на химични реакции на съответните индивидуални съединения). В градска среда обикновено концентрациите на NO_2 са толкова големи, че образуването на HNO_3 доминира реакциите на OH радикалите (механизъм (ii)), което води до това, че образуването на O_3 е малка. Тези условия са наречени ЛОС-ограничение, защото образуването на O_3 се интензифицира с увеличаване концентрациите на ЛОС. Далеч от града концентрациите на NO_2 в даден обем въздух трайно намаляват, защото NO_2 реагира с наличните OH радикали, както, разбира се, и поради дифузията. Намаляването на NO_2 променя доминирането на механизъм (ii) над механизъм (i), благоприятствайки главно механизъм (i) и съответно локалната продукция на O_3 се увеличава. Когато концентрациите на NO_x са достатъчно намалели, сместа от органични и NO_x концентрации преминава през състояние, при което съотношението на концентрациите на озоновите прекурсори е такова, че продукцията на O_3 става максимална, което е наречено "режим на преход". При по-нататъшно намаляване концентрациите на NO_x (чрез механизъм (ii)) локалната продукция на O_3 се ограничава от наличността на NO_x, режим който се нарича NO_x-ограничение.

Проследявайки концентрациите на NO_2 (от глава II.), а също така и от показаните по-горе оценки на приноса на биогенните емисии, може да се направи извод, че както за страната като цяло, така и за отделните точки по отношение на климата на озоново замърсяване преобладаващият режим е този на NO_x-ограничение.

ГЛАВА IV ОЦЕНКА ПРИНОСА НА РАЗЛИЧНИТЕ ПРОЦЕСИ КЪМ ФОРМИРАНЕ ОБЩАТА КАРТИНА НА ЗАМЪРСЯВАНЕ В СТРАНАТА

Атмосферното замърсяване и съответно неговият климат се формират в резултат на взаимодействието на различни динамични и химични процеси (включително хетерогенна и аерозолна химия и динамика). Познаването на тези процеси, на тяхното взаимодействие и принос, очевидно е изключително важно за обяснение на общата картина на замърсяване в страната и отделни нейни точки.

Използвания при симулациите модел CMAQ има опция, наречена "Integrated Process Rate Analysis", която позволява да се оцени ролята на всеки от отделните процеси при формиране на атмосферното замърсяване, като изменението на концентрацията за даден интервал от време Δc се представи като сума от приноса на различните процеси.

Процесите, които влияят върху формиране картината на замърсяване са следните: хоризонтална и вертикална дифузия, хоризонтална и вертикална адвекция, емисии, сухо отлагане, химически трансформации, аерозолни процеси, хетерогенна химия и облачни процеси, съхранение на масите.

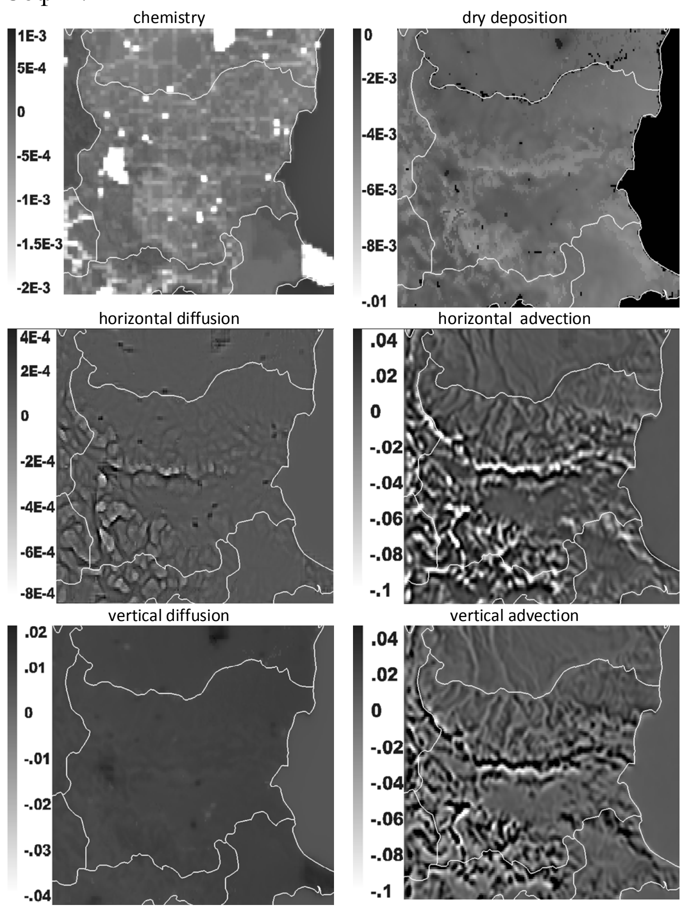
В тази глава на дисертацията са представени главно някои резултати от компютърните симулации, оценяващи приноса на различните динамични процеси на пренос и трансформация на замърсителите, които формират климатът на замърсяването на въздуха в България. В IV.2. са представени двумерни картини на някои осреднени по ансамбъл приземни (всъщност за първия слой в областта на интегриране) приноси на отделните процеси за територията на България. В IV.3. са представени някои оценки на осреднените по ансамбъл приземни приноси на отделните процеси на транспорт и трансформация на замърсителите, осреднени за територията на България и за отделни точки.

Включването на опцията за изследването на приносите на отделните процеси, дава възможност да се определят не само приносите на отделните процеси за определен замърсител, но също така и за група (семейство) от замърсители. В тази глава се разглеждат само една група от газовите замърсители GNOY, а също така и две групи от праховите замърсители ACOARSE и A2.5 (едри и фини прахови частици).

Двумерни полета на осреднените приземни приноси на отделните процеси

Изследването на отделни процеси на транспорт и трансформация на замърсителите има за цел да покаже, кой или кои процеси са водещи при определяне замърсяването на въздуха. Това силно зависи не само от емисиите на даденият замърсител, релефа, подложната повърхност и метеорологията, но също така и от спецификата на даденият замърсител, като например дали той е газ или аерозол, а от тук дали, до колко и как ще му влияят химичните и аерозолните процеси при изменението на неговите концентрации.

Годишно осреднени карти за полетата на приземните приноси на отделните процеси водещи до образуването на азотен диоксид (NO_2): Хоризонталната и вертикалната адвекция се изменят в един и същи диапазон, и като се съпоставят една с друга, добре се вижда влиянието на релефа. Хоризонталната и вертикална адвекция имат като правило обратен знак, което е отражение на уравнението на непрекъснатост (несвиваемост на атмосферата). В полетата и на хоризонталната и на вертикалната адвекция много добре се открояват планинските вериги – отражение на ефектите на обтичане и, може би, склонов вятър. И на двете фигури добре се откроява техният отрицателен принос, най-вече над големите градове и ТЕЦ-овете, като при хоризонталната адвекция се вижда, че максималният принос е изнесен в страни от основните източници на NO_2 и по това може да се съди за преобладаващите ветрове в зоните около тях. Приносът на хоризонталната дифузия е положителен само по високите части на планините и около източниците на NO_2 и е отрицателен в подножията на планините и над самите източници. Както се вижда над останалата част от страната той е почти нулев. Приносът на вертикалната дифузия е отрицателен и много добре се открояват София и предприятията (приземни и ниски източници), където тя има най-голям отрицателен принос. Изключение правят само ТЕЦ-овете Марица Изток, Бобов дол, Варна, Бургас, Русе и Пловдив, които се откроят, като места с положителен и в отделни части от денонощието дори максимален принос на вертикалната дифузия (високи източници). Приносът тези двете двойки адвекции и дифузии се мени в един и същи диапазон, и като цяло техният най-голям отрицателен принос е съсредоточен най-вече над района на София.



Фиг. **IV.1.** Хоризонтално разпределение на приносите [μg/hour] на различни процеси към часовите изменения на приземния озон в 06.00GMT (08.00 местно време).

Приносът на сухото отлагане е най-голям над София и ТЕЦ-овете Бобов дол, Марица Изток и Хасково, което не е странно имайки в предвид, че именно там се открояват местата с едни от най-високите концентрации в страната. Местата с нулеви приноси на сухото отлагане са точно където се очаква да бъдат, а именно над морето, реките и язовирите, като и те също така добре се открояват на картата. Приносът на облачните процеси/ водната химия също е изцяло отрицателен, но е пренебрежимо малък, като той е най-голям над планините и в определени части на деня се открояват София и ТЕЦ-овете Перник и Бобов дол. Приносът на химичните процеси е изцяло положителен и е най-голям в сравнение с останалите процеси, като местата на които той е максимален са над точковите източници на NO_2.

Годишно осреднени карти за полетата на приземните приноси на отделните процеси водещи до образуването на азотни окиси (GNOY): Средно годишните приноси на приземните процеси водещи до образуването на азотни окиси доста наподобяват тези за азотният диоксид. Хоризонталната и вертикалната адвекция и тук се изменят в един и същи диапазон и са с обратни знаци над и покрай планините. Освен това приносите на адвекциите и на вертикалната дифузия са равни и са два пъти по-големи от тези на азотният диоксид, като само хоризонталната дифузия има равен на него принос. Сухото отлагане има по-голям отрицателен принос, като в 11:00 часа той е максимален над абсолютно цялата страна.

От разглеждането на приносите на отделните процеси за това семейство от замърсители се вижда, че при него се появява още един процес, а именно този на образуването на аерозоли. При него през цялото денонощие приносът му е изцяло положителен и най-голям само над планините, като по обяд почти над цялата страна той става положителен. Аерозолните процеси имат най-голям отрицателен принос през цялото денонощие над София, а също така и над предприятията в отделни часове от деня. Освен това се вижда, че приносът на ТЕЦ-овете също е положителен, като този на ТЕЦ София и Перник в 05:00 и 17:00 часа е максимален.

Годишно осреднени карти за полетата на приземните приноси на отделните процеси водещи до образуването на озон (O_3): Хоризонталната и вертикалната адвекция се изменят в един и същи диапазон, и като се съпоставят една с друга, добре се вижда влиянието на релефа. Местата на които хоризонталната адвекция има най-голям отрицателен принос (планините в даден момент), то вертикалната адвекция в същият този момент там е положителна. Приносът на хоризонталната дифузия почти навсякъде е отрицателен и клони към нулата, като планините се открояват с максимален отрицателен принос, а долините с максимален положителен. Приносът на вертикалната дифузия се отличава от този на азотният диоксид, и това не е странно имайки предвид, че двата замърсителя са в противофаза и единият води до трансформирането му в другият. Разликата в знаците на приноса на вертикалната дифузия се обяснява и с това, че азотните оксиди в голяма степен произхождат от приземни източници, докато значителна част от приземният озон е резултат от пренос от по-високите слоеве. През цялото денонощие над почти цялата страна той е положителен, изключение прави само ТЕЦ Марица Изток в 05:00 и 17:00 часа, като точка с максимален отрицателен принос, а София и планините се открояват като места с най-голям положителен принос през денонощието. Приносът на сухото отлагане е най-голям над планините, като в 11:00 часа над цялата област той е максимален, разпределен равномерно над цялата страна и не се открояват по-особени точки. Приносът на облачните процеси/ водната химия, също е изцяло отрицателен, разпределен е почти равномерно и е пренебрежимо малък, като планинските върхове се открояват с по-висок отрицателен принос, а над някой ТЕЦ-ове и предприятия той е максимален. Химичните процеси през по-голямата част от денонощието имат отрицателен принос, като само по обяд почти навсякъде той е положителен. През цялото време София, Девня и Бургас се открояват с максимален отрицателен принос, като в 05:00 и 17:00 часа много добре се виждат ТЕЦ-овете, предприятията и конфигурацията на пътната мрежа, като места с максимален отрицателен принос.

Годишно осреднени карти за полетата на приземните приноси на отделните процеси водещи до образуването на серен диоксид (SO_2): Въпреки, че не са в едни и същи скали може да се види, че местата на които хоризонталната адвекция има най-голям отрицателен принос (планините в даден момент), то вертикалната адвекция в същият този момент там е положителна. Над ТЕЦ-овете най-силно изпъкват максималните отрицателни приноси на хоризонталната адвекция и положителният на вертикалната адвекция. Приносът на хоризонталната дифузия почти навсякъде е отрицателен и клони към нулата, като ТЕЦ-овете се открояват с максимален отрицателен принос, а околностите около тях с повишен положителен и на места максимален. Приносът на вертикалната дифузия през цялото денонощие почти навсякъде е отрицателен и клонящ към нулата, като изключение правят ТЕЦ-овете с максимален положителен принос (високи източници на SO_2). Приносът над София през цялото денонощие е най-силно отрицателен (ниски и приземни източници. Приносът на сухото отлагане е най-голям над ТЕЦ-овете, докато над останалата част почти навсякъде клони към нулата. Приносът на облачните процеси/ водната химия е пренебрежимо малък и също е изцяло отрицателен. Планинските върхове се открояват с по-висок отрицателен принос, от този в областта около тях. Отрицателният принос на облачните процеси/ водната химия е максимален над ТЕЦ-овете и се откроява на откроява на обширни територии около тях. Химичните процеси през по-голямата част от денонощието имат почти нулев принос, като само ТЕЦ-овете се открояват с леко по-голям отрицателен принос. По обяд приносът навсякъде нараства, като над планините той е по-малък, а влиянието на ТЕЦ-овете е максимално и се разпростира над почти цялата страна.

Годишно осреднени карти за полетата на приземните приноси на отделните процеси водещи до образуването на амоняк/ амония (NH_3): Въпреки, че не са в едни и същи скали може да се види, че местата на които хоризонталната адвекция има най-голям отрицателен принос (планините в даден момент), то вертикалната адвекция в същият този момент там е положителна. Над предприятията свързани с производството на амоняк най-силно изпъкват максималните отрицателни приноси на хоризонталната адвекция и положителният на вертикалната адвекция. Приносът на хоризонталната дифузия почти навсякъде е отрицателен и клони към нулата, като предприятията се открояват с максимален отрицателен принос, а околностите около тях с повишен положителен принос. Приносът на вертикалната дифузия навсякъде през цялото денонощие е отрицателен и клонящ към нулата, като изключение правят някои от предприятията в 11:00 часа с положителен принос. Приносите на сухото отлагане и облачните процеси/ водната химия са най-големи над предприятията, докато над останалата част почти навсякъде клони към нулата. Аерозолните процеси през цялото денонощие почти навсякъде имат отрицателен принос, с изключение над планинските върхове през нощта, където той е леко положителен. Максимален отрицателен принос през цялото денонощие се наблюдава над София, докато над предприятията в 05:00 и 17:00 часа. Над ТЕЦ-овете приносът на аерозолните процеси също е максимален и се наблюдава почти през цялото денонощие, като това се дължи на процесите на десулфуризация.

Годишно осреднени карти за полетата на приземните приноси на отделните процеси водещи до образуването на амоний/ амониум (NH_4): Въпреки, че не са в едни и същи скали може да се види, че местата на които хоризонталната адвекция има най-голям отрицателен принос (планините в даден момент), то вертикалната адвекция в същият този момент там е положителна. Приносът на хоризонталната дифузия почти навсякъде е отрицателен и клони към нулата и максимално отрицателен над ТЕЦ-овете. Планините се открояват с положителен принос, а на отделни места покрай някои от ТЕЦ-овете е максимален. Приносът на вертикалната дифузия почти навсякъде през цялото денонощие е отрицателен, клонящ към нулата и е максимално отрицателен над София. Над предприятията също е максимално отрицателен в 05:00 и 17:00 часа, а над ТЕЦ-овете в 11:00 часа. Приносът на вертикалната дифузия става положителен над предприятията в 11:00 и 23:00 часа, а над ТЕЦ-овете в 05:00 и 17:00 часа. Приносът на сухото отлагане е най-голям над планините, като над останалата част почти навсякъде клони към нулата, а в 11:00 часа почти над цялата страна той става максимално отрицателен. Приносът на облачните процеси/ водната химия също е най-голям над планините и ТЕЦ-овете, докато над останалата част почти навсякъде клони към нулата. Аерозолните процеси през цялото денонощие почти навсякъде имат положителен принос, с изключение над планинските върхове през нощта, където той е леко отрицателен. Максимален положителен принос през цялото денонощие се наблюдава над София и ТЕЦ-овете, докато над предприятията само в 05:00 и 17:00 часа. Над ТЕЦ-овете приносът на аерозолните процеси също е максимално положителен, най-вече в 11:00 часа. От тук и от приносът на вертикалната дифузия и от приносите на химичните процеси на серният диоксид в този момент може да се направи хипотезата, че това най-вероятно се дължи на процесите на десулфуризация.

Годишно осреднени карти за полетата на приземните приноси на отделните процеси водещи до образуването на фини прахови частици (A2.5): Въпреки, че не са в едни и същи скали може да се види, че местата на които хоризонталната адвекция има най-голям отрицателен принос (планините в даден момент), то вертикалната адвекция в същият този момент там е положителна, като максималният отрицателен принос над ТЕЦ-овете на хоризонталната адвекция много добре се откроява в 11:00 часа. Приносът на хоризонталната дифузия почти навсякъде е отрицателен и клони към нулата и максимално отрицателен над ТЕЦ-овете. Планините се открояват с положителен принос, а на отделни места покрай някои от ТЕЦ-овете е максимален. Приносът на вертикалната дифузия почти навсякъде през цялото денонощие е отрицателен, клонящ към нулата и е максимално отрицателен над София. Над самите ТЕЦ-овете той е максимално положителен, а в околностите около ТЕЦ-овете отрицателен, което добре се вижда в 11:00 часа. Приносът на сухото отлагане е най-голям над планините, като над останалата част почти навсякъде клони към нулата, а в 11:00 часа почти над цялата страна той нараства и над ТЕЦ Марица Изток става максимално отрицателен.

Приносът на облачните процеси/ водната химия е максимално отрицателен над планините, над останалата част от страната е положителен но клонящ към нулата, а над ТЕЦ Марица Изток е максимално положителен. Аерозолните процеси през цялото денонощие почти навсякъде имат положителен принос, с изключение над планинските върхове, където той е леко отрицателен. Максимален положителен принос през цялото денонощие се наблюдава над София и ТЕЦ-овете, докато над предприятията само в 05:00 и 17:00 часа. В 11:00 часа приносът на аерозолните процеси показват влиянието на ТЕЦ-овете, като се вижда, че почти над цяла южна България той е положителен, а над почти цяла северна отрицателен.

Оценки на годишно и сезонно осреднените приземни приноси на различните процеси за територията на България и за отделни точки.

Показаните по-горе резултати за приземният принос на различните процеси осреднени по осем годишният ансамбъл, получени чрез компютърно симулиране, могат да бъдат използвани, за да се определят приносите на отделните процеси водещи до образуването на даден замърсител както осреднени за страната, така и за която и да е точка от областта. Това е ценна информация, която може да бъде използвана при изучаване природата на замърсяването в дадена точка за определен замърсител или семейство от замърсители.

Оценки на годишно и сезонно осреднените приземни приноси на различните процеси водещи до образуването на различни замърсители осреднени за територията на България: Приземните приноси на отделните процеси водещи до образуването на азотен диоксид (NO_2) за България показват, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите, бива както положително така и отрицателно, с добре изразен денонощен ход, а също така е и различно през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности но с противоположен знак и фази, като за NO_2 това са основно положителният принос на химичните процеси и отрицателният на вертикалната дифузия. Приносът на емисиите, вертикалната и хоризонталната адвекция е доста малък, като приносът на останалите процеси е дори и почти нулев, а това са хоризонталната дифузия, сухото отлагане и облачните процеси.

Приземните приноси на отделните процеси водещи до образуването на GNOY в България показват, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите, бива както положително така и отрицателно, а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойностите но с противоположен знак и фази, като за GNOY това са главно положителният принос на емисиите и отрицателният на вертикалната дифузия. Приносът на вертикалната и хоризонталната адвекция е доста малък, като приносът на останалите процеси е дори и почти нулев, а това са хоризонталната дифузия, сухото отлагане, химичните, аерозолните и облачните процеси.

Приземните приноси на отделните процеси водещи до образуването на озон в България показват, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC за различните сезони се определя главно от различни брой процеси, които са с големи стойности но с противоположен знак и фази, като вертикалната дифузия е водещият процес с положителен принос през деня при годишно осреднения случай, а и за всички сезони с изключение през зимата. През зимата и през нощта за всички случай хоризонталната адвекция е доминиращият процес с положителен принос с изключение на лятото между 12:00 и 16:00 часа когато тя става отрицателна. Приносът на вертикалната адвекция е в противофаза с хоризонталната адвекция и изцяло отрицателен с изключение през лятото от обяд до към 18:00 когато става положителен. През всички сезони за този часови интервал приносът на вертикалната адвекция водещ до изменението на O_3 най-силно намаля . Сухото отлагане е с много добре изразена противофаза с вертикалната дифузия, като през лятото той е доминиращият процес с отрицателен принос през деня. Приносът на химичните процеси е малък и предимно отрицателен с изключение през лятото в интервала между 07:00 и 12:00 часа когато той става положителен. Приносът на хоризонталната дифузия и облачните процеси в сравнение с останалите процеси е практически нулев.

Приносът на хоризонталната дифузия, осреднен по територията на страната, всъщност е нормирания по площта пренос на съответната субстанция през границите. Преобладаващо положителният принос на хоризонталната адвекция (с изключение на часовете около пладне през лятото) говори за предимно чуждестранния произход на приземния озон в България. За това говори и преобладаващо отрицателния принос на химичните трансформации (отново с изключение на часовете около пладне през лятото).

Приземните приноси на отделните процеси водещи до образуването на NH_3 в България показват, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с леко изразен денонощен ход (което бива както положително така и отрицателно), като през различните сезони то е много малко и почти не се наблюдава значително изменение в ходът му. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности но с противоположен знак и фази, като за NH_3 това са положителният принос на емисиите и отрицателният на вертикалната дифузия. Освен това на графиките се вижда, че приносът на останалите процеси е доста малък, като само леко се открояват хоризонталната адвекция с положителен и аерозолните процеси с отрицателен принос.

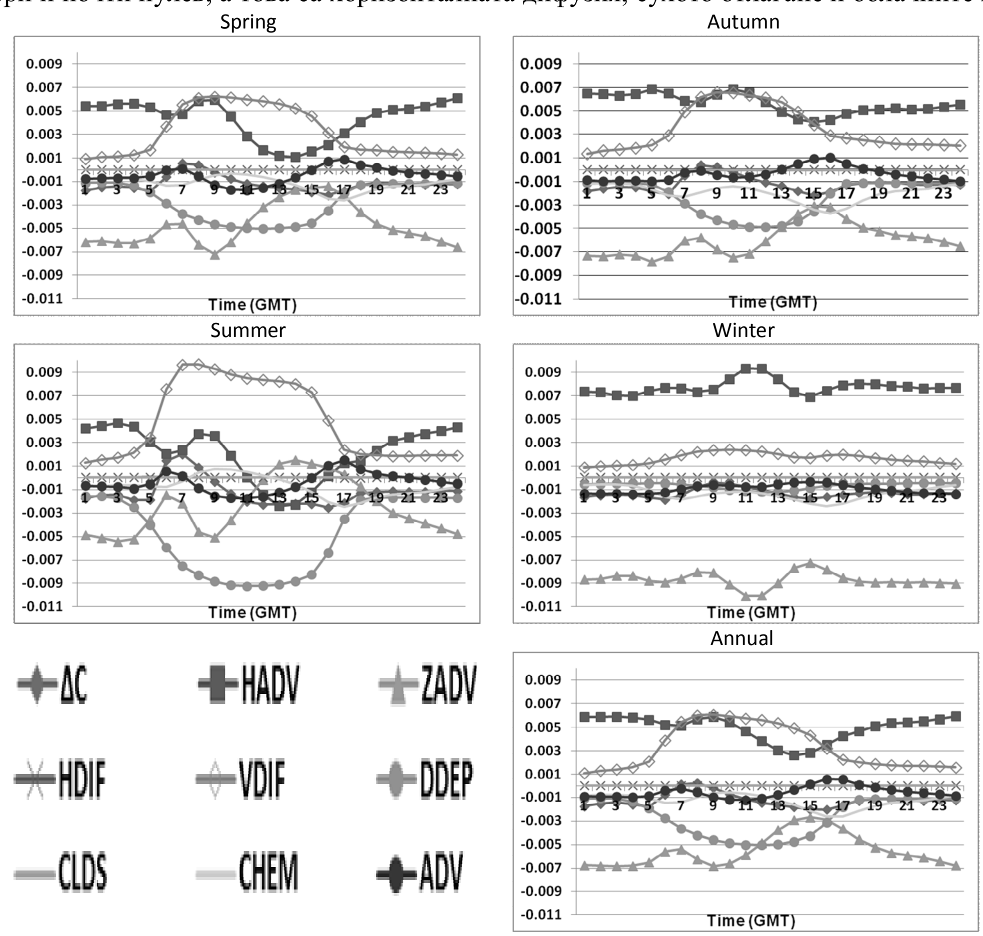
Приземните приноси на отделните процеси водещи до образуването на NH_4 в България показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите, бива както положително така и отрицателно и с добре изразен денонощен ход, а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности но с противоположен знак и фази, като за NH_4 това са положителният принос на аерозолните процеси и отрицателният принос на вертикалната дифузия през деня и вертикалната адвекция през нощта. Също така приносът на хоризонталната адвекция е доста голям и предимно положителен с изключение през следобедните часове на лятото и есента когато тя става леко отрицателна. Приносът на останалите процеси е почти нулев, като това са хоризонталната дифузия, сухото отлагане, химичните и облачните процеси.

Приземните приноси на отделните процеси водещи до образуването на SO_2 в България показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности но с противоположен знак и фази, като за SO_2 това са положителният принос на емисиите и отрицателният на вертикалната дифузия. Отрицателният приносът на сухото отлагане и вертикалната и адвекция, също е добре представен, а приносът хоризонталната адвекция е с предимно положителен с изключение по изгрев и залез слънце. Приносът на останалите процеси е почти нулев, а това са хоризонталната дифузия, химичните и облачните процеси.

Приземните приноси на отделните процеси водещи до образуването на ACOARSE в България показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности но с противоположен знак и фази, като за ACOARSE това са положителният принос на емисиите и отрицателният на сухото отлагане и вертикалната дифузия. Приносът на вертикалната и хоризонталната адвекция е доста малък, като приносът на останалите процеси е дори и почти нулев, а това са хоризонталната дифузия, химичните, аерозолните и облачните процеси.

Приземните приноси на отделните процеси водещи до формирането на A2.5 в България показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности но с противоположен знак и фази, като за A2.5 това са отрицателният принос на вертикалните адвекция и дифузия и положителният принос на емисиите, аерозолните процеси и хоризонталната адвекция с изключение през лятото около 17:00 часа когато хоризонталната адвекция става леко отрицателна. Приносът на останалите процеси е почти нулев, а това са хоризонталната дифузия, сухото отлагане, химичните и облачните процеси.

Оценки на годишно и сезонно осреднените приземни приноси на различните процеси водещи до образуването на различни замърсители осреднени за територията на София: Приземните приноси на отделните процеси водещи до формирането на NO_2 над София показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности но с противоположен знак и фази, като за NO_2 това са отрицателният принос на вертикалната адвекция през нощта и на вертикалната дифузия през деня с изключение през зимата когато доминира само вертикалната адвекция. Химичните процеси са с доминиращ положителният принос с изключение през зимата когато приносът и е равен на този на хоризонталната адвекция. Приносът на хоризонталната адвекция е доста различен за различните сезони - докато през лятото е предимно отрицателен то през зимата е само положителен. Приносът на останалите процеси е доста малък, дори и почти нулев, а това са хоризонталната дифузия, сухото отлагане и облачните процеси.



Фиг. **IV.1.** Графики на "типичен" годишен и сезонен денонощен ход на осреднените за територията на България приноси на хоризонталната адвекция (HADV),вертикалната адвекция (ZADV), сумарната (хоризонтална + вертикална) адвекция (ADV), хоризонталната дифузия (HDIF), вертикалната дифузия (VDIF), сухото отлагане (DDEP), химичните процеси (CHEM), облачни процеси/водна химия (CLDS) към часовите изменения (ΔC) на приземния O_3.

Приземните приноси на отделните процеси водещи до формирането на GNOY в България показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности, но с противоположен знак и фази, като за GNOY това са положителният принос на емисиите и отрицателният на вертикалната дифузия през деня и вертикалната адвекция през нощта. Изключение прави само зимата когато положителният принос на емисиите е почти колкото приносът на хоризонталната адвекция, а вертикалната адвекция е с изцяло доминиращ отрицателен принос. Освен това приносът на останалите процеси е доста малък и е почти нулев, а това са хоризонталната дифузия, сухото отлагане, химичните, аерозолните и облачните процеси.

Приземните приноси на отделните процеси водещи до формирането на O_3 в София показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC за различните сезони се определя главно от различни брой процеси, които са с големи стойности, но с противоположен знак и фази, като хоризонталната адвекция и вертикалната дифузия са водещите процеси с положителен принос. Вертикалната адвекция е с доминиращ отрицателен принос през всички сезони с изключение през лятото след 07:00 часа, когато тя става положителна и си сменя знакът с хоризонталната адвекция който пък става отрицателен (вероятно резултат от по-развити конвективни процеси през лятото). Приносът на химичните процеси е малък и е изцяло отрицателен, а приносът на хоризонталната дифузия, сухото отлагане и облачните процеси в сравнение с останалите процеси е практически нулев.

Приземните приноси на отделните процеси водещи до формирането на NH_3 в София показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности, но с противоположен знак и фази, като за NH_3 това са положителният принос на емисиите и в по-малка степен на хоризонталната адвекция до около 16:00 часа след което тя става с отрицателен принос. Отрицателният принос на аерозолните процеси и в по-голяма степен на вертикалната дифузия през деня и на вертикалната адвекция през нощта е добре изразен на всички плотове. Изключение прави само зимата, когато аерозолните процеси са доминиращи с отрицателен принос, а хоризонталната адвекция е изцяло положителна. Освен това приносът на останалите процеси е доста малък, дори почти е нулев за сухото отлагане, хоризонталната дифузия, химичните и облачните процеси.

Приземните приноси на отделните процеси водещи до формирането на NH_4 в София показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности, но с противоположен знак и фази, като за NH_4 това са положителният принос на аерозолните процеси и хоризонталната адвекция, с изключение през лятото, когато след изгрев тя става изцяло отрицателна. Отрицателният принос на вертикалната адвекция също е добре изразен през всички сезони, но отново през лятото след изгрев тя става положителна. Приносът на вертикалната дифузия е изцяло отрицателен но доста малък в сравнение с изброените процеси. Останалите процеси имат почти нулев принос, а това са хоризонталната дифузия, сухото отлагане, химичните и облачните процеси.

Приземните приноси на отделните процеси водещи до формирането на SO_2 в София показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности, но с противоположен знак и фази, като за SO_2 това са положителният принос на емисиите и хоризонталната адвекция, с изключение на лятото. Доминиращите отрицателни приноси на вертикалната адвекция през нощта и на вертикалната дифузия през деня също са добре изразени през всички сезони. През лятото до 08:00 часа приноса на хоризонталната адвекция е положителен, след което става леко отрицателен до 22:00 когато отново става положителен, а приноса на вертикалната адвекция е подобен но с обратен знак. Приносът на останалите процеси е почти нулев, а това са хоризонталната дифузия, химичните и облачните процеси.

Приземните приноси на отделните процеси водещи до формирането на ACOARSE в София показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности, но с противоположен знак и фази, като за ACOARSE това са положителният принос на емисиите и през отделните сезони на хоризонталната адвекция, и отрицателният принос на сухото отлагане и вертикалната адвекция. Приносът на вертикалната дифузия е доста малък, а на останалите процеси е дори и почти нулев, а това са хоризонталната дифузия, химичните, аерозолните и облачните процеси.

Приземните приноси на отделните процеси водещи до формирането на A2.5 в София показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности, но с противоположен знак и фази, като за A2.5 това са отрицателният принос на вертикалните адвекция и дифузия и положителният принос на емисиите и хоризонталната адвекция с изключение през лятото. Тогава от 07:00 до 23:00 часа хоризонталната адвекция става отрицателна, а вертикалните адвекция положителна. Аерозолните процеси се открояват, но техният принос е доста по-малък в сравнение с този на изброените по-горе. Приносът на останалите процеси е почти нулев, а това са хоризонталната дифузия, сухото отлагане, химичните и облачните процеси.

Оценки на годишно и сезонно осреднените приземни приноси на различните процеси водещи до образуването на различни замърсители осреднени за територията на Стара Загора: Приземните приноси на отделните процеси водещи до формирането на NO_2 над Стара Загора показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности, но с противоположен знак и фази, като за NO_2 това са положителният принос на химичните процеси и хоризонталната адвекция, и отрицателният на вертикалната дифузия през деня и вертикалната адвекция през нощта. Освен това приносът на останалите процеси е дори и почти нулев, а това са хоризонталната дифузия, емисиите, сухото отлагане и облачните процеси.

Приземните приноси на отделните процеси водещи до формирането на GNOY в Стара Загора показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности, но с противоположен знак и фази, като за GNOY това са положителният принос на емисиите през деня и хоризонталната адвекция през нощта, и отрицателният на вертикалната дифузия през деня и вертикалната адвекция през нощта. През пролетта и есента хоризонталната и вертикалната адвекция си смеят знака по обяд, а през лятото през целият ден. Освен това приносът на останалите процеси е дори и почти нулев, а това са хоризонталната дифузия, сухото отлагане, аерозолните, химичните и облачните процеси.

Приземните приноси на отделните процеси водещи до формирането на O_3 в Стара Загора показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC за различните сезони се определя главно от различни брой процеси, които са с големи стойности, но с противоположен знак и фази, като вертикалната дифузия е водещият процес с положителен принос през деня и хоризонталната адвекция през нощта с изключение през зимата. През зимата и през нощта за всички случай хоризонталната адвекция е доминиращият процес с положителен принос. Приносът на вертикалната адвекция е в противофаза с хоризонталната адвекция. Сухото отлагане е в много добре изразена противофаза с вертикалната дифузия и то най-вече през лятото. Приносът на хоризонталната дифузия, химичните и облачните процеси в сравнение с останалите процеси е практически нулев.

Приземните приноси на отделните процеси водещи до формирането на NH_3 в Стара Загора показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с постоянно изменящ се денонощен ход, който бива както положително така и отрицателно, а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности, но с противоположен знак и фази, като за NH_3 това са положителният принос на емисиите и отрицателният на вертикалната дифузия. Освен това приносът на останалите процеси е доста малък, като леко се открояват само хоризонталната и вертикалната адвекция и аерозолните процеси. Постоянното изменение на денонощният ход в приносът на емисиите над Стара Загора се забелязва, че през всички сезони периодите на минимумите и максимумите му съвпадат.

Приземните приноси на отделните процеси водещи до формирането на NH_4 в Стара Загора показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с постоянно изменящ се денонощен ход, който бива както положително така и отрицателно, а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности, но с противоположен знак и фази, като за NH_4 това са положителният принос на аерозолните процеси, хоризонталната адвекция през нощта и вертикалната адвекция през деня, а също така и на отрицателният принос на хоризонталната адвекция и вертикалната дифузия през деня и вертикалната адвекция през нощта. Изключение прави само зимата когато хоризонталната адвекция е изцяло положителна а вертикалната адвекция изцяло отрицателна. Приносът на останалите процеси е почти нулев, а това са хоризонталната дифузия, сухото отлагане, химичните и облачните процеси. Постоянното изменение на денонощният ход в приносът на аерозолните процеси над Стара Загора се забелязва, че през всички сезони периодите на минимумите и максимумите му съвпадат, като това най-добре се вижда през деня.

Приземните приноси на отделните процеси водещи до формирането на SO_2 в Стара Загора показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности, но с противоположен знак и фази, като за SO_2 това са положителният принос на емисиите и хоризонталната адвекция през нощта и вертикалната адвекция през деня. Отрицателният принос на сухото отлагане е добре изразен, като също така добре се вижда и приносът на хоризонталната адвекция през деня и вертикалната адвекция през нощта. Приносът на останалите процеси е почти нулев, а това са хоризонталната дифузия, химичните и облачните процеси.

Приземните приноси на отделните процеси водещи до формирането на ACOARSE в Стара Загора показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности, но с противоположен знак и фази, като за ACOARSE това са положителният принос на емисиите и хоризонталната адвекция през нощта и вертикалната адвекция и дифузия през деня. Отрицателният принос на сухото отлагане е добре изразен, като също така добре се вижда и приносът на хоризонталната адвекция през деня и вертикалната адвекция през нощта. Освен това приносът на останалите процеси е и почти нулев, а това са хоризонталната дифузия, химичните, аерозолните и облачните процеси.

Приземните приноси на отделните процеси водещи до формирането на A2.5 в Стара Загора показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности, но с противоположен знак и фази, като за A2.5 това са положителният принос на аерозолните процеси и хоризонталната адвекция през нощта и вертикалната адвекция през деня. Отрицателният принос хоризонталната адвекция през деня и вертикалната адвекция през нощта също е добре представен. Приносът на останалите процеси е почти нулев, а това са хоризонталната и вертикалната дифузия, химичните и облачните процеси. изключение прави само зимата когато хоризонталната адвекция е изцяло положителна, вертикалната адвекция изцяло отрицателна, а също така приносът на вертикалната дифузия е по-добре изразен в сравнение с останалите случаи.

Оценки на годишно и сезонно осреднените приземни приноси на различните процеси водещи до образуването на различни замърсители осреднени за територията на Рожен: Приземните приноси на отделните процеси водещи до формирането на NO_2 над Рожен показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности, но с противоположен знак и фази, като за NO_2 това са положителният принос на вертикалната адвекция през нощта и химичните процеси. Приносът е отрицателен за хоризонталната адвекция през нощта, вертикалната адвекция през деня и вертикалната дифузия. Приносът за останалите процеси е доста малък дори и е почти нулев, а това са хоризонталната дифузия, сухото отлагане и облачните процеси. Единствено есента се различава в денонощният ход на приносите на отделните процеси, като хоризонталната адвекция е почти изцяло отрицателна с изключение на интервалите между 15:00-17:00 и 20:00-21:00 часа, вертикалната адвекция е положителна само от 07:00-13:00 часа, а вертикалната дифузия през нощта си мени на около всеки два часа знака.

Приземните приноси на отделните процеси водещи до формирането на GNOY в Рожен показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности, но с противоположен знак и фази, като за GNOY това са положителният принос на емисиите и хоризонталната адвекция през деня и вертикалната адвекция през нощта. Отрицателният принос на вертикалната адвекция през деня и хоризонталната адвекция през нощта, а също така и на вертикалната дифузия и сухото отлагане са добре откроими. Освен това приносът на останалите процеси е дори и почти нулев, а това са хоризонталната дифузия, аерозолните, химичните и облачните процеси.

Приземните приноси на отделните процеси водещи до формирането на O_3 в Рожен показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC за различните сезони се определя главно от различни брой процеси, които са с големи стойности но с противоположен знак и фази. През деня е хоризонталната адвекция, а през нощта вертикалната адвекция са с положителен принос, като през есента хоризонталната адвекция е с изцяло положителен принос, а вертикалната адвекция с изцяло отрицателен, като максимумите им са по-малки и изместени с няколко часа по-късно. Отрицателният принос на сухото отлагане е в противофаза с положителният на вертикалната дифузия. Приносът на хоризонталната дифузия, химичните и облачните процеси в сравнение с останалите процеси е практически нулев.

Приземните приноси на отделните процеси водещи до формирането на NH_3 в Рожен показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности, но с противоположен знак и фази, като за NH_3 това са положителният принос на емисиите и отрицателният на вертикалната дифузия, аерозолните процеси и през есента и лятото на сухото отлагане. Освен това приносът на останалите процеси е доста малък и е почти нулев, като само леко се открояват хоризонталната адвекция с положителен принос през деня и отрицателен през нощта и обратното за вертикалната адвекция.

Приземните приноси на отделните процеси водещи до формирането на NH_4 в Рожен показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности, но с противоположен знак и фази, като за NH_4 това са положителният принос на аерозолните процеси и отрицателният на вертикалната дифузия през деня и вертикалната адвекция през нощта. Също така приносът на хоризонталната адвекция е доста голям и положителен през деня и отрицателен през нощта, като приносът на вертикалната адвекция е в противофаза с този на хоризонталната адвекция. Приносът на останалите процеси е почти нулев, а това са хоризонталната дифузия, сухото отлагане, химичните и облачните процеси.

Приземните приноси на отделните процеси водещи до формирането на SO_2 в Рожен показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности, но с противоположен знак и фази, като за SO_2 това са положителният принос на емисиите, хоризонталната адвекция през деня и вертикалната адвекция през нощта с изключение през есента. Отрицателният принос на сухото отлагане се вижда през всички сезони с изключение през лятото. Приносът на хоризонталната адвекция през нощта и вертикалната адвекция през деня е отрицателен с изключение през есента. През есента доминиращи са вертикалната дифузия с положителен принос и хоризонталната адвекция с отрицателен, като именно тогава приносът на сухото отлагане е най-голям. Приносът на останалите процеси е почти нулев, а това са хоризонталната дифузия, химичните и облачните процеси.

Приземните приноси на отделните процеси водещи до формирането на ACOARSE в Рожен показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности, но с противоположен знак и фази, като за ACOARSE това са положителният принос на емисиите и отрицателният на сухото отлагане. Приносът на вертикалната адвекция през нощта е положителен а през деня отрицателен, а за хоризонталната адвекция обратно. Приносът на останалите процеси е почти нулев, а това са хоризонталната дифузия, химичните, аерозолните и облачните процеси и вертикалната дифузия с изключение през есента. През есента приносът на вертикалната дифузия е положителен и доста голям.

Приземните приноси на отделните процеси водещи до формирането на A2.5 в Рожен показва, че сумарното изменение на процесите (ΔC) водещо до изменението на концентрациите е с добре изразен денонощен ход (което бива както положително така и отрицателно), а също така и с различен ход през различните сезони. Изменението на ΔC се определя главно от малък на брой процеси, които са с големи стойности, но с противоположен знак и фази, като за A2.5 това са положителният принос на емисиите и аерозолните процеси, и отрицателният на вертикалната дифузия. Също така се вижда, че приносът на хоризонталната адвекция е доста голям и положителен през деня и отрицателен през нощта, като приносът на вертикалната адвекция е в противофаза с този на хоризонталната адвекция. Приносът на останалите процеси е почти нулев, а това са хоризонталната дифузия, сухото отлагане, химичните и облачните процеси.

ЗАКЛЮЧЕНИЕ

Настоящото изследване беше извършено с методите на компютърната симулация. При това беше използван набор **световно признати** и широко използвани модели с **доказани симулационни качества**, а именно US EPA Models-3 system.

При изследването бяха използвани **надеждни** бази данни, а именно инвентаризация на емисиите и емисионните времеви профили, разработени от TNO, Нидерландия и крупномащабни метеорологични полета, взети от US NCEP "Global Analysis Data".

Компютърните симулации бяха извършени чрез последователно решаване на задачата в няколко последователни, вместени една в друга области, при използване възможностите за 'nesting' на моделите MM5 и CMAQ. При това от една страна беше постигната висока разрешаваща способност от 3 km за територията на България, а от друга беше отчетено и влиянието на външните за страната европейски емисии върху нивата на замърсяване в България.

Резултатите от компютърните симулации бяха надлежно проверени чрез сравнение с данните от измервания в станциите от НАСЕМ. Сравненията показаха, че в голяма степен е удовлетворено изискването за не повече от 50% неопределеност за едночасовите нива на замърсяване, дефинирано в съответните европейски директиви (European Parliament, 2002) и Приложение №4 към чл.15, т.2 от Наредба №4 от 5.07.2004. Това изискване е категорично удовлетворено за 8-часовите пълзящи средни стойности на озоновите концентрации.

Като цяло от проверката на компютърно симулираните приземни концентрации следва, че като ансамбъл те са достатъчно достоверни и надеждни и **могат да се използват за оценки на замърсяването на страната**.

Компютърните симулации бяха извършени за дълъг период от време - 2000-2007 г. По този начин беше генериран ансамбъл от симулирани приземни концентрации за пет емисионни сценария, който е **изчерпателен** – отразява възможното многообразие на метеорологични условия, а именно целият набор типични и екстремни ситуации с тяхната характерна повторяемост във времето. По този начин симулираните приземни концентрации и други характеристики на замърсяването и при петте емисионни сценария следва да се приемат за **представителни**, т.е. такива които съдържат, както типичните, така и екстремни конфигурации на полетата с типичната им повторяемост. Така, генерираният ансамбъл може да се разглежда като характеристика на **климата** на замърсяване на страната. Съответно с това получените ансамблови оценки на нивата на замърсяване при всички емисионни сценарии са **универсални** – направените на тяхна основа изводи могат, при равни други условия, да бъдат отнесени към всеки друг период от време.

Анализът на ансамбъла от симулации позволи да бъдат разкрити някои от основните факти относно климата на атмосферно замърсяване в България, изведени от резултатите от компютърните симулации: осреднени по ансамбъла приземни концентрации на замърсители за територията на България и за отделни точки, тяхната денонощна и сезонна изменчивост, границите в които те се изменят с различна вероятност и пр. Бяха определени и абсолютните максимални, получени при анализ на целия ансамбъл, концентрации за съответния замърсител с техния денонощен ход. Бяха пресметнати и показани някои от най-използваните и важни индекси на озоново замърсяване, които са важни не само за човешкото здраве, но също така и за горското и селското стопанство.

Съпоставянето на резултатите от петте емисионни сценария позволи да бъдат оценени, отново в климатичен смисъл (осреднени по целия ансамбъл), приносите на източниците от съответните категории към общата картина на замърсяване в страната с тяхната денонощна и сезонна изменчивост.

Замърсяването на въздуха силно зависи от емисиите на примеси. Ето защо изследването на приноса на емисиите от отделни категории източници (SNAP категории) към общата картина на замърсяване в страната е очевидно задача с голямо практическо значение, чиито резултати могат да бъдат пряко използвани при формулирането на краткосрочни (текущи) решения и дългосрочни стратегии за намаляване на замърсяването на въздуха.

Използвания при симулациите модел CMAQ има опция, наречена “Integrated Process Rate Analysis”, която позволява да се оцени ролята на всеки от отделните процеси при формиране на атмосферното замърсяване. Чрез осредняването на тези приноси по ансамбъл беше изяснена тяхната денонощна и сезонна изменчивост и беше анализирана ролята на отделните процеси за формиране на замърсяването, както за страната като цяло, така и за отделни нейни точки.

Атмосферното замърсяване и съответно неговият климат се формират в резултат на взаимодействието на различни динамични и химични процеси (включително хетерогенна и аерозолна химия и динамика). Познаването на тези процеси, на тяхното взаимодействие и принос, очевидно е изключително важно за обяснение на общата картина на замърсяване в страната и отделни нейни точки.

Един много важен и нов резултат, получен при настоящото изследване е изводът за произхода на приземния озон в България. Анализът както на приноса на емисиите от различните категории източници, така и на ролята на отделните процеси при формиране на приземния озон показва, че характерен за страната е режимът на NO_x лимитация, който ограничава образуването на приземен озон, така че озонът в България произхожда в голяма степен от външни за страната източници.

Анализът на ансамбълът от компютърни симулации, представен в настоящия дисертационен труд, далеч не е изчерпателен.

Например, не са показани резултатите за сухото и влажно отлагане, които са важни характеристики на въздействието на качеството на въздуха върху екосистемите, както и приноса на отделните категории източници към формирането им.

Не са показани и пресметнатите статистически моменти от по-висок порядък, като асиметрия, уплътняване и пр. Изобщо, ансамбълът като цяло търпи по-детайлен и задълбочен статистически анализ.

Могат, също така да се пресметнат и още много индекси на замърсяване и комфорт.

Всички тези задачи ще стоят при бъдещата работа на автора.

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Grid computing for atmospheric composition studies in Bulgaria

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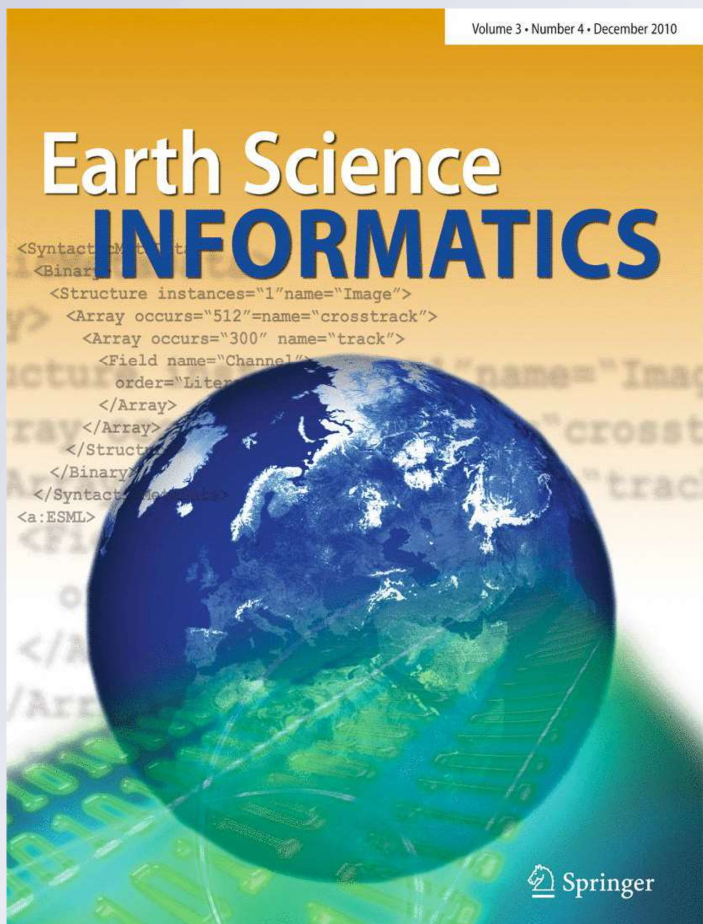

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RESEARCH ARTICLE

Grid computing for atmospheric composition studies in Bulgaria

Angelina Todorova · Dimiter Syrakov · Georgi Gadjhev · Georgi Georgiev · Kostadin G. Ganev · Maria Prodanova · Nikolai Miloshev · Valery Spiridonov · Andrej Bogatchev · Kiril Slavov

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Abstract Three Grid applications from the SEE-GRID-SCI Environmental VO are developed by the Bulgarian project team: Climate Change Impact on Air Quality (CCIAQ); Multi-scale atmospheric composition modeling (MSACM); Modeling System for Emergency Response to the Release of Harmful Substances in the Atmosphere (MSERRHSA). The three applications concern problems of significant socio-economic significance. They are all dedicated to air pollution studies, but address different goals and so face different problems and requirements. The applications are briefly presented in the paper. Examples of the different applications validations are given. Some application results are shown and commented.

Keywords Atmospheric composition · Regional scale transport and transformation · Numerical modeling · Grid computing

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Introduction

Three Grid applications from the SEE-GRID-SCI Environmental VO (http://www.see-grid-sci.eu/), developed by the Bulgarian project team will be presented in the paper. The Environmental VO applications are the following:

– Climate Change Impact on Air Quality (CCIAQ)
– Multi-scale atmospheric composition modeling (MSACM)
– Modeling System for Emergency Response to the Release of Harmful Substances in the Atmosphere (MSERRHSA)

The applications concern different aspects of atmospheric composition studies, so they are closely related in many ways, which is the reason to be presented in one paper. They are based on almost the same modeling tools and use to great extend common databases. All the three tasks require substantial computer resources and this is the reason why the Grid is chosen as a computational platform.

The applications face different problems, however, so below they will be considered separately, respectively in chapters 2, 3 and 4.

Climate change impact assessment of air quality over Bulgaria

Study objectives

Extremely many scientific projects and related publications are aimed to assessment of the impact of climate changes on various areas of human activity and environment. The impact of climate changes on pollution levels uses to be object

Ivan Lirkov
Svetozar Margenov (Eds.)

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Process Analysis of Atmospheric Composition Fields in Urban Area (Sofia City)

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Abstract. The air pollution pattern is formed as a result of interaction of different processes, so knowing the contribution of each one of the processes for different meteorological conditions and given emission spatial configuration and temporal profiles could be helpful for understanding the atmospheric composition and air pollutants behavior. Analysis of the contribution of these different processes (chemical and dynamical) which form the atmospheric composition in chosen region will be demonstrated in the present paper. To analyze the contribution of different dynamic and chemical processes for the air pollution formation over Sofia the CMAQ Integrated Process Rate Analysis option was applied. The procedure allows the concentration change for each compound to be presented as a sum of the contribution of each one of the processes, which determine the air pollution concentration. A statistically robust ensemble of the atmospheric composition over Sofia, taking into account the two-way interactions of local to urban scale and tracking the main pathways and processes, which lead to different scale atmospheric composition formation should be constructed in order to understand the atmospheric composition climate and air pollutants behavior.

On the basis of 3D modeling tools an extensive data base was created and this data was used for different studies of the atmospheric composition, carried out with good resolution using up-to-date modeling tools and detailed and reliable input data. All the simulations were based on the US EPA (Environmental Protection Agency) Model–3 system for the 7 years period (2008 to 2014). The modeling system consists of 3 models, meteorological pre–processor, the emission pre–processor SMOKE and Chemical Transport Model (CTM) CMAQ.

Keywords: Air pollution modeling · Dynamical and chemical processes · Ensemble of numerical simulation · Atmospheric composition · Process analysis

1 Introduction

An ensemble of the atmospheric composition over Sofia, taking to account the two-way interactions of different processes and track the main pathways and

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Numerical study of the atmospheric composition in Bulgaria

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ABSTRACT

The present work aims at studying the local to regional atmospheric pollution transport and transformation processes over Bulgaria and at tracking and characterizing the main pathways and processes that lead to atmospheric composition formation in the region.

The US EPA Models-3 system is chosen as a modeling tool. As the NCEP Global Analysis Data with 1 degree resolution is used as meteorological background, the MM5 and CMAQ nesting capabilities are applied for downscaling the simulations to a 9 km resolution over Balkans and 3 km over Bulgaria. The TNO emission inventory is used as emission input. Special pre-processing procedures are created for introducing temporal profiles and speciation of the emissions.

The study is based on a large number of numerical simulations carried out day by day for the years 2000–2007 and four emission scenarios—with all the emissions and with biogenic emissions, emissions from energetics and road transport excluded. Results from the numerical simulations concerning the main features of the atmospheric composition in Bulgaria and the contribution of the different emission categories are demonstrated in the paper. Some results from the CMAQ "Integrated Process Rate Analysis" are also given.

1. Introduction

Air Quality (AQ) is a key element for the well-being and quality of life of European citizens. Bulgaria also faces AQ problems. It should be noted that, while in Western Europe the photo-oxidant and PM air pollution is at present the major environmental problem, in Bulgaria the classic acidifying pollutants (SO_2, NO_x), the heavy metals (Hg, Cd, Pb) and the persistent organic pollutants are still a serious problem and so the study of their environmental impact is absolutely necessary. The reduction of the emissions of these compounds is a major task in the environmental policy of the country.

Regional studies of the air pollution over the Balkans, including country-to-country pollution exchange, had been carried out for quite a long time—see for example [1–8]. These studies were focused on both studying some specific air pollution episodes and long-term simulations and produced valuable knowledge and experience about the regional to local processes that form the air pollution pattern over Southeast Europe. It seems, however, that the atmospheric composition status in Bulgaria is still not enough comprehensively studied. The word "comprehensive" in the context of the present study should mean:

– simulations performed for a long enough period, which would grant that all the most typical for the country meteorological situations will appear with their typical recurrence;

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– simulations performed for different emission scenarios, which will make the evaluation of the contribution of different source types to the air pollution pattern of the country possible;
– attempt for generalization and joint consideration of all the obtained simulation results.

Carrying out such a comprehensive study with up-to-date modeling tools detailed and reliable input data and good resolution is the aim of the present work.

The air pollution transport is subject to different scale phenomena, each characterized by specific atmospheric dynamics mechanisms, chemical transformations, typical time scales, etc. The specifics of each transport scale define a set of requirements for appropriate treatment of the pollutants transport and transformation processes, respectively for suitable modeling tools, data bases, scenarios and time scales for air pollution evaluation. The air pollution pattern is formed as a result of interaction of different processes, so knowing the contribution of each for different meteorological conditions and given emission spatial configuration and temporal behavior is by all means important. That is why the one of the overall study goals is to make some evaluations of the contribution of different processes to the local to regional pollution over the Balkans and/or Bulgaria.

The main scientific challenge of local to regional atmospheric composition pattern modeling probably is the accounting for the strong dependence of concentrations on fluctuations of local and regional meteorological conditions, the complex interaction of transport scales (different life times of the pollutants make it even more complex), uncertainties and responses to emission forcing and boundary conditions, both introducing information noise. This is even more valid for the Balkan Peninsula—a region with complex topography, which causes significant disturbances of air flows. These mesoscale disturbances may have a great influence not only on the local pollution transport and hence on the detailed pollution pattern, but also on the trans-boundary transport of substances (see for example [3,9,10]). That is why the multi-scale modeling is an important issue in the study strategy.

Atmospheric composition modeling methods include statistical, deterministic and hybrid systems. The approach presented in the present paper is deterministic—a combination of meteorological input, weather diagnosis/forecasting, additional meteorological pre-processing and chemical composition simulations. This is a fruitful approach for indicating exceedances of limit and target values, evaluating different emission sources impact on air pollution and formulating possible long and short term measures to abate air pollution. The deterministic approach could also help the better understanding the role of different transport scales and phenomena in the formation of the air pollution model, thus contributing to the model validation.

Multi-scale numerical experiments have to be carried out, which to some extent account for different scale process interactions. Model interfaces from synoptic through meso- to local scale have to be tailored (two-way nesting effects have to be checked). In shortly, extensive sensitivity studies have to be carried out, tailoring the model set-up and parameters.

Performing extensive simulations of this kind with up to date highly sophisticated numerical models obviously requires computer resources of the order of magnitude of those provided by the so-called supercomputers. Using supercomputers, however, is rather expensive and far beyond what most of the research groups can afford. Luckily an alternative technology—grid computing [11–13], is recently very intensively developing, which makes formulating and solving problems already quite relevant.

2. Methodology and input data

2.1. Modeling tools

All the simulations were based on the US EPA Models-3 system, which was chosen as a modeling tool because it appears to be one of the most widely used models with proved simulation abilities. At the same time, this is a modeling tool of large flexibility with a range of options and possibilities to be used for different applications/purposes. Many research groups in Europe already use the Models-3 system or some of its elements and this number is going to increase rapidly.

The system consists of three components:

– MM5—the 5th generation PSU/NCAR Meso-meteorological Model MM5 [14,15] used as meteorological pre-processor;
– CMAQ—the Community Multiscale Air Quality System [16,17]—the Chemical Transport Model (CTM) of the system, and
– SMOKE—the Sparse Matrix Operator Kernel Emissions Modeling System [18]—the emission pre-processor of Models-3 system.

The next-generation mesoscale numerical weather prediction system WRF is already available and even used in Bulgaria for some other studies [19]. Nevertheless it was decided that the MM5 model be applied for the present study. The reasons for this choice are the following: the teams experience is mostly in using MM5; some model validation experiments for the above described US EPA Models-3 system have already been carried out; the Bulgarian operational air pollution forecast system is also based on the US EPA Models-3 system, so some consistency of the present "pollution climate" simulations with the air pollution forecast will make it possible for conclusions from the current study to be compared in the future with air pollution forecast results.

Each of these models consists of a number of programs that can be run in different schedules depending of the task to be solved. The output of one module is input to others. Taking into account that they had to be run for multiple days it occurred

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that very complicated LINUX scripts were necessary to be created. The obtained results have been visualized by several graphical packages – GRAPH, GRADS, PAVE, SURFER, IDV – supplemented by meta-languages for automation of drawing. All this presumes high experience in Linux and different programming languages.

2.2. Integrated Process Rate Analysis

The Models-3 ''Integrated Process Rate Analysis'' option was applied to discriminate the role of different dynamic and chemical processes for the air pollution pattern formation. The procedure allows the concentration change for each compound for an hour Δc to be presented as a sum of the contribution of the processes, which determine the concentration:

$$\Delta c = \sum_{i=1}^{N} \Delta c_i. \tag{1}$$

The processes that were considered are: advection, diffusion, mass adjustment, emissions, dry deposition, chemistry, aerosol processes and cloud processes/aqueous chemistry.

2.3. Emission scenarios

Studying the air pollution fields response to emission changes (model sensitivity to emission input) is obviously a task of great practical importance, obviously connected with formulating short-term (current) pollution mitigating decisions and long-term pollution abatement strategies.

In the chosen domain let there be N countries and the total number of source categories is M (generally $M = 12$ if maritime and biogenic emissions are accounted for). Let an arbitrary (concentration, deposition, columnar value, process contribution, etc.) pollution characteristic, obtained with all the emissions accounted for is denoted by ϕ. Let ϕ_{nm} is the respective characteristic obtained when the emissions form source category m in country n are reduced by a factor of α. In such a case the quantity φ_{nm}:

$$\varphi_{nm} = \frac{1}{1-\alpha}\frac{\phi - \phi_{nm}}{\phi} \cdot 100 \tag{2}$$

can be interpreted as the relative (in %) contributions of emission category m in country n to the formation of the characteristic ϕ.

It is obvious that more than one Selected Nomenclature for sources of Air Pollution (SNAP) category emissions in more than one country can be reduced by a factor of α and so the quantities $\phi_{n1m1,n2m2,\ldots,nLmL}$ $(n1,\ n2,\ldots,nL \le N, m1,\ m2,\ldots,mL \le M)$ can be simulated and the respective estimations $\varphi_{n1m1,n2m2,\ldots,nLmL}$ of the joint influence of the L pairs of chosen SNAP categories in chosen countries in the formation of the pollution characteristic ϕ can be evaluated. It is possible, in particular, to evaluate the contribution of all the emissions from a chosen country, or of the emissions from a chosen SNAP category in the whole domain.

As some of the chemical reactions are none-linear, there is mutual influence between the pollution from different sources. In such a case the question ''What is the influence of the emissions from SNAP category $m1$ located in country $n1$ to the air pollution from sources from SNAP category $m2$ located in country $n2$?'' is not meaningless. If the quantities ϕ, ϕ_{n1m1}, ϕ_{n2m2} and $\phi_{n1m1,n2m2}$ are simulated some more ''sophisticated'' properties, like the above mentioned impact of the emissions from SNAP category $m1$ in country $n1$ on the air pollution from sources from SNAP category $m2$ in country $n2$ (the ratio $\phi_{n2m2}|_{n1m1}$ or vice versa $-\phi_{n1m1}|_{n2m2}$) can also be defined:

$$\varphi_{n2m2}|_{n1m1} = \frac{\phi_{n1m1} - \phi_{n1m1,\ n2m2}}{\phi - \phi_{n2m2}} \cdot 100, \qquad \varphi_{n1m1}|_{n2m2} = \frac{\phi_{n2m2} - \phi_{n1m1,\ n2m2}}{\phi - \phi_{n1m1}} \cdot 100. \tag{3}$$

Obtaining such complex characteristics like (3), however, requires much more numerical experiments and the results are not easy for interpretation. That is why numerical experiments of this kind were not carried out in the framework of the present study.

2.4. Input data

The large scale (background) meteorological data used in the study is the NCEP Global Analysis Data with $1^\circ \times 1^\circ$ resolution. At the moment the created database contains all the necessary information since the year 2000.

The TNO high resolution emission inventory [20] was exploited. The inventory is produced by proper disaggregation of the EMEP 50 km inventory data base [21,22]. GIS technology was applied as to produce area and large point source input from this data base. It must be mentioned that the TNO emissions are distributed over 10 SNAPs classifying pollution sources according the processes leading to harmful material release to the atmosphere. The inventory contains 8 pollutants: CH_4, CO, NH_3, NMVOC (Non-Methane Volatile Organic Compounds), NO_x, SO_x, PM10 (Particle Matter with $d < 10\ \mu m$) and PM2.5 (Particle Matter with $d < 2.5\ \mu m$).

The TNO emission inventory was also used in the innermost domain D4 with no further disaggregation, so the emission resolution in this domain is again the one of the TNO inventory. GIS software was used only to interpolate the emissions in

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the respective computational grid. The possibility of using more detailed national emission inventory was not considered, simply because the national emission inventory was not available when the simulations started.

The biogenic emissions, which depend on the vegetation type and the meteorological conditions, were calculated by the SMOKE model.

2.5. Emission modeling

CMAQ demands its emission input in specific format reflecting the time evolution of all polluters accounted for in the used chemical mechanism. The emission inventory usually is made on an annual basis for, as a rule, big territories (municipalities, counties, countries, etc.) and many pollutants are estimated as groups like NO_x, SO_x, VOC (Volatile Organic Compounds), PM2.5. In preparing CMAQ emission file a number of specific estimates must be done. First, all this information must be gridded. Secondly, time variation profiles must be over-posed on these annual values to account for seasonal, weekly and daily variations. Finally, organic gas emission estimates, and to a lesser extent SO_x, NO_x and PM2.5, must be split, or "speciated", into more defined compounds in order to be properly modeled for chemical transformations and deposition.

The different types of sources: Area Sources (AS), Large Point Sources (LPS) and Biogenic Sources (BS) were treated in a specific way. Obviously, emission models are needed as reliable emission pre-processors to the chemical transport models. Such a component in EPA Models-3 system is SMOKE. Unfortunately, it is highly adapted to the US conditions—emission inventory, administrative division, motor fleet, etc.

For the needs of the present study anthropogenic emission files (AS and LPS) were prepared by interface programs AEmis and PEmis, which use as an input the above cited emission inventory, gridded according to each computational domain.

The temporal allocation was made on the basis of daily, weekly and monthly profiles, provided in [23,24]. The temporal profiles are country-, pollutant- and SNAP-specific. The speciation procedure is dependent on the Chemical Mechanism (CM) used [25]. CMAQ supports different CMs. Here, the Carbon Bond, v.4 (CB4) was exploited [26]. In the used Version 4.6 of CMAQ the CB4 is upgraded with the Version 1.7 of the ISORROPIA aerosol model [26]. It requires splitting of VOC into 10 lump pollutants (Isoprene – ISOP, Olefin – OLE, Paraffin – PAR, Acetaldehyde – ALD2, Terpenes – TERPB, XYLENE – XYL, Ethanol – ETH, Reactive Nitrogen – NR, Formaldehyde – FORM, Toluene – TOL) and PM2.5 into 5 groups of aerosol (PSO_4, PNO_3, Primary Organic Aerosol – POA, Elemental Carbon – PEC, PMFINE).

The speciation profilers were created following the technology elaborated by US EPA Emission Factor and Inventory Group and described in [27]. All necessary information can be downloaded from the respective EPA web site. In the same location VOC, PM2.5, NO_x and SO_x speciation profiles for all types of sources described in US EPA SCC (Source Category Code) can be found. It is quite convenient that the profiles are chemical mechanism specific giving direct splitting coefficients from VOC, PM2.5, NO_x and SO_x quantities in (g/s) to lump pollutants in (moles/s), which is the CMAQ emission input requirement.

Taking into account that the TNO emission inventory classifies the pollution sources to only 10 categories (SNAPs), the following approach was used for creating the respective speciation profiles: First of all a correspondence between American and European sources was detected. For each SNAP a number of American typical sources were chosen from SCC and their relative share of the total emission from the respective SNAP was approximately evaluated. Each of these sources possesses its own speciation profile. Those profiles were averaged for each SNAP. The averaging is weighted, weights being the share of the total emission from the respective SNAP that each one of the respective sources has. The weights were redetermined based on [28]. The produced in such a way speciation profiles are specific for Bulgaria and differ for the various SNAPs and pollutants.

SMOKE was used to produce biogenic emission file. For biogenic emissions, the temporal processing is a true simulation model driven by ambient meteorology and other data. SMOKE currently supports BEIS (Biogenic Emissions Inventory System) mechanism, versions 2 and 3 [29,30]. BEIS2 and BEIS3 are fed with spatial allocation of land use data as the first processing step. They next compute normalized emissions for each grid cell and land use category. The final step is adjusting the normalized emissions based on gridded, hourly meteorology data and assigning the chemical species to output a model-ready biogenic emissions file. In the current version of SMOKE BEIS3.13 is built [31].

The SMOKE's MrgGrid Processor was used to merge AS, LPS and BS files as a common 3D NetCDF file—the CMAQ-ready emission input.

3. Brief description of the numerical experiments

As far as the background meteorological data is the NCEP Global Analysis Data with $1^\circ \times 1^\circ$ resolution, it is necessary to use MM5 and CMAQ nesting capabilities to downscale the simulations to a 3 km step for the innermost domain. The MM5 pre-processing program TERRAIN was used to define four domains with 81 (D1), 27 (D2), 9 (D3) and 3 (D4) km horizontal resolution. These four nested domains were chosen in such a way that the finest resolution domain contains the whole territory of Bulgaria and the domain with a horizontal resolution of 9 km contains the whole Balkan Peninsula. The three inner nested domains are demonstrated in Fig. 1(a). A map of Bulgaria, with the major cities, roads and power plants is shown in Fig. 1(b).

The meteorological pre-processor MM5 was forced by the NCEP global scale data. In the D1 domain the model was set to relax toward observed temperature, wind and humidity through four dimensional data assimilation (FDDA) [32]. FDDA

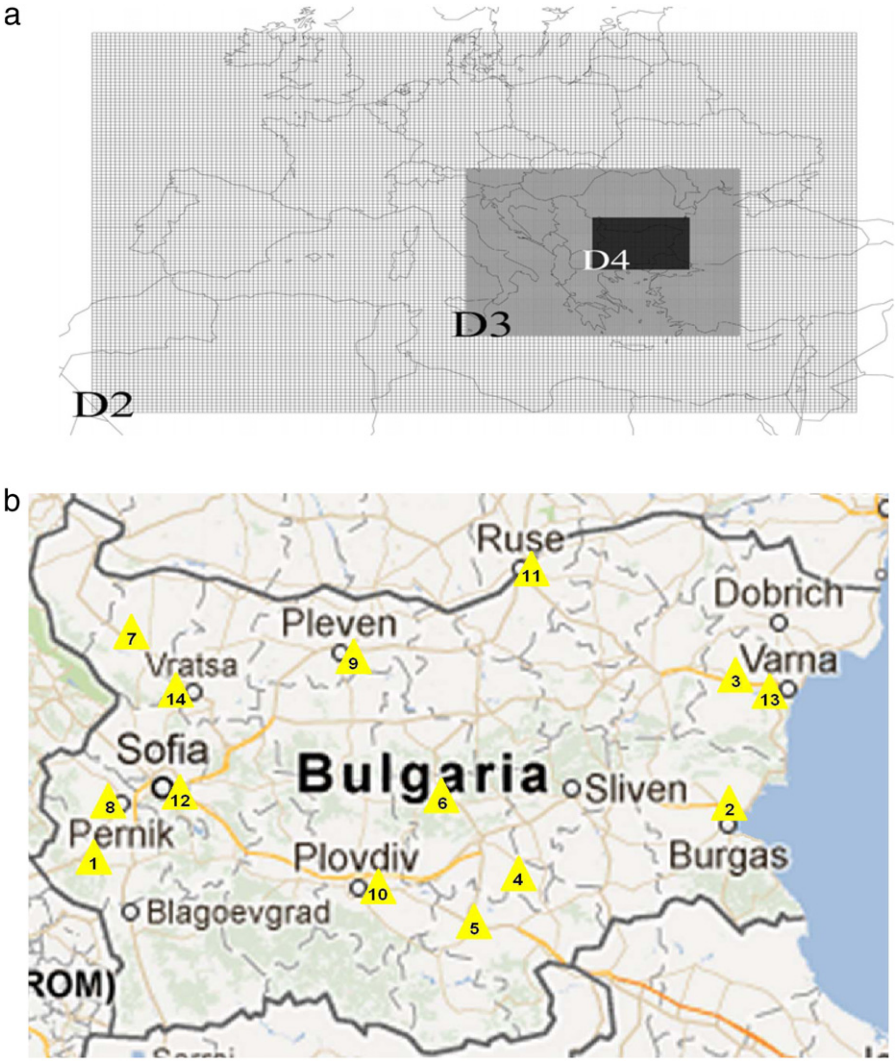

Fig. 1. The three inner computational domains (a) and Map of Bulgaria, with the major cities, roads and power plants (▲ 1 Bobov dol, 2 Burgas, 3 Devnia, 4 Galabovo, 5 Haskovo, 6 Kazanlak, 7 Montana, 8 Pernik, 9 Pleven, 10 Plovdiv, 11 Ruse, 12 Sofia, 13 Varna and 14 Vratsa) (b). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

amounts to adding an additional term to the prognostic equations that serves to "nudge" the model solution toward the individual observations. This significantly reduces the drift in the solution for simulations of several days or more. The NCEP data set does not include observations, but analyzed data every 6 h in all its grid points. MM5 is configured with FDDA option on as to nudge the model toward analyzed data in D1 only. For all the domains (D1, D2, D3, D4) MM5 was run simultaneously with "two-way" nesting mode on. All simulations were made with 23 σ-levels going up to 100 hPa height. The MM5 simulations were made on portions of 3 days. Every portion has additional 12 h that are an initial spin-up period that overlaps the last 12 h of the preceding run.

CMAQ meteorological input was created from the MM5 output exploiting the CMAQ meteorology-chemistry interface—MCIP, v2.3. CMAQ simulations were performed in D2, D3 and D4 domains. The CMAQ pre-defined (default) concentration profiles were used as boundary conditions for D2. The boundary conditions for the inner domains were determined through the nesting capabilities of CMAQ. The CB-4 chemical mechanism with Aqueous-Phase Chemistry and MEBI solver has been exploited for all the domains. The CMAQ simulations were made with 15 σ-levels vertical resolution.

Four emission scenarios will be considered in the present paper: Simulations with all the emissions, simulations with biogenic emissions and the emissions of SNAP categories 1 (energetics) and 7 (road transport) for Bulgaria reduced by a factor of 0.8.

As it can be seen from Table 1 the computer resource requirements are quite big. On the other hand the very nature of the numerical experiments planned make it possible to organize the computations in a grid effective manner. The MM5 simulations were carried out in 3-day packages for all the 4 domains, using the two-way nesting mode of the model. This

Table 1
Computer requirements for 3-day real time simulations.

Domain:	D1	D2	D3	D4	Total
MM5 on 8 processors—23 sigma vertical level					
HDD (input/output)	396 MB	919 MB	1.27 GB	1.42 GB	4 GB
Computational time	–	–	–	–	19 h 20 min
CMAQ on 4 processors—15 sigma vertical level					
HDD (input/output)	–	7.59 GB	10.68 GB	10.57 GB	28.84 GB
Computational time	–	1 h 10 min	2 h 10 min	4 h 40 min	8 h 00 min
CMAQ on 8 processors—15 sigma vertical level					
Computational time	–	50 min	1 h 30 min	3 h 40 min	6 h 00 min
CMAQ on 16 processors—15 sigma vertical level					
Computational time	–	30 min	1 h 10 min	2 h 20 min	4 h 00 min
CMAQ on 32 processors—15 sigma vertical level					
Computational time	–	30 min	45 min	1 h 45 min	3 h 00 min
XTRACT—1 sigma vertical level					
HDD (input/output)	–	1.43 GB	2.02 GB	1.99 GB	5.44 GB
Computational time	–	30 min	30 min	30 min	+1 h 30 min

will make a total run time of less than 20 h, which means that the successful execution of the jobs on the Grid is quite probable.

The CMAQ simulations for domains D2 and D3 and those for D4 were organized in separate jobs, which again makes the jobs run time for 3 days real time fairly reasonable.

The model output storage, however, is too large. As not all the output information is so valuable for further air quality and environmental considerations a post-processing procedure and respective software were developed, in order for the output to be "filtered" and only the necessary information to be kept. What is recently kept from the CMAQ output on an hourly basis are the surface concentrations of the following most important pollutants:

- NO_2, NO, O_3, NO_3, OH, HO_2, N_2O_5, HNO_3, HONO, PNA (Peroxynitric acid), H_2O_2, CO, FORM, ALD2, C_2O_3, PAN (Peroxyacetylnitrat), PACD (Peroxyacetic acid), PAR, OLE, FACD (Formic acid), AACD (Acetic Acid), ETH, TOL, CRES (Cresol), TO_2, XYL, MGLY (Methylglyoxal), ISOP, ISPD (Products of isoprene rxns), SO_2, SULF (H_2SO_4 Sulfuric acid), UMHP (Methanediol), TERP, NH_3 (gases—34)
- PSO_4, PNH_4, PNO_3, POA, PEC (aerosol—5)
- SOAA, SOAB (Anthropogenic and Biogenic secondary organic aerosol—2)
- FPRM, CPRM (fine and coarse PM—2).

The MM5/CMAQ simulations were performed day by day for 8 years—from 2000 to 2007. Thus a quite extensive data base was created, which could be used for different studies and considerations of the main features and origins of the atmospheric composition in Bulgaria.

4. Results, comments and discussion

All the modeling system (models, input data, emission treatment) was well validated by previous works [13,33,34] and showed fairly good simulation abilities. The validation showed that the discrepancies between simulations and measured data is mostly within the ± 50% margins, which means that the quality of simulations complies with the European legislation. That is why the results, which will be demonstrated below could be considered reliable enough and so be trusted, in particular when qualitative conclusions are made. A massive validation, with using all the available measured data and applying objective validation techniques is a job, which still has to be done.

The data base, obtained by the numerical experiments allows statistical treatment for retrieving various and most sophisticated atmospheric composition evaluations. The illustrations and comments in the present paper consider some very simple generalizations—mostly mean annual and seasonal characteristics.

4.1. Some basic facts about the atmospheric composition status in Bulgaria

The surface concentrations are the most interesting, because of their direct impact on human health and vegetation. By averaging over the 8-year simulated fields ensemble the mean annual and seasonal surface concentrations can be obtained and treated as respective "typical" daily concentration patterns. Maps of some of these "typical" for the year, summer and winter periods surface concentrations are shown in Figs. 2–6 for some of the most popular compounds—NO_2, SO_2, Ozone, Fine and Coarse Particulate Matter (PM) for 05.00 and 17.00 GMT (7 am and 7 pm local time). What can be seen from the

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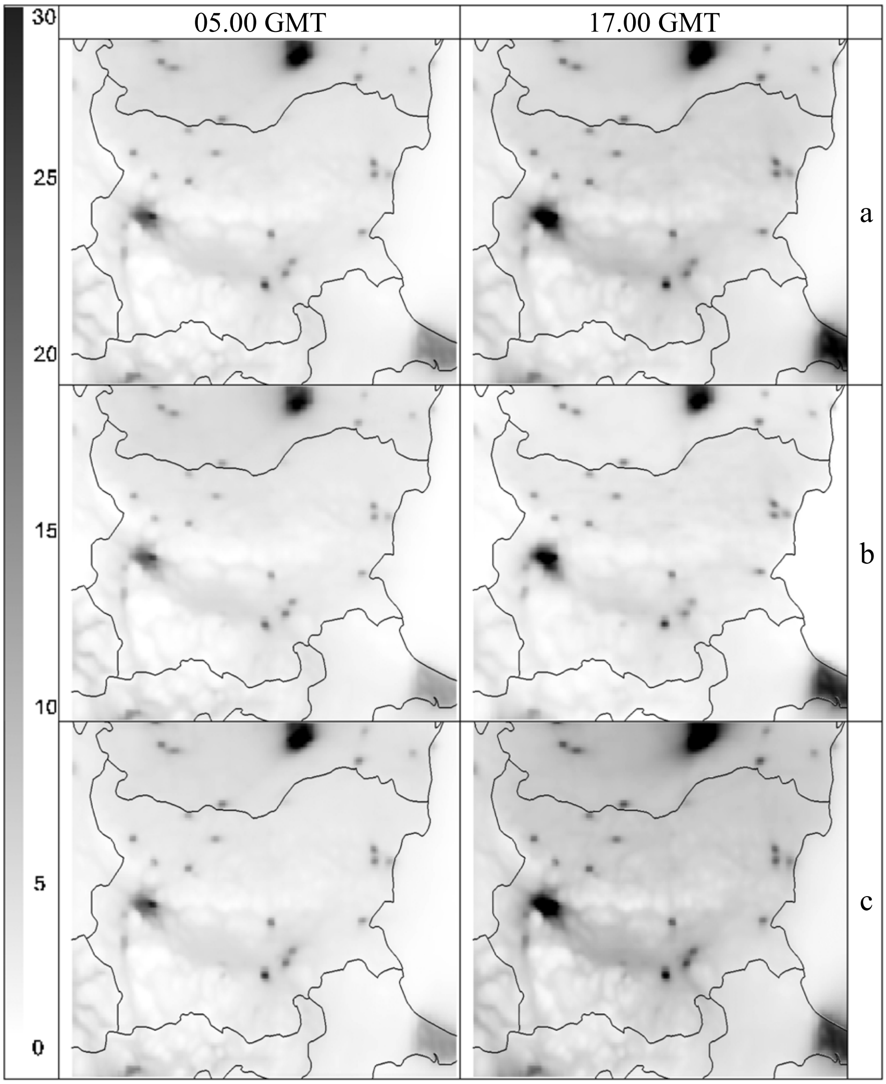

Fig. 2. Surface concentrations of NO_2 ($\mu g/m^3$) averaged annually (a), for the summer (b) and winter (c) periods at 05.00 and 17.00 GMT.

maps is not surprising: the big cities and the road network are clearly outlined in the NO_2 surface concentrations, the big power plants in the SO_2 surface concentrations, the Fine and Coarse Particulate Matter plots reflect both influences.

The ozone fields are much more complex. What should be mentioned is the expected effect of ozone minimums over big cities. The road network can also be followed in the plots as lines with lower ozone concentrations. This is in a good agreement with the ozone chemistry scheme.

The means of the multi-year 2-D concentration fields were averaged over the territory of Bulgaria to obtain typical diurnal cycles on a yearly base and the four seasons. This enables the interpretation and comparison of the variability of different compounds on these time scales (Fig. 7). What can be seen in the plots does not defy common sense and does not oppose the schematic concepts about how the air pollution near the earth surface is formed: NO_2, SO_2, Primary Organic Aerosol, Coarse Particulate Matter and Fine Particulate Matter have their minimums during daytime and their concentrations for the cold period (autumn, winter) are higher than those for the warm period (spring, summer). The ozone concentrations, as they should, have their maximum during daytime and are higher for the warmer part of the year.

It should be kept in mind that the diurnal evolutions, shown in Fig. 7 are obtained once by averaging over the whole ensemble and second by averaging over the territory of the country. Thus, they do not explicitly reflect heterogeneity in meteorological and emission fields, but only the emissions diurnal evolution and as it seems, mostly the atmospheric stability course and for some of the compounds the role of photochemical reactions.

The behavior of SOAB – Secondary Organic Aerosol Biogenic is a little bit surprising – again have their minimums during daytime and their concentrations for the cold period (autumn, winter) are higher than those for the warm period (spring, summer), while one expects it to be just the other way round. It should be kept in mind, however, that the SOAB are products

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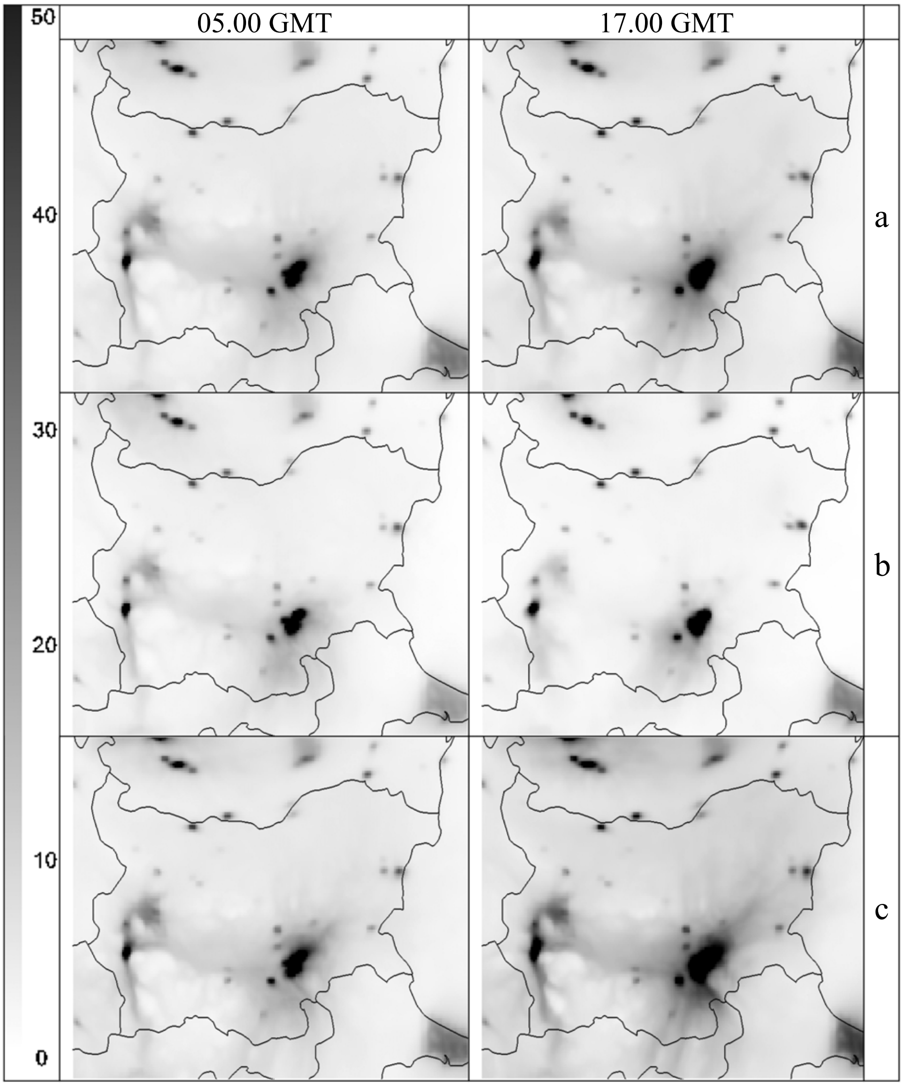

Fig. 3. Surface concentrations of SO_2 ($\mu g/m^3$) averaged annually (a), for the summer (b) and winter (c) periods at 05.00 and 17.00 GMT.

of some chemical reactions of biogenic with some other species, so even if the biogenic emissions are higher during daytime and in the warm periods of the year, the SOAB behavior may follow the one of the non-biogenic compounds.

The behavior of SO_2 is a little bit surprising as well. One could expect that, because a significant SO_2 amount comes from elevated sources (power plants) during the day its surface concentrations may have a maximum. The effect of stratification on the surface SO_2 from high sources can be followed locally (Fig. 3) and in the diurnal course of SNAP 1 summer emission contribution to SO_2 surface concentrations (see Fig. 12). Nevertheless the competition of both the effects of better mixing during the day—diffusion transport of SO_2 from elevated sources to the ground and diffusion transport of SO_2 from low sources aloft is won by the second effect and so the SO_2 surface concentrations have their minimum during the day.

The SOAA concentrations diurnal course is different from these of the most of the compounds. The concentration starts increasing in the morning until it reaches a maximum or a plateau in the evening. This is probably due to the fact that there is an effect of steady SOAA accumulation, which dominates the effect of turbulent mixing.

The conventional behavior of the species is, perhaps, good news—unexpected effects could be a novel and interesting result, but more often they indicate some shortcomings in the numerical simulations.

Shortcomings in the current simulations, however, do exist and should be noted. For example, the levels of coarse PM are grossly underestimated (probably by half or even one order of magnitude). This is a well known problem for almost all models (see for example [35] and was also manifested in some experiments for validation of the system used in the current study [34,36]).

Plots of the diurnal course of the averaged for the territory of Bulgaria maximal concentrations for the year and the four seasons are given in Fig. 8 for the same compounds as in Fig. 7. As it can be seen the behavior of the maximal concentrations

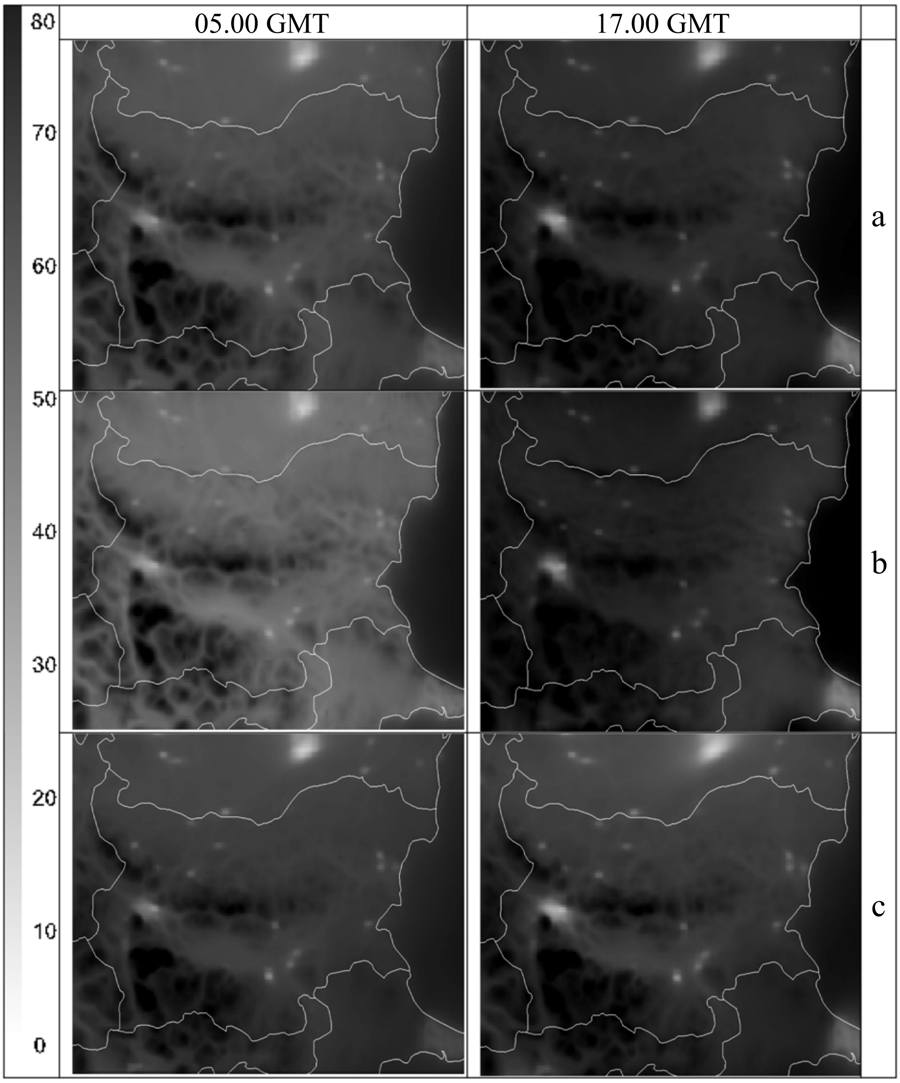

Fig. 4. Surface concentrations of O_3 ($\mu g/m^3$) averaged annually (a), for the summer (b) and winter (c) periods at 05.00 and 17.00 GMT.

is qualitatively similar to the behavior of the "typical" ones. The annual maximum is, naturally, the biggest one—it is the maximum of all maximums and at each moment closely follows the maximal of the seasonal maximums. It does not coincide with any of the seasonal maximums, however, because, as already stated, what is presented in Fig. 8 are the maximal seasonal and annual concentrations averaged for the territory of Bulgaria, not the maximums of averaged for the territory of Bulgaria seasonal and annual concentrations.

4.2. Impact of different emission categories to the atmospheric composition status in Bulgaria

Four emission scenarios will be considered in the present paper: Simulations with all the emissions, simulations with biogenic emissions and the emissions of SNAP categories 1 (energetics) and 7 (road transport) for Bulgaria reduced by a factor of 0.8. This makes it possible, according to (2), to evaluate the contribution of road transport, energetics and biogenic emissions to the atmospheric composition in Bulgaria. These relative contributions were calculated day by day and then, by averaging over the 8-year ensemble the "typical" contributions for the four seasons and annually were obtained. Some illustrations of the emission impact evaluations will be given in the present paper only.

Maps of the diurnal evolution of the "typical" summer relative contribution of biogenic emissions and the emissions of SNAP categories 1 and 7 to the surface ozone concentrations in Bulgaria are shown in Figs. 9–11. It can be seen, that at the very location of the big power plants, where the nitrogen oxide concentration is very high all the time, the impact on the surface ozone is negative all day. The SNAP 1 emissions contribution for the rest of the territory of the country, however, is mostly positive, in particular after sunrise. The contribution of the SNAP 7 emissions is negative almost everywhere in the

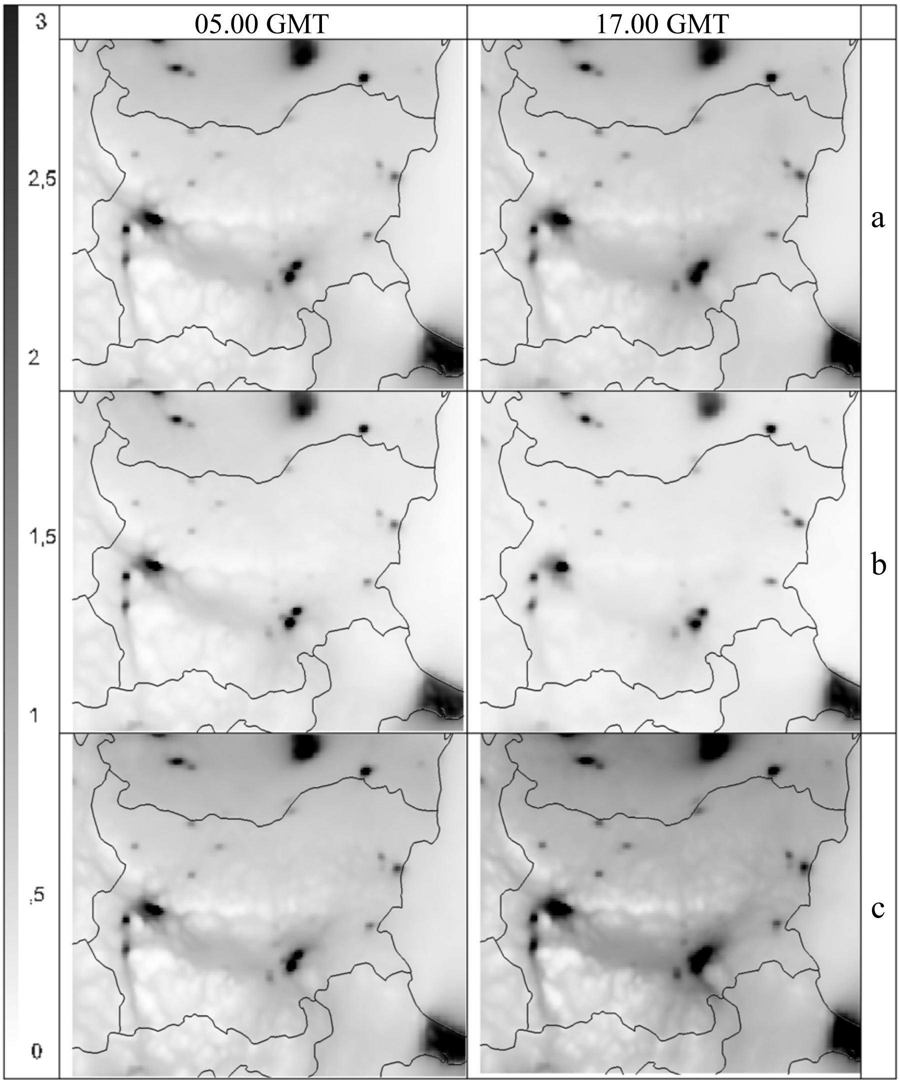

Fig. 5. Surface concentrations of FPRM ($\mu g/m^3$) averaged annually (a), for the summer (b) and winter (c) periods at 05.00 and 17.00 GMT.

country before sunrise. The city of Sofia negative contribution is particularly prominent and remains so during the whole day. Even the road network can be followed as the ozone sink in the 5.00 GMT plot. Gradually during the day, the contribution of SNAP 7 emissions becomes positive almost everywhere and then, late in the afternoon, again tends toward the negative, except for the mountain regions.

The contribution of biogenic emissions is negative before sunrise in quite a big part of the country, except for mostly the mountain regions. Then during the day the contribution becomes positive everywhere.

For all the emission categories the pattern of the contribution fields is rather complex, which reflects the emission source configuration, the heterogeneity of topography, land use and meteorological conditions.

Plots of this kind are rather interesting to look at and can give a good qualitative impression of the spatial complexity of the emission contribution. In order to demonstrate the emission contribution behavior in a more simple and easy to comprehend way, the respective fields can be averaged over some domain (in this case the territory of Bulgaria), which makes it possible to jointly follow and compare the diurnal behavior of the respective contributions for different species. Such plots for some of the compounds are given in Figs. 12–13.

The following comments on Figs. 12–13 could be made: First of all it could be seen that the different emissions relative contribution to the concentration of different species could be rather different, varying from almost 100 to several %. The contributions of different emission categories to different species surface concentrations have different diurnal courses and different importance. The biogenic emissions have near zero or even negative contributions for some species SO_2, CPRM and FPRM.

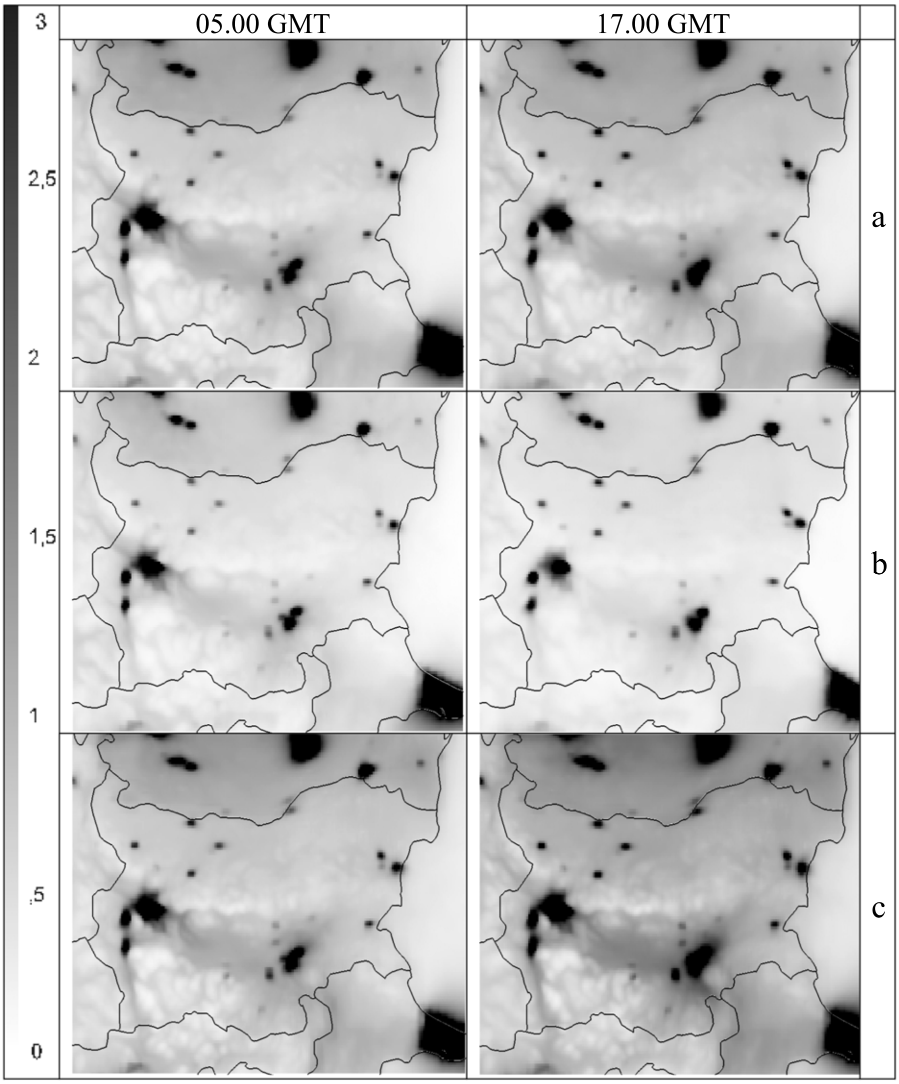

Fig. 6. Surface concentrations of CPRM ($\mu g/m^3$) averaged annually (a), for the summer (b) and winter (c) periods at 05.00 and 17.00 GMT.

Another general comment, which can be made, is that the winter contributions of biogenic emissions are, for almost all the species, much smaller than the one for summer. This is quite natural, of course, having in mind that in the warm period of the year the biogenic emissions are higher.

It should be noted that the SNAP 1 contribution to the surface SO_2 concentrations is smaller than one should expect, having in mind that the "Maritza" power plants are among the biggest sulfur sources in Europe. Probably, a significant amount of SO_2 from these sources becomes a subject of larger scale transport and so is moved outside the country.

There are significant differences between the summer and winter contributions. The most important thing that should be noted is that the contribution of all the three emission categories to the surface ozone in Bulgaria is negative, though small by absolute values. This is an important result, which means, in particular, that the ozone in Bulgaria during the winter is mostly due to transport from other countries.

One cannot help but notice the small contribution of biogenic emissions to surface ozone. At first glance this may seem strange; moreover that the biogenic emissions contribution to major VOC like ISOP, TERP is large and the VOCs are one of the major ozone precursors. This can be explained, however, by the ozone photochemistry [37–39], more precisely by the RO_x/HO_x radical chain reaction system: OH radicals can react (i) with organic compounds leading to peroxyradical formation which produces O_3 by oxidizing NO to NO_2 or (ii) OH can react with NO_2 forming HNO_3 which is a termination reaction suppressing O_3 formation. The dominance of pathway (i) over (ii) depends on the NO_2 concentration versus the sum of NM-VOC concentrations in the air parcel (weighted over the reaction rates of the individual species). In urban environments NO_2 concentrations are usually that large that HNO_3 formation dominates the reactions of OH radicals (pathway (ii)), which implies that local O_3 production is small. These conditions are also called VOC-limitation because O_3 production

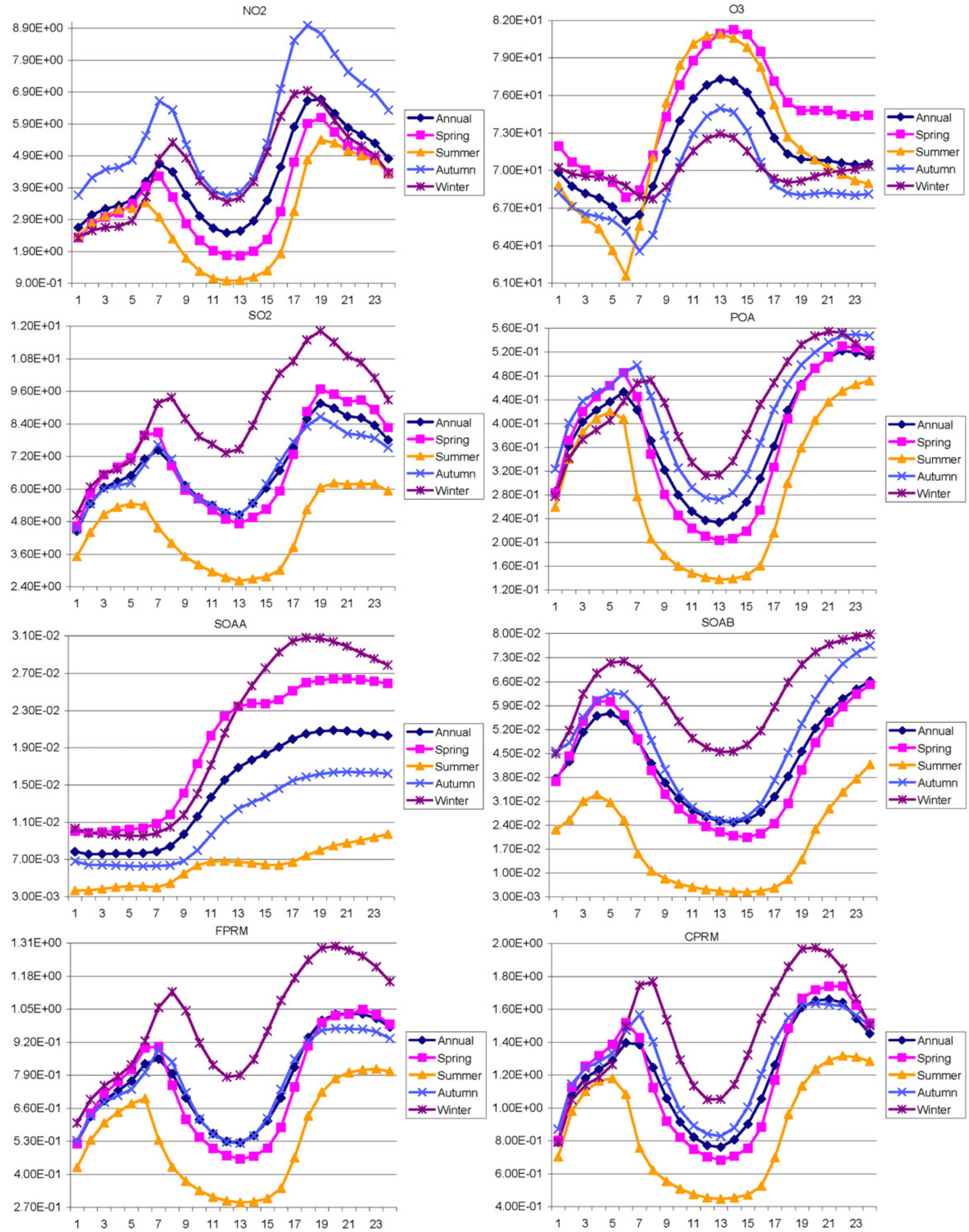

Fig. 7. Plots of the ''typical'' diurnal course of the averaged for the territory of Bulgaria concentrations of NO_2, SO_2, O_3 ($\mu g/m^3$), POA (Primary Organic Aerosol), SOAA, SOAB (Anthropogenic and Biogenic Secondary Organic Aerosol), CPRM, FPRM (Coarse and Fine Particulates) ($\mu g/m^3$) averaged annually, for the spring, summer, autumn and winter.

increases with increasing VOC concentration. When the air parcel moves along the trajectory from an urban to a suburban environment, NO_2 concentration in the air parcel steadily decreases because NO_2 reacts with the available OH radicals. The decrease in NO_2 changes the dominance of pathways (ii) over (i) favoring pathway (i) more and therefore local O_3 production increases. When NO_x concentration is decreasing steadily the mixture of organic vs. NO_x concentration passes through a

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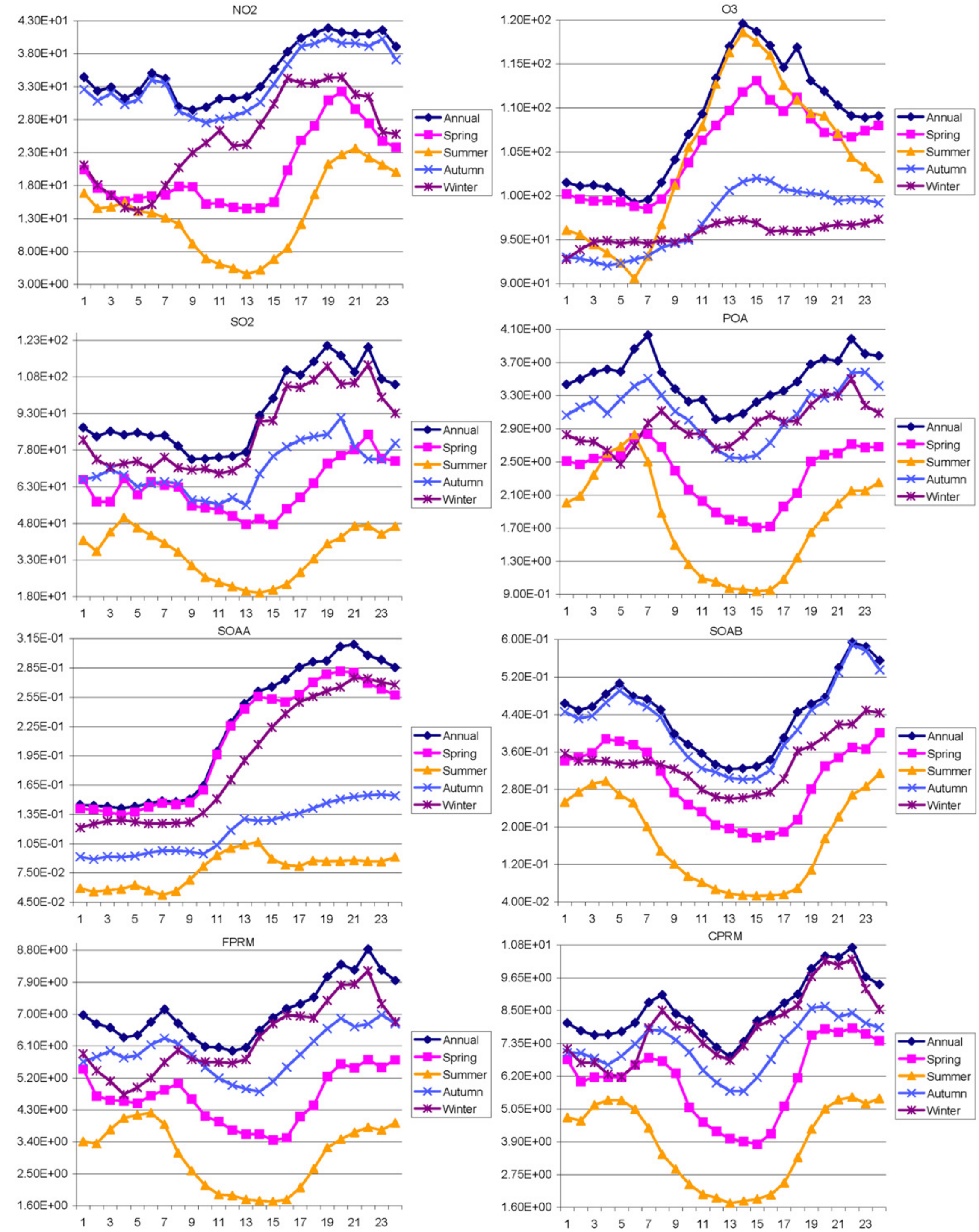

Fig. 8. Plots of the diurnal course of the averaged for the territory of Bulgaria maximal concentrations of NO_2, SO_2, O_3 ($\mu g/m^3$), POA (Primary Organic Aerosol), SOAA, SOAB (Anthropogenic and Biogenic Secondary Organic Aerosol), CPRM, FPRM (Coarse and Fine Particulates) ($\mu g/m^3$) averaged annually, for the spring, summer, autumn and winter.

state in which the ratio of ozone precursor concentration is such that local O_3 production maximizes, which is called the transition regime. When NO_x concentration is decreasing further (by pathway (ii)) local O_3 production rate becomes limited by the availability of NO_x concentration, a regime which is called NO_x-limitation. Such conditions usually occur in rural environments. Obviously from the point of view of atmospheric composition climate the Balkan Peninsula and Bulgaria are predominantly "rural" environments which explains the ozone photochemistry specifics in the region.

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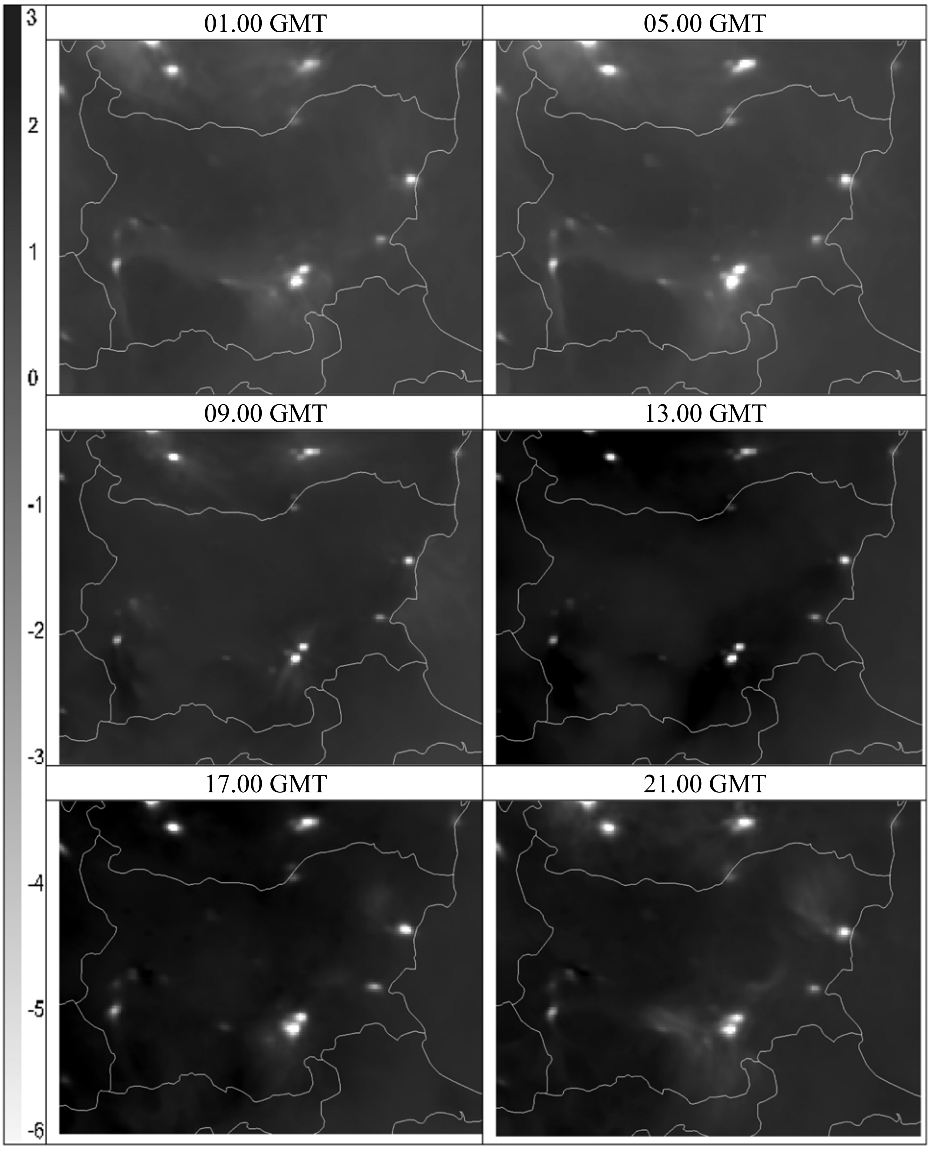

Fig. 9. Diurnal evolution of the "typical" summer relative contribution (%) of the emissions from SNAP category 1 to the surface ozone concentrations in Bulgaria.

The contribution of the emission from SNAP categories 1 and 7, which are the major sources of the other ozone precursor—nitrogen oxides, is also small. This, once again is an indirect indicator, that the surface ozone in Bulgaria is to a small extend due to domestic sources, but is mostly imported.

4.3. Some results from the Integrated Process Rate Analysis

Similarly to the evaluations, described in paragraphs 4.1 and 4.2, the outputs from the Integrated Process Rate Analysis were averaged over the 8-year ensemble and so the "typical" seasonal and annual evaluations were obtained. An example of the special distribution of some of the processes contribution to the surface ozone is given in Fig. 14. It can be seen that the chemical processes have mostly negative impact, especially later in the day and the big cities and the road network (powerful nitrogen oxide sources) can be clearly followed as ozone sinks. The vertical diffusion impact is mostly positive (turbulent transport of ozone from the upper layers). The effect is very prominent in the big cities, where the very large nitrogen oxide surface sources cause big ozone deficiency (big negative vertical gradients) and so the turbulent transport is more intensive. Some small spots of vertical diffusion negative impact can be seen at the location of big power plants. This is probably due to the fact that these are high sources of nitrogen oxide, which cause ozone deficiency aloft, so the ozone vertical gradients near surface are positive.

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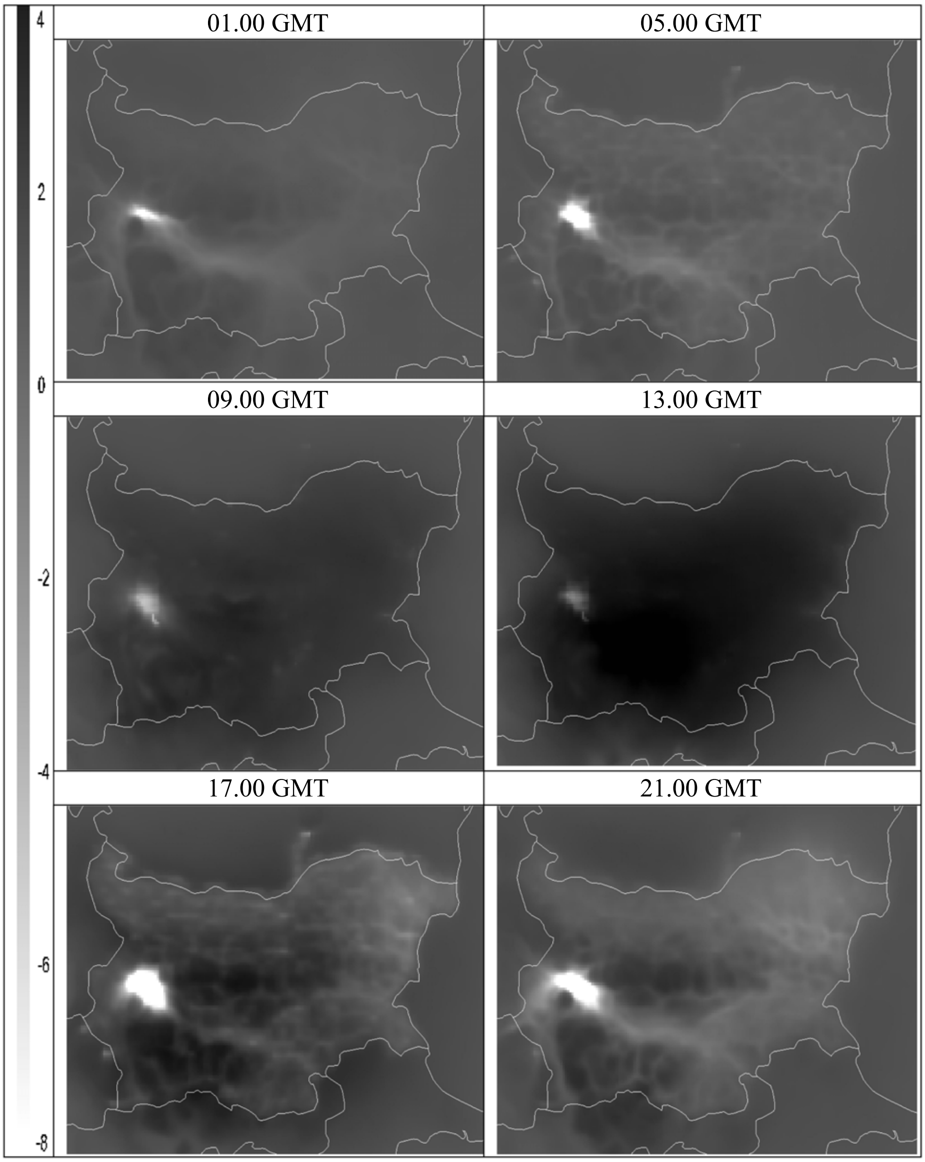

Fig. 10. Diurnal evolution of the "typical" summer relative contribution (%) of the emissions from SNAP category 7 to the surface ozone concentrations in Bulgaria.

The vertical advection contributions pattern is very complex and clearly reflects topography induced vertical motions.

The averaged over the territory of Bulgaria contributions of some of the processes will be also demonstrated (Fig. 15). A detailed description even of these much simpler images will take a lot of space and probably is not necessary. Some more general features could be mentioned, however:

- The temporal behavior of the processes is also complex.
- For some processes the contribution sign is obvious (like emissions or dry deposition), but some can have different signs for different species.
- For most of the compounds some of the advection/diffusion process have significant role.

5. Conclusions

The numerical experiments performed produced a huge volume of information, which have to be carefully analyzed and generalized so that some final conclusions could be made. Simulations for emission scenarios concerning the contribution of the other SNAP categories have to be performed.

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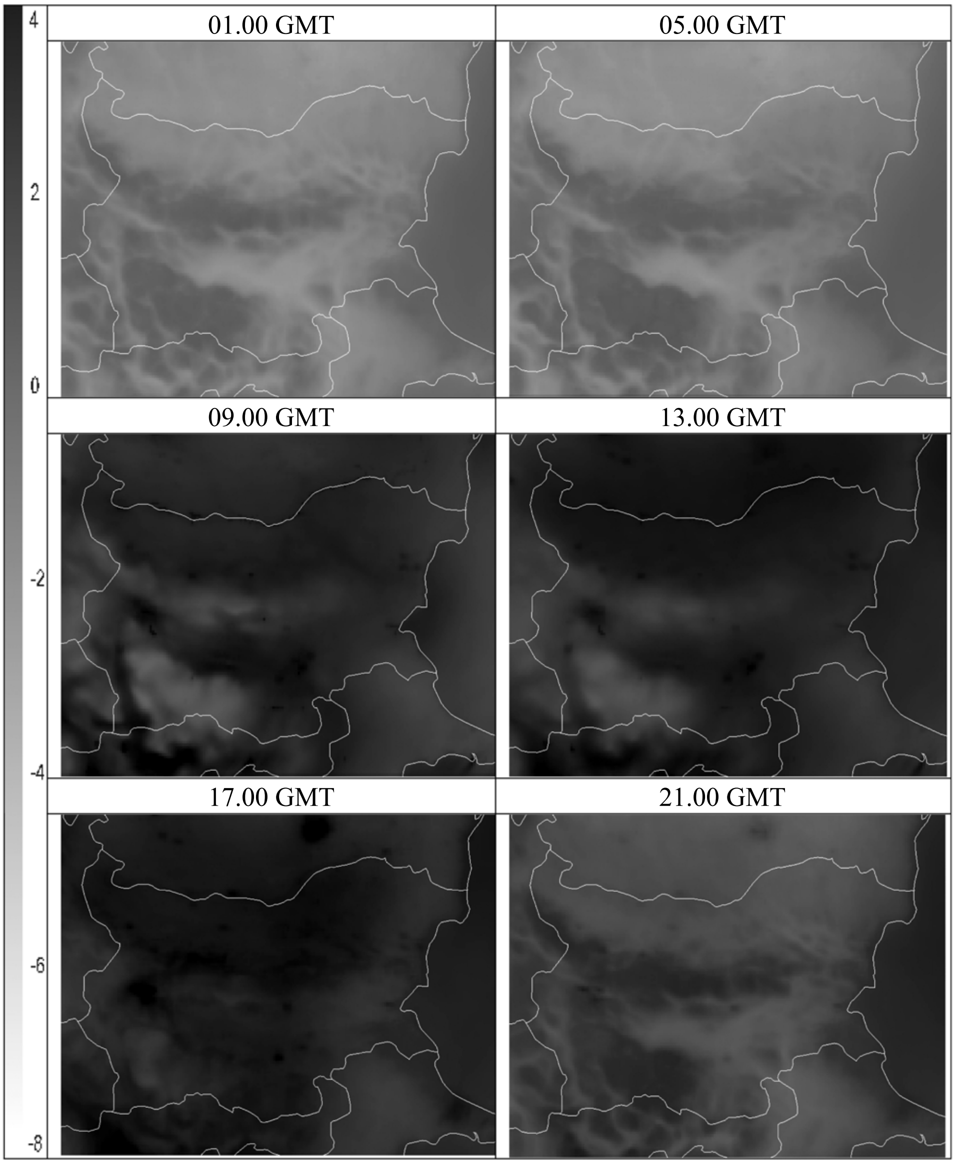

Fig. 11. Diurnal evolution of the "typical" summer relative contribution (%) of the biogenic emissions to the surface ozone concentrations in Bulgaria.

The demonstrations, presented in the present paper are just a first glance on the atmospheric composition status in Bulgaria, so very few decisive conclusions can be made at this stage of the study. Nevertheless, some of the major findings so far will be listed below:

- the behavior of the surface concentrations, averaged over the ensemble annually, or for the four seasons and over the territory of the country is reasonable and demonstrates effects which for most of the compounds can be explained from the point of view of the generally accepted schemes of dynamic influences (in particular the role of turbulent transport and its dependence on atmospheric stability) and/or chemical transformations;
- the surface concentrations of coarse PM are probably underestimated by the simulations, which is a well known problem for practically all models;
- some of the compounds (mostly secondary aerosols) manifest a diurnal course, which is not so easy to explain, which is probably a result of a complex interaction of dynamic, chemical and aerosol processes;
- the SNAP 1 contribution to the surface SO_2 concentrations is smaller than one should expect, having in mind that the "Maritza" power plants are among the biggest sulfur sources in Europe. Probably, a significant amount of SO_2 from these sources becomes a subject of larger scale transport and so is moved outside the country;

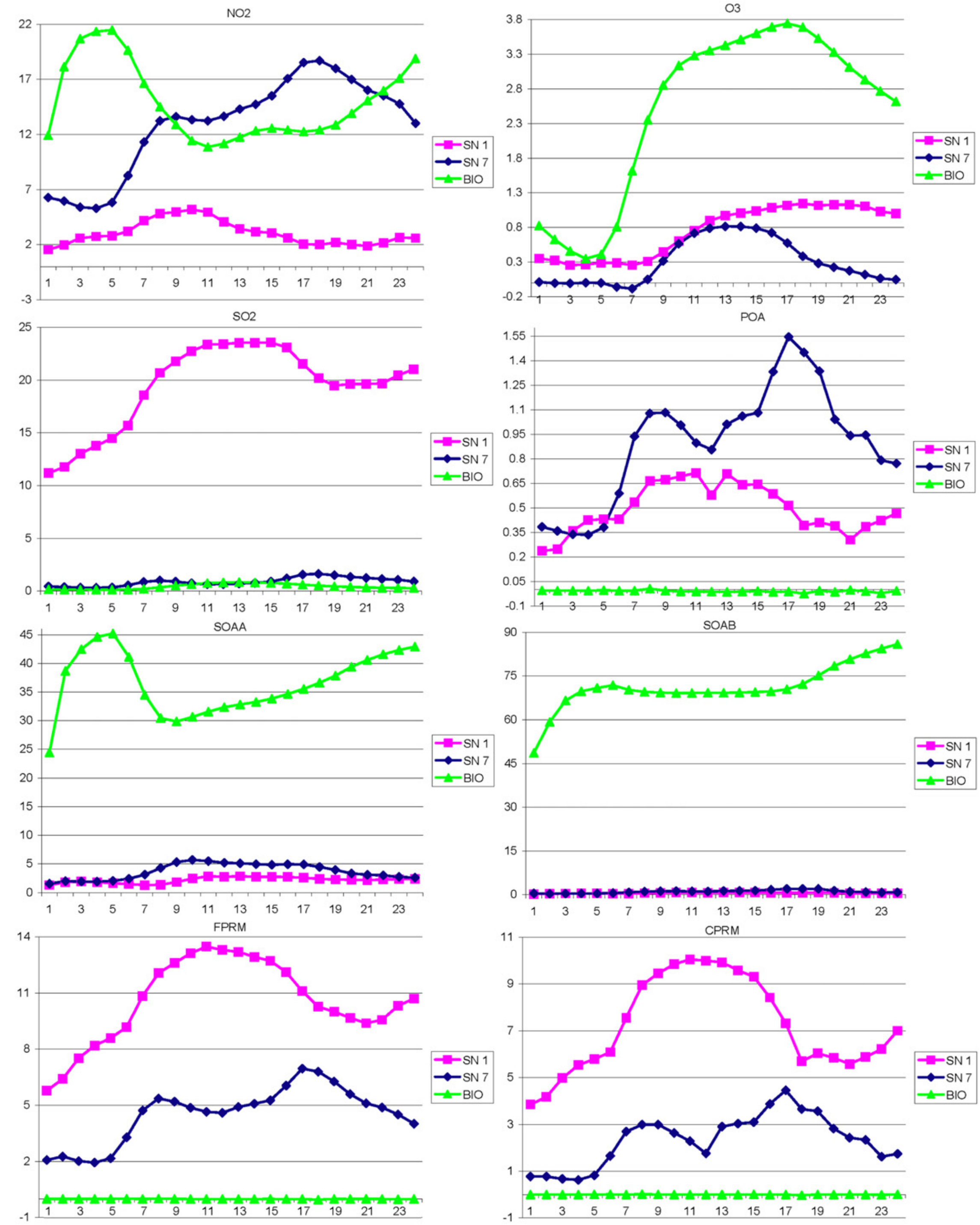

Fig. 12. Plots of the "typical" summer diurnal course of the averaged for the territory of Bulgaria relative contributions (%) of emissions from SNAP categories 1 (SN1) and 7 (SN7) and of the biogenic emissions (BIO) to the concentrations of NO_2, SO_2, O_3 ($\mu g/m^3$), POA (Primary Organic Aerosol), SOAA, SOAB (Anthropogenic and Biogenic Secondary Organic Aerosol), CPRM, FPRM (Coarse and Fine Particulates).

– the contribution of biogenic emissions to surface ozone in the country is relatively small. This indicates that local O_3 production rate is limited by the availability of NO_x concentration, a regime which is called NO_x-limitation. Obviously from a point of view of atmospheric composition climate the Balkan Peninsula and Bulgaria are predominantly "rural" environment which explains the ozone photochemistry specifics in the region;

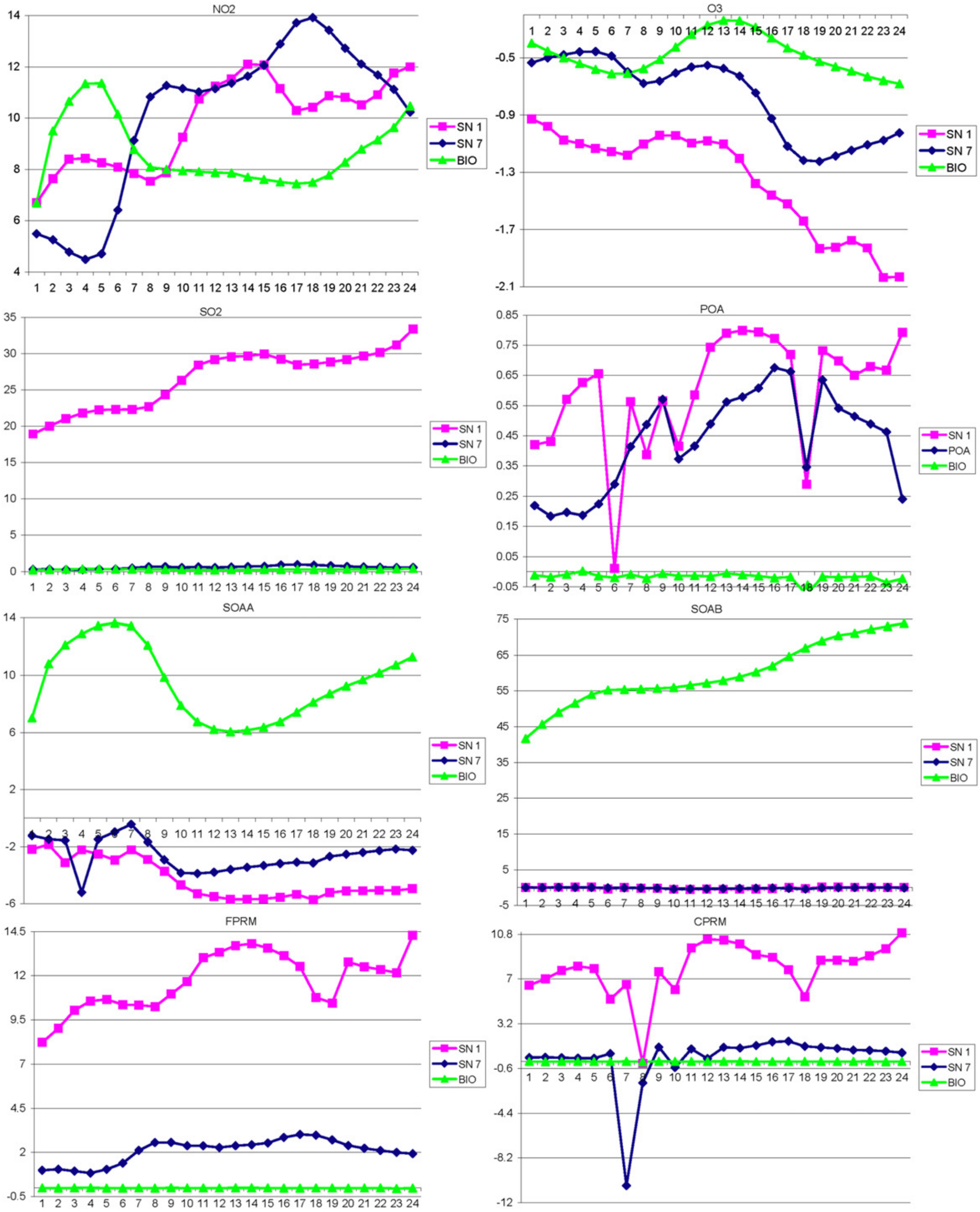

Fig. 13. Plots of the "typical" winter diurnal course of the averaged for the territory of Bulgaria relative contributions (%) of emissions from SNAP categories 1 (SN1) and 7 (SN7) and of the biogenic emissions (BIO) to the concentrations of NO_2, SO_2, O_3 ($\mu g/m^3$), POA (Primary Organic Aerosol), SOAA, SOAB (Anthropogenic and Biogenic Secondary Organic Aerosol), CPRM, FPRM (Coarse and Fine Particulates).

– the contribution of the emission from SNAP categories 1 and 7, which are the major sources of the other ozone precursor—nitrogen oxides, is also small. This, once again is an indirect indicator, that the surface ozone in Bulgaria is to a small extend due to domestic sources, but is mostly imported;
– the results produced by the CMAQ "Integrated Process Rate Analysis" demonstrate the very complex behavior and interaction of the different processes. The analysis of the behavior of different processes does not give a simple answer

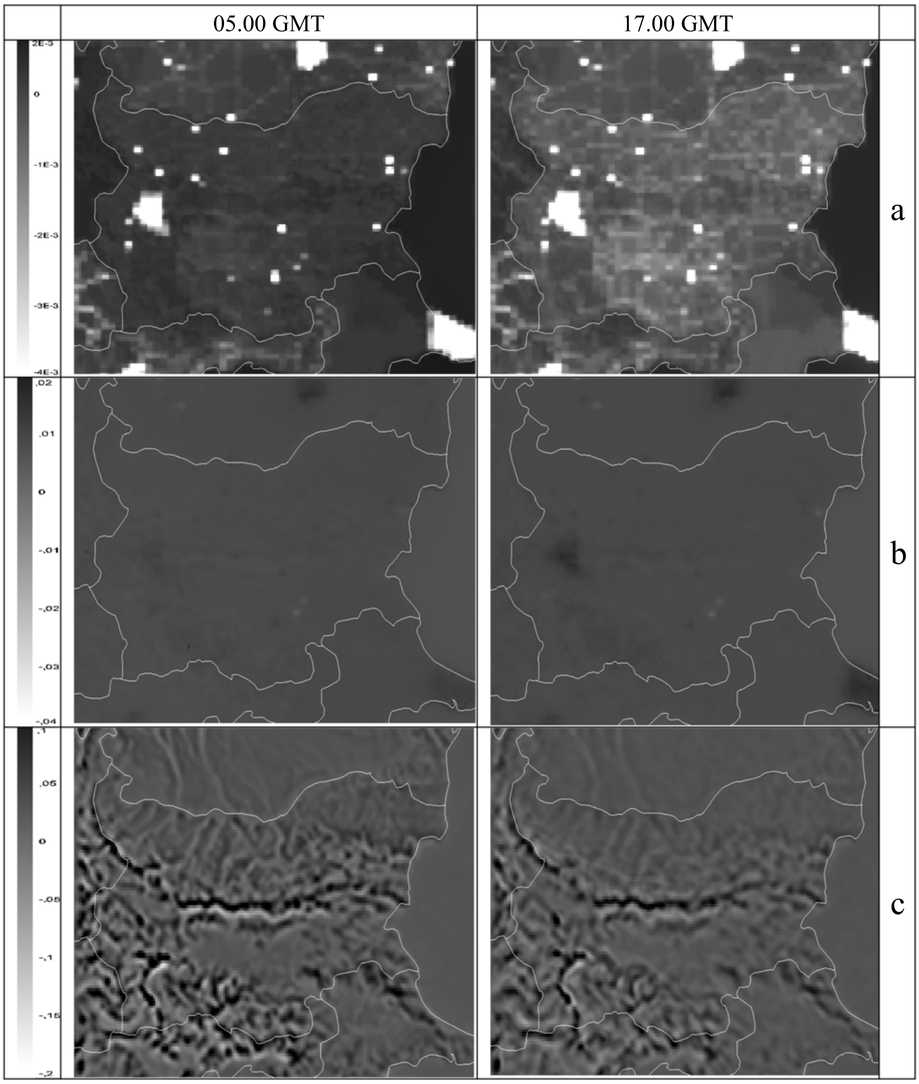

Fig. 14. Diurnal evolution of the "typical" summer contributions (μg/h) of chemical processes (a), vertical diffusion (b) and vertical advection (c) to the hourly surface ozone changes.

of the question of how the air pollution in a given point or region is formed.

The obtained ensemble of numerical simulation results is extensive enough to allow statistical treatment—calculating not only the mean concentrations and different SNAP categories contribution mean fields, but also standard deviations, skewness, etc., with their dominant temporal modes (seasonal and/or diurnal variations) Some advanced and sophisticated methods for statistical treatment of the results should also be appropriately applied in order to:

– clarify the role of the atmospheric pollution transport and transformation processes (accounting also for heterogeneous chemistry and the importance of aerosols for air quality and climate) from urban to local to regional (Balkan and country) scales,
– track and characterize the main pathways and processes that lead to atmospheric composition formation in different scales,
– provide high quality scientifically robust assessments of the atmospheric composition and its origin—the air pollution fields response to emission changes (model sensitivity to emission input) is obviously a task of great practical importance, obviously connected with formulating short-term (current) pollution mitigating decisions and long-term pollution abatement strategies.

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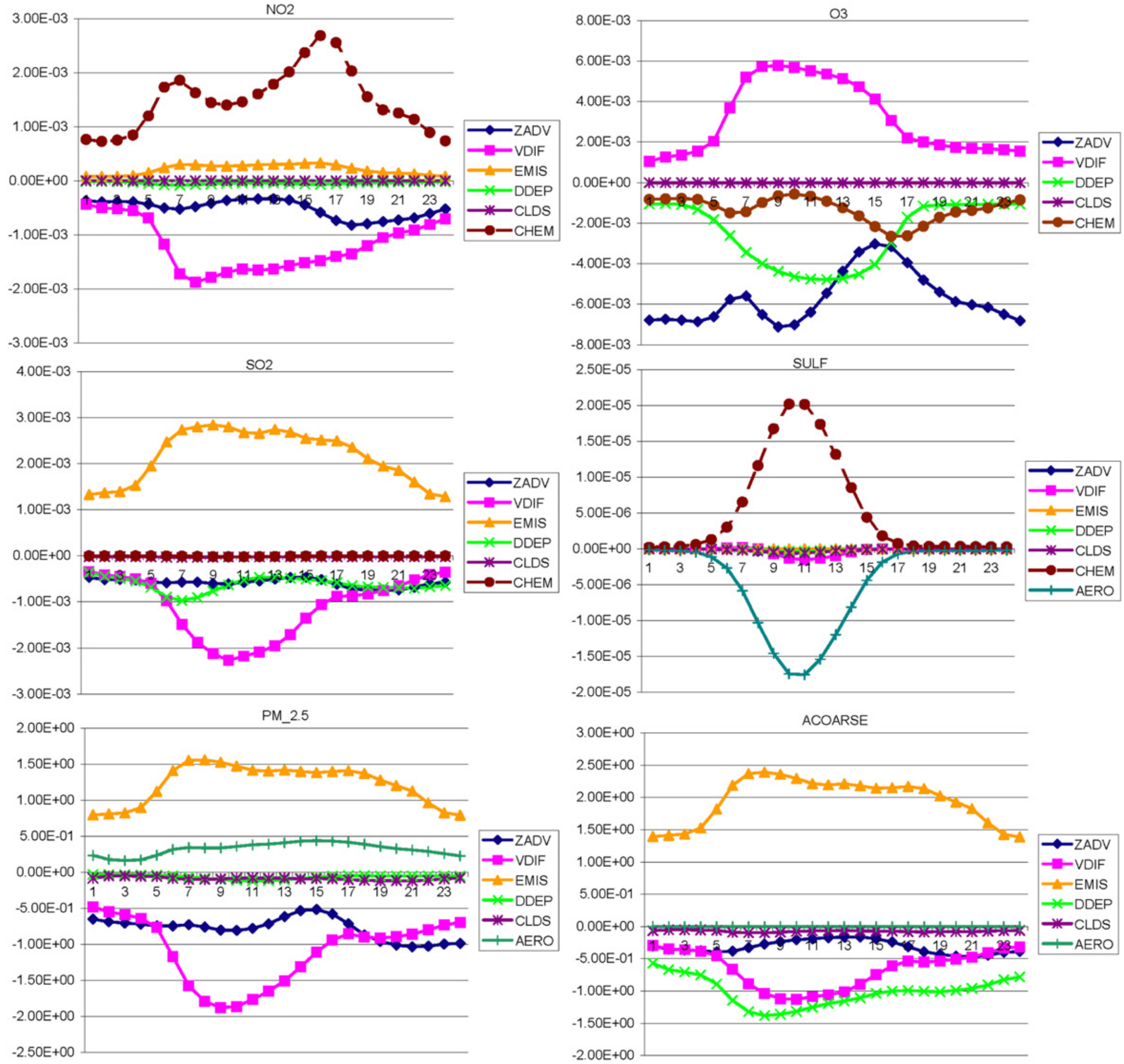

Fig. 15. Plots of the "typical" annual diurnal course of the averaged for the territory of Bulgaria contributions of vertical advection (ZADV), vertical diffusion (VDIF), emissions (EMIS), dry deposition (DDEP), chemistry (CHEM), aerosol processes (AERO) and cloud processes/aqueous chemistry (CLDS) to the hourly changes of surface NO_2, O_3, SO_2, sulphate (SULF), PM2.5 and PM-coarse (ACOARSE).

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High Performance Computing Simulations of the Atmospheric Composition in Bulgaria and the City of Sofia

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Abstract: *Some extensive numerical simulations of the atmospheric composition fields in Bulgaria and Sofia have been recently performed. The US EPA Model-3 system was chosen as a modeling tool. A very extensive database was created from simulations which was used for different studies of the atmospheric composition, including the Air Quality* (*AQ*) *climate.*

Keywords: *High Performance Computing* (*HPC*)*, simulations, atmospheric composition, air pollutants.*

1. Introduction

The atmospheric composition studies were based on extensive computer simulations carried out with good resolution using up-to-date modelling tools and detailed and reliable input data. All the simulations were based on the US EPA (Environmental Protection Agency) Model-3 system, which consists of three models: WRF (Weather Research and Forecasting) used as meteorological pre-processor; CMAQ – the Community Multiscale Air Quality System, being the Chemical Transport Model (CTM); SMOKE (Sparse Matrix Operator Kernel Emissions) Modelling System– the emission pre-processor. The simulations were performed for 7-year period (2008-2014) with Two-Way Nesting mod on. Carrying out reliable, comprehensive and detailed studies of the influence of the parameters and characteristics of lower atmosphere requires various types of data such as meteorological and chemical fields and measurements – Air Quality (AQ) data, emission inventories and physiographic data. The data is necessary as an input to the respective studies, as well as for evaluation and validation of the modelling approaches and tools [1-5].

A very extensive database was created from the numerical simulations and this data was used for different studies of the atmospheric composition, including the AQ climate. The air pollution pattern is formed as a result of interaction of different processes, so knowing the contribution of each one of these processes for different meteorological conditions and given emission spatial configuration and temporal behaviour could be helpful for understanding the atmospheric composition and air pollutants behaviour. Therefore the CMAQ "Integrated Process Rate Analysis" option was applied to discriminate the role of different dynamic and chemical processes for the air pollution formation. Different characteristics of the numerically obtained concentration fields, as well as evaluating the impact of air pollutants on quality of life in the term of AQI and of the contribution of different processes will be demonstrated in the present paper.

2. Methodology

The simulations were performed using the US EPA models three system.

Meteorological model WRF [6]. The Weather Research and Forecasting (WRF) model is a Numerical Weather Prediction (NWP) and atmospheric simulation system designed for both research and operational applications. It supplies various dispersion models, including presented below model CMAQ with input meteorological fields. WRF is suitable for a broad span of applications across scales ranging from large-eddy to global simulations.

Meteorological data. The large-scale (background) meteorological fields, used by the application were taken from the NCEP Global Analysis Data with 1°×1° resolution. The WRF and CMAQ nesting capabilities were used to downscale the simulations to a 9 km for domain D3 – Bulgaria, and to a 1 km horizontal resolution for the innermost domain – Sofia. The simulations were carried out for five nested domains (Fig. 1).

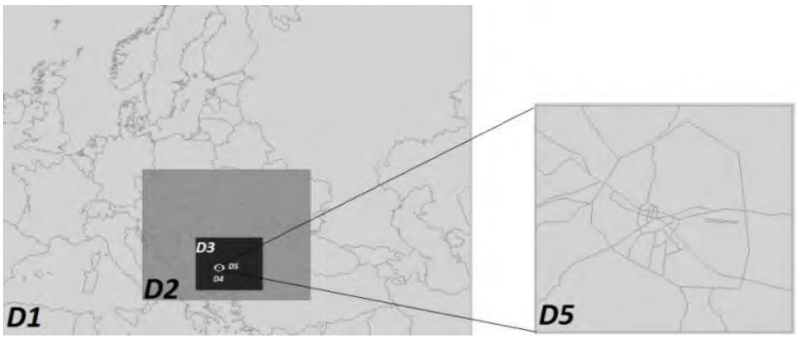

Fig. 1. Model domains: D1 81×81 km (Europe); D2 27×27 km (Balkan Peninsula); D3 9×9 km (Bulgaria); D4 3×3 km (Sofia municipality); D5 1×1 km (Sofia city)

Emission model SMOKE [7]. The Sparse Matrix Operator Kernel Emissions (SMOKE) was designed to integrate the emission data using sparse-matrix algorithms. SMOKE was created to allow emissions data for the AQ model's needs.

SMOKE provides a mechanism for preparing specialized inputs for AQ modelling research, and it makes AQ forecasting possible. SMOKE can process criteria gaseous pollutants and has no limitation regarding the number or types of pollutants it can process. The purpose of SMOKE is to convert the resolution of the emission inventory data to the resolution needed by an AQ model.

Emission data. The Bulgarian emission inventory was used as an emission input for Bulgaria. Special pre-processing procedures were created for introducing temporal profiles and speciation of the emissions. GIS (Geographic Information System) technology is applied as to produce area and large point source input from this data base. Outside the country the TNO (Netherlands Organisation for Applied Scientific Research) high resolution inventory was exploited 0.25º×0.125º (about 20×15 km) and the emissions were distributed over 10 SNAPs category [8]. The inventory is produced by proper disaggregation of the EMEP 50-km inventory data base [9, 10]. Currently, SMOKE supports Area, Mobile and Point Sources emissions processing and also includes biogenic emissions modelling through both a rewrite of the Biogenic Emission Inventory System (BEIS3) [11].

The Atmosphere Composition Model CMAQ [12-14]. The Community Multiscale Air Quality (CMAQ) modelling system is a tool for transport and chemical transformations of pollutants in the atmosphere and it is a part of US EPA Models-3 System. CMAQ as part of the system used meteorological data prepared by the model WRF and emission data, prepared by the model SMOKE. CMAQ is Eulerian model, "one atmosphere", which takes into account interactions between pollutants (about 100 species) in various dynamic scales. The model handles complex compositions of pollutants and configuration of sources, modelled transport and diffusion in a dynamic environment in wide time range – from minutes to days and weeks, and in the corresponding spatial scales – from local to global.

3. Grid computing

As it was stated above the WRF/CMAQ simulations were performed day by day for 7-year period. Thus a very extensive database was created, which could be used for different studies and considerations of the main features and origins of the atmospheric composition in different scales, including the AQ climate. The computer resource requirements for the model (WRF, SMOKE and CMAQ) simulations are rather big [15] (Tables 1 and 2) and that is why the numerical experiments were organized in effective HPC environment. The simulations were organized in two separate jobs: one job for WRF simulations and one for SMOKE, CMAQ and post-processing procedures. This makes the jobs run time for 6 days real time fairly reasonable. The calculations were implemented on the Supercomputer System Avitohol at IICT-BAS (Institute of Information and Communication Technologies-Bulgarian Academy of Sciences). This supercomputer consists of 150 HP Cluster Platform SL250S GEN8 servers, each one equipped with two Intel Xeon E5-2650 V2 8C 2600 GHz CPUs and 64GB RAM per server. The storage system is HP MSA 2040 SAN with a total of 96 TB of raw disk storage capacity. All the servers are interconnected with fully non-blocking FDR Infiniband, using a fat-tree topology.

Table 1. Computer resource requirements for models

Time/HDD	1 Day simulation at 16 CPU		
	WRF	CMAQ and SMOKE	Total
Time	3 h	2 h	5 h
HDD	530 MB	970 MB	1.5 GB

Table 2. Computer resource requirements for CMAQ model

Time	CPU/HDD	D2/27 km	D3/9 km	D4/3 km	D5/1 km	Total
	2 CPU (min)	2 h 40 min	1 h 10 min	1 h 36 min	32 min	5 h 58 min
	4 CPU (min)	1 h 20 min	35 min	30 min	10 min	2 h 35 min
	8 CPU (min)	20 min	20 min	17 min	6 min	63 min
	16 CPU (min)	30 min	20 min	12 min	5 min	67 min
1 day	HDD (MB)	255 MB	420 MB	70 MB	145 MB	890 MB
7 years	HDD (GB)	636 MB	1048 MB	175 MB	362 MB	2221 MB

The model output storage, however, is too large. Not all the information from the model output is so valuable for further air quality and environmental considerations, so an additional post-processing procedure and respective software (the program XTRACT) were developed, to reduce the information (only the necessary information to be kept) and the needed storage space. This procedure allows not only the number of output compounds to be reduced but also the number of the vertical levels. Another post-processing procedure was applied for statistical treatment of the results to present different statistical characteristics as the mean, minimum and maximum concentrations, probability density, bias, errors and etc., not only for the whole domain but also for selected points of interest. What are recently kept from the CMAQ output on an hourly basis are the surface concentrations of the following most important pollutants:

- 34 gases – NO_2, NO, O_3, NO_3, OH, HO_2, N_2O_5, HNO_3, HONO, PNA, H_2O_2, CO, FORM, ALD_2, C_2O_3, PAN, PACD, PAR, OLE, FACD, AACD, ETH, TOL, CRES, TO2, XYL, MGLY, ISOP, ISPD, SO_2, SULF (H_2SO_4), UMHP, TERP, NH_3;
- 5 aerosols – PSO_4, PNH_4, PNO_3, POA, PEC;
- 2 Anthropogenic and Biogenic secondary organic aerosols – SOAA, SOAB;
- 2 fine and coarse PM – FPRM, CPRM.

A key factor in the present work is the appropriate choice of metrics, which evaluate the impact of air environment on quality of life and human health, respectively elaboration of software, which to calculate the introduced metrics on the basis of the atmospheric composition. An integral characteristic, which reflects the impact of the atmospheric composition on general population health and quality of life will be presented in this paper – the Air Quality Index (AQI).

4. Results

As mentioned above, a very extensive database was created from the numerical simulations and this data was used for different studies of the atmospheric composition, including the AQ climate.

The most simple and natural atmospheric composition evaluations are the surface concentrations, so by averaging over the whole simulated fields' ensemble the mean annual and seasonal surface concentrations can be obtained and treated like "typical" daily concentration patterns. The simulated ensemble is large enough to allow different statistical treatment. The probability density functions for each of the atmospheric compounds can be calculated for each grid point, or averaged over a chosen territory, with the respective seasonal and diurnal variations. Knowing the probability density functions means to know everything about the ensemble.

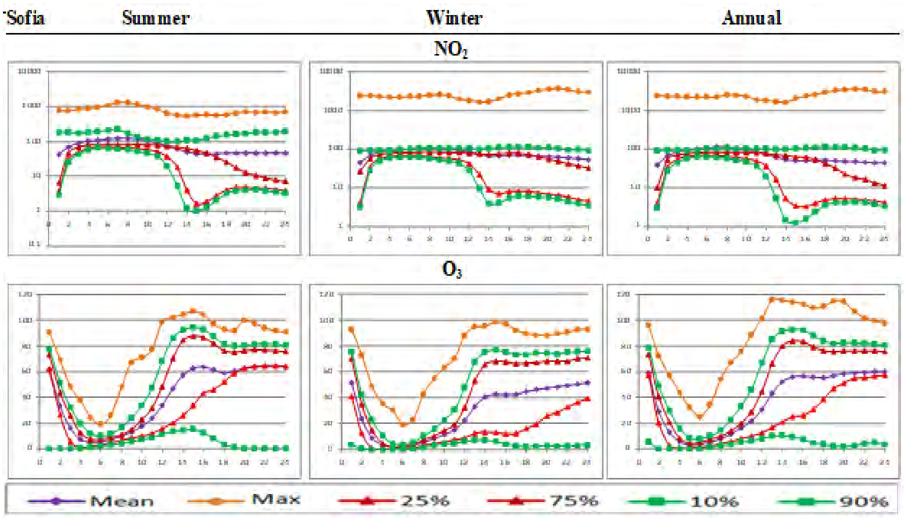

Fig. 2. Seasonal and diurnal variations of the "typical" surface concentrations for NO_2 and O_3, averaged for the territory of the city of Sofia

In Fig. 2 the seasonal and diurnal variations of the "typical" surface concentrations for NO_2 and O_3, averaged for the territory of the city of Sofia are presented. The curves in the graphics present the diurnal course of mean and maximal concentrations. The curves denoted by 25, 75, 10 and 90% show the imaginary concentrations for which the probability of the simulated ones to be smaller respectively than 25th, 75th, 10th and 90th percentiles of all. Thus the band 25-75 contains 50% and the band 10-90 contains 80% of the possible cases.

The diurnal variations of surface concentration fields are very well manifested.

Calculation of the Air Quality (AQ) impact on human health and quality of life. The AQ impact on human health and quality of life is an issue of great social significance. Evaluating this impact will give scientifically robust basis for elaborating efficient short term measures and long term strategies for mitigation of the harmful effects of air pollution on human health and quality of life. The AQ impact on human health and quality of life is evaluated in the terms of AQ Indices (AQI), which give an integrated assessment of the impact of pollutants and directly measuring the effects of AQ on human health. In the current study the AQI evaluations are based on extensive computer simulations of the AQ for Bulgaria and Sofia city carried out with good resolution using up-to-date modelling tools and detailed and reliable input data [16-19], which makes it possible to revile the climate of AQI spatial/temporal distribution and behaviour on the basis of air pollutant concentrations obtained from the numerical modelling. The index is defined in several segments, each of which is a linear function of the concentration of each pollutant considered: [20]. In that calculation the index falls in the ranges of a dimensionless scale. In each range index values are associated with an intuitive colour code, a linguistic description and a health description.

In different countries the indices are different and have their different scales. In Bulgaria the index, calculated in the frame of Bulgarian Chemical Weather Forecast System [21-23] and follows the UK Daily Air Quality Index [24]. This index has ten grades, which are further grouped into four bands: low, moderate, high and very high (Fig. 3). The index is based on the concentrations of five pollutants – Ozone, Nitrogen Dioxide, Sulphur Dioxide, Carbon Oxide and PM10. The breakpoints between index values are defined for each pollutant separately and the overall index is defined as the maximum value of the index.

Banding	Value	Health Descriptor
Low	1–3	Effects are unlikely to be noticed even by individuals who know they are sensitive to air pollutants
Moderate	4–6	Mild effects, unlikely to require action, may be noticed amongst sensitive individuals.
High	7–9	Significant effects may be noticed by sensitive individuals and action to avoid or reduce these effects may be needed (e.g. reducing exposure by spending less time in polluted areas outdoors). Asthmatics will find that their 'reliever' inhaler is likely to reverse the effects on the lung.
Very High	10	The effects on sensitive individuals described for 'High' levels of pollution may worsen.

Fig. 3. Air pollution bandings and Index impact on human health

Different averaging periods are used for different pollutants. The reference levels and Health Descriptor used in the tables are based on the health-protection related limit, target or guideline values set by the European regulations, at national or local level or by the World Health Organisation [25, 26].

Annually and seasonally averaged hourly values of the AQI for both domains with different horizontal grid resolution are presented in Fig. 4. The graphs represent the daily and seasonal percent recurrence of the AQI (1-10) over territory of Bulgaria and Sofia. These results, allow to follow which one of the indices has the highest recurrence through the day and during the seasons, and to analyze what are the possible reasons for high values of the index in High and Very High bands - meteorological conditions, dominant pollutants, and etc. Such a representation of the index makes it possible to evaluate the atmospheric composition in the context of impacts on human health and quality of life.

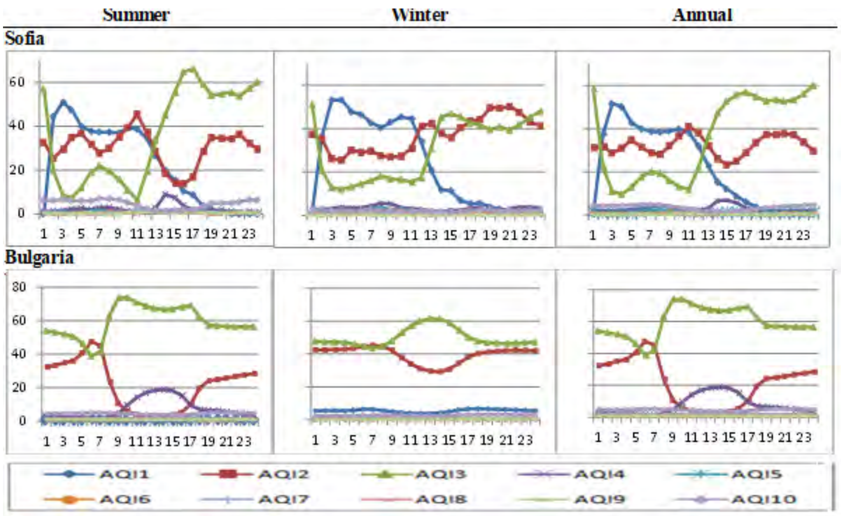

Fig. 4. Diurnal and seasonal variations (%) of the different AQI (1-10) integrated over territory of Bulgaria and Sofia

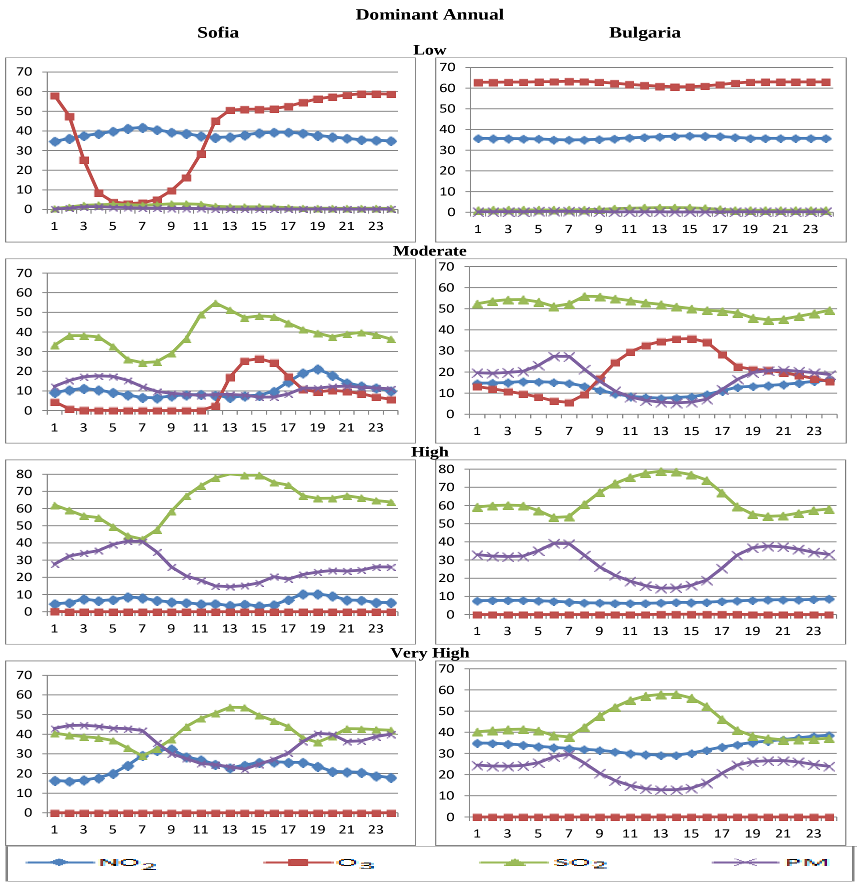

Fig. 5. Annual diurnal variations (%) of the dominant pollutant

The graphics that demonstrate the annual recurrence of the dominant pollutant (the pollutant with highest AQI, which determines the overall AQI) are presented in Fig. 5 for the four bands. The considered pollutants – NO_2, O_3, SO_2 and PM are presented in different colours. Of course the seasonal cases differ from the annually averaged graphics and the dominant pollutants are different for different band with well displayed seasonal and diurnal course.

Determining the contribution of different types of pollution sources to the AQ of the city of Sofia. The used emission inventory is made for a 10 emission categories (SNAP – Selected Nomenclature for sources of Air Pollution) and allows the evaluation of the contribution of various anthropogenic activities to the overall picture of air pollution:

1. SNAP 1 (Combustion in energy).
2. SNAP 2 (Non-industrial combustion plants).
3. SNAP 3 (Combustion in manufacturing industry).
4. Production processes.
5. Extraction and distribution of fossil fuels.
6. Solvent and other product use.
7. SNAP 7 (Road transport).
8. Other mobile sources and machinery.
9. Waste treatment and disposal.
10. Agriculture.

Six emission scenarios will be considered in the present paper: Simulations with all the emissions, with the emissions of SNAP categories 1 (energetic), 2 (non-industrial combustions), 3(industrial combustions) and 7 (road transport), and all the emissions for Sofia reduced by a factor of 0.8. This makes it possible to evaluate the contribution of road transport, energetic, industrial and non-industrial combustions to the atmospheric composition in the city. The concentrations for each scenario of reduced SNAP's were also calculated for each day of this 7-year period. The relative contribution of the emissions for each of the scenarios are calculated in the following way:

Let an arbitrary (concentration, deposition, columnar value, process contribution, etc.) pollution characteristic, for a given grid point, or averaged over chosen domain, obtained with all the emissions accounted for is denoted by φ. Let φ_m is the respective characteristic obtained when the emissions form source category m are reduced by a factor of α. In such a case the quantity

$$\phi_m = \frac{1}{1-\alpha} \cdot \frac{\varphi - \varphi_m}{\varphi} .100, \tag{1}$$

can be interpreted as the relative (in %) contributions of emission category m to the formation of the characteristic φ. It is obvious that more than one Selected Nomenclature for sources of Air Pollution (SNAP) category emissions can be reduced by a factor of α and so the joint contribution of several or all SNAP categories to the formation of the pollution characteristic φ can be evaluated.

Thus obtained relative source contributions can also be averaged for the whole ensemble, thus providing the "climate" of the emission contributions, in particular the "typical" annual and seasonal contributions.

For all the emission categories the pattern of the contribution fields is rather complex, which reflects the emission source configuration, the heterogeneity of topography, land use and meteorological conditions. Plots of this kind can give a good qualitative impression of the spatial complexity of the emission contribution. In order to demonstrate the emission contribution behavior in a more simple and easy to comprehend way, the respective fields can be averaged over some domain, which makes it possible to follow and compare the diurnal behavior of the respective contributions of different species.

Graphics of the diurnal evolution of the "typical" annual and seasonal relative contributions of the emissions from the already mentioned SNAP categories to the surface concentrations of NO_2, FPRM (Fine PaRticulate Matter) and CPRM (Coarse PaRticulate Matter) for the territory of Sofia city are shown in Fig. 6. The relative contributions for the territory of Sofia have well displayed diurnal and seasonal course.

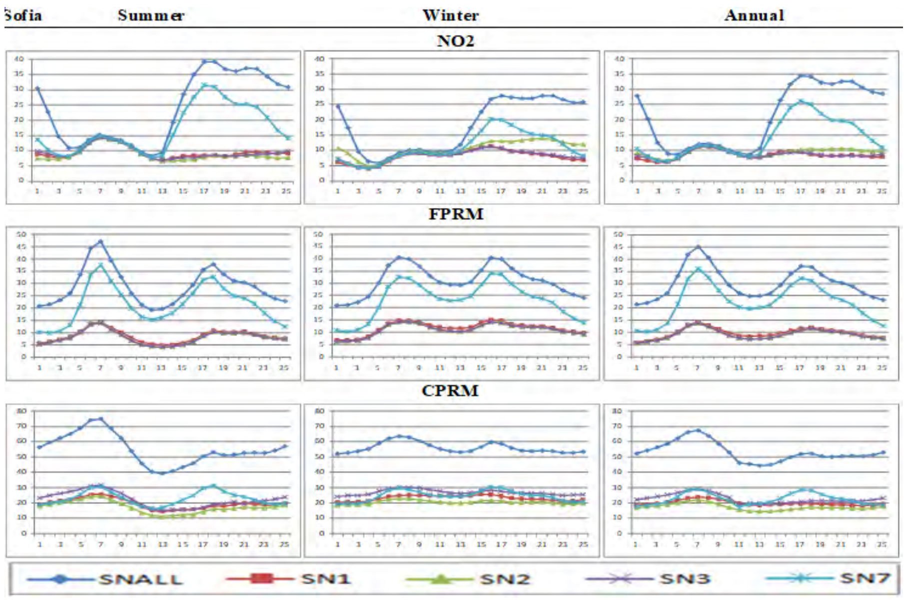

Fig. 6. Annually and seasonal averaged contribution of different SNAP categories (%) to the formation of NO_2, FPRM and CPRM for the territory of Sofia city

Determining the contribution of different processes to the surface concentration of pollutants. The Models-3 "Integrated Process Rate Analysis" option was applied to discriminate the role of different dynamic and chemical processes for the air pollution pattern formation. The procedure allows the concentration change for each compound for an hour ΔC to be presented as a sum of the contribution of the processes, which determine the concentration:

(2) $$\Delta C = \sum_{i=1}^{N} \Delta c_i .$$

The outputs from the Integrated Process Rate Analysis were averaged over the 7-year ensemble and so the "typical" seasonal and annual evaluations were obtained.

An example of the diurnal/seasonal behavior of some of the processes contributing to the surface concentrations of the pollutant NO_2, FPRM and CPRM, averaged for the city of Sofia, is given in Fig. 7. The processes that were considered are: advection, diffusion, mass adjustment, emissions, dry deposition, chemistry, aerosol processes and cloud processes/aqueous chemistry.

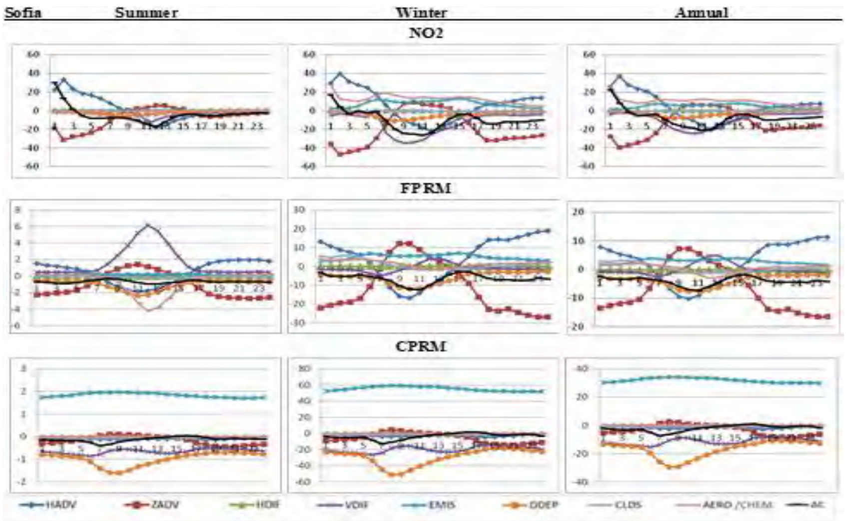

Fig. 7. Annually and seasonal averaged contribution of the different processes to the formation of NO_2, FPRM and CPRM (μg/m^3 per 1 h) for Sofia city

For the whole domain Sofia city, and for each of the selected items, the total concentration change (ΔC), leading to a change in a concentration is determined mainly by a small number of dominating processes which have large values, and could be with opposite sign and phases. The total concentration change (ΔC) is different for each pollutant and during the seasons. The sign of the contributions of some of the processes is obvious, but some of them may have different sign depending on the type of emissions, as well as weather conditions and topography.

5. Conclusion

A very small part of the obtained results is presented in the present paper, just to demonstrate the opportunity HPC platforms give for detailed and extensive study of the atmospheric composition – its behaviour, origin and health impact. Due to volume limitations the spatial variability of the air pollution characteristics is not demonstrated at all.

The generated ensembles of atmospheric composition characteristics have still to be carefully and extensively treated and analysed, which will be objective of the future work of the authors.

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Contribution of different emission sources to the atmospheric composition formation in the city of Sofia

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Abstract: Some extensive numerical simulations of the atmospheric composition fields in Sofia city have been recently performed and an ensemble, comprehensive enough to provide statistically reliable assessment of the atmospheric composition climate has been constructed. The US EPA Models-3 system was chosen as a modelling tool. As the NCEP Global Analysis Data with one degree resolution is used as meteorological background, the system nesting capabilities were applied for downscaling the simulations to a 1 km resolution. The national emission inventory and the TNO inventory were used as an emission input. The study is based on a large number of numerical simulations carried out day by day for years 2008–2014 for six emission scenarios – with all the emissions included and with reduced: all the emissions, emissions from energetics, from non-industrial, industrial combustions and road transport. Results concerning the contribution of the different emission categories are demonstrated in the paper.

Keywords: urban air pollution; computer simulations; SNAP categories; contribution of different emission sources.

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Degree-Day Climatology over Central and Southeast Europe for the Period 1961-2018 – Evaluation in High Resolution

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Abstract**:** *The ongoing climate change over Central and Southeast Europe has a great potential to affect significantly the public energy demands and in particular the energy consumption in the residential heating and cooling sector. The linkage of the ambient daily extreme and mean temperatures and the energy needs for condition or heat buildings can be quantified as numerical indicators as the heating and cooling degree-days. In the present study, these indicators are calculated according the UK Met Office methodology from the daily mean and extreme temperatures, which, in turn, are computed from the output of the MESCAN-SURFEX system in the frame the FP7 UERRA project. The study, which is performed in a very high resolution, is dedicated on the analysis of the spatial patterns as well as assessment of the magnitude and statistical significance of the temporal evolution of the heating and cooling degree-days. It reveals general tendencies which are coherent with the regional climate warming, but with high spatial heterogeneities. The study confirms the essential impact of the ongoing climate change on the heating, ventilating and air-conditioning industry over Central and Southeast Europe.*

Keywords**:** *Degree-days, MESCAN-SURFEX, UERRA Project, trend analysis.*

1. Introduction

According to the high-level synthesis report of the United Nations, titled "United In Science" (**https://public.wmo.int/en/resources/unitedinscience**), the climate change is the defining challenge of our time which exert influence on the ecosystems, on all branches of the international economy, and on the quality of life. The globally averaged surface temperature of the Earth increased 0.85 °C over the 1880 to 2012 period [19]. The global warming effects and the associated regional climatic changes over Central and Southeast Europe (CSE) have been widely documented in the last decades based on in situ measurements [1, 3, 16], assimilated surface observations [6, 9, 14, 22-24], reanalysis [11] global [10, 26] and regional climate models [5, 19, 20]. Most of these studies are focused on the second half of the twentieth and the first decade of the 21st century, clearly evidencing that, similarly to the global and continental trends, the regional temperature got warmer during the period. The study of near past climate provides an essential baseline from which to understand and contextualize changes in the contemporary and future climate.

As evidenced in many recent publications (e.g., [7, 21, 28]), the changes in climate have direct and indirect impact on managed systems like heating, ventilating and air-conditioning industry. Space heating and cooling is responsible for a large fraction of European energy use [18]. The linkage of the ambient daily extreme and mean temperatures and the energy needs for air-conditioning or heat buildings can be quantified as numerical indicators as the Heating Degree-Days (HDD) and Cooling Degree-Days (CDD). Thus, HDD and CDD are rough surrogates for how climate change is likely to affect energy use for heating and cooling. In the present study, these indicators are calculated according the UK Met Office (UKMO) methodology from the daily minimum, mean and maximum temperatures, denoted tn, tg and tx respectively, which, in turn, are computed from the output of the MESCAN-SURFEX system in the frame the FP7 UERRA project. The study, which is performed in a very high resolution, is dedicated on the analysis of the spatial patterns as well as on the assessment of the magnitude and statistical significance of the temporal evolution of the HDD and CDD over CSE Europe.

The article is structured as follows. The used input data are described in Section 2 titled "Short Description of UERRA and MESCAN-SURFEX". A brief explanation of the UKMO definition of the HDD and CDD is placed in Section 3. The core of the article is Section 4, containing 2 subsections and titled "Performed Calculations and Obtained Results". The concluding remarks are in Section 5.

2. Short description of UERRA and MESCAN-SURFEX

Accurate and reliable sources of information are crucial for building energy simulations and analyses [7] and thus we have exploited modern and reliable weather data in a very high spatial resolution.

The objective of the project-driven collaborative initiative FP7 UERRA (Uncertainties in Ensembles of Regional ReAnalyses (RRA); **www.uerra.eu**) is to produce ensembles of European RRA of essential climate variables for several decades and estimate the associated uncertainties in the data sets [25, 30]. It also includes recovery of historical (last century) data and creation of user friendly data services. Within UERRA three different Numerical Weather Prediction (NWP) models have been employed to generate European RRA and subsequent surface reanalysis products.

The MESCAN-SURFEX system analysis uses the 2D-analysis system MESCAN [27] and the land surface platform SURFEX [4] to generate a coherent surface and soil analysis. The UERRA-NWP HARMONIE-ALADIN at 11 km grid spacing is used as a starting point to further downscaling. Beside the other parameters, MESCAN-SURFEX produces air temperature at 2 m above the surface in 6-hour temporal resolution, i.e., at 00, 06, 12 and 18 UTC for the period 1961-2018. Based on the availability of this data, the tn, tg and tx are derived in regular 0.05°×0.05° grid and validated against independent data sets as documented in [12].

The applicability of the derived in such fashion temperature data for assessment of agro-meteorological indices over CSE Europe in the context of climate change is demonstrated in [13].

3. HDD and CDD

HDD and CDD are, similarly to the climate and agro-meteorological indices [1], an attempt to objectively extract information from daily weather data (observations or model as in current study) that answers questions concerning energy demand and/or consumption in the residential and domestic heating and cooling sector. Thus, they are likely to display the same types of variability as the temperature data on which they are based. The heating and cooling requirements for a given structure at a specific location are considered, beside the impact of the other factors, proportional to the number of HDDs and CDDs at that location [7]. Recently, many studies have focused on the use of HDD and CDD to estimate annual and seasonal trends in the energy demand for heating and cooling residential, commercial, and industrial buildings, especially in the context of climate change (see [21, 28, 29] and references therein). Hence, the theoretical formulation of both indicators is not standardised, their computation can be performed in different ways, depending on the nature and scope of the study as well as availability of input data. Computation methods range from simple models based on monthly or annual temperature to more sophisticated approaches [28, 29]. In the present study we use the developed by the UKMO [15] and successfully applied in [29] method. According it, daily HDD and CDD are calculated based on a comparison of tn, tg and tx with the selected base temperature (tb), taking account of fluctuations of daily air temperature around the base temperature, as well as the asymmetry between daily mean temperature and diurnal temperature variations, as shown on Table 1.

Table 1. UKMO methodology for computing daily HDD and CDD

Condition	HDD	CDD
tx ≤ tb (uniformly cold day)	HDD=tb–tg	CDD=0(No cooling is required)
tg ≤ tb <tx (mostly cold day)	HDD=(tb–tn)/2–(tx–tb)/4	CDD=(tx–tb)/4
tn < tb < tg (mostly warm day)	HDD=(tb–tn)/4	CDD=(tx–tb)/2– (tb–tn)/4
tn ≥ tb (uniformly warm day)	HDD=0 (No heating is required)	CDD=tg–tb

Hence, as the study is on annual basis, we summed up the daily values. The base temperature is the outdoor temperature below or above which heating or cooling is needed [7]. As in the original proposal [15], tb is set on 15.5 °C for the HDD-computation and on 22.0 °C for the CDD-computation. Previous versions of these indicators, based solely on tg, have a jump discontinuity when daily mean temperature falls below the base temperature. UK Met Office methodology does not exhibit such a discontinuity [18]. It is worth to emphasize also, that in present work the daily mean temperature is independent input parameter, rather than estimated as arithmetic average between tn and tx as in [28, 29].

The units of measurement of the HDD and CDD are degree-days, noted further °D as properly proposed in [21].

4. Performed calculations and obtained results

4.1. Spatial patterns and temporal evolution

First, in order to reveal long term inter-annual changes for the considered indices, the spatial patterns of the Multiyear Means (MM) for the first 30-year, i.e., 1961-1990, are superimposed to the multiyear means for the second 30-year period, i.e., 1989-2018 as shown on Fig. 1. Such comparison is acceptable, hence the both periods overlaps in only two years. The long-term changes are estimated by means of the relative bias, i.e., the difference between the MMs for the second and first period in respect to the first period.

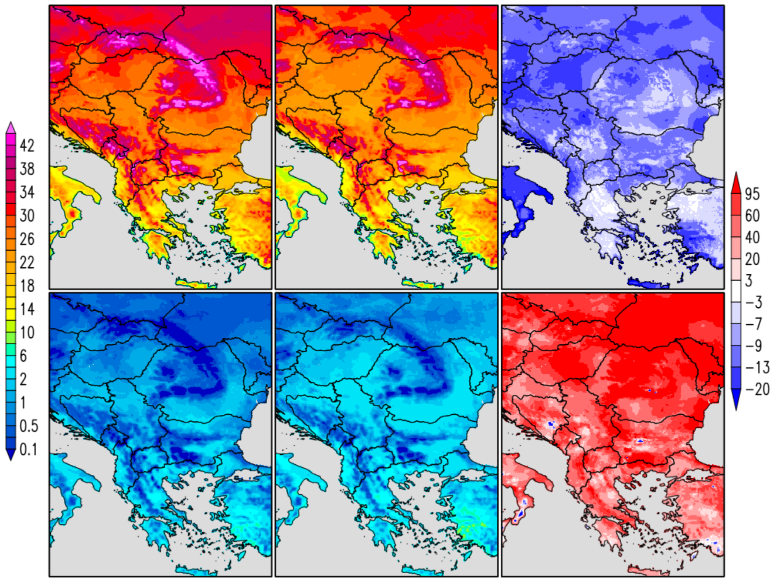

Fig. 1. Multiyear means of HDD (first row) and CDD (second row) in the first and second column correspondingly for 1961-1990 and for 1989-2018. The units are 100 °D. The relative biases (in %) are shown in the third column

The spatial patterns of the variables considered are generally consistent in both time spans. The vertical gradients are reproduced in detail that is direct consequence from the high grid spacing. The landscape of CSE Europe contains large plains, high mountains, mountain chains and fragmented coastlines and is quite non-uniform. The exploitation of datasets with coarser grid spacing could lead to overlooking of local spatial details, essential for some end-user applications. As stated in the regional study [6], based on the 0.1°×0.1° dataset CARPATCLIM [22], the regional differences in the HDD and CDD trends within the considered domain are related more to altitude, rather than latitude.

The most obvious result from the analysis of Fig. 1 is the substantial decrease of the HDD and, vice versa, increase of CDD over the entire domain. Both biases are quite uniform and the relative increase of the CDD is significantly higher than the decrease of the HDD. Some recent papers (e.g., [6, 9-11, 16, 17]) have noted the asymmetrical evolution patterns of the regional warming in the near past but depending of the considered input data, time span and methodology the different studies have yielded mixed results.

The temporal evolution of the Area-weighted over land Averages (AA) of the HDD and CDD are shown on Fig. 2.

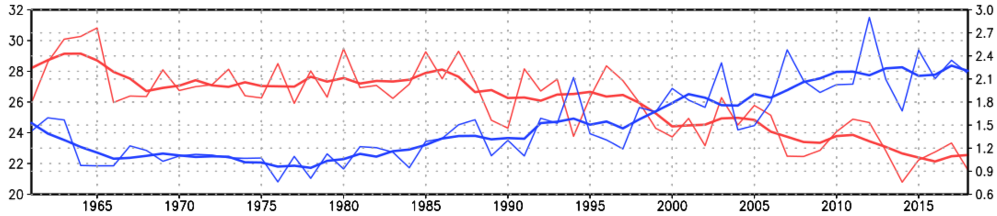

Fig. 2. Temporal evolution of the HDD (red line, left ordinate) and CDD (blue line, right ordinate). The units are 100 °D. The fat lines are the running 5-year means

In agreement with the results from the analysis of Fig. 1, the evolution of HDD and CDD shows fairly clear tendencies: Despite some colder episodes as, for example, the noted in [13] 1965, there is general decrease of the HDD and increase of the CDD. It is worth to emphasize also that the inter-annual course of the HDD is somewhat anti-correlated with the inter-annual course of the CDD. This is reflection of the fact that generally warm years are characterized most frequently with low values of HDD and high CDD and vice versa.

4.2. Trend analysis

The magnitude of the trend is estimated by the Theil-Sen Estimator (TSE), which is preferably used in many geophysical and engineering branches as a superior alternative of the ordinary least squares [8]. The statistical significance is analysed with the Mann-Kendall (MK) test. As, like the TSE, the MK test is non-parametric, rank-based procedure has been applied, especially suitable for non-normally distributed data, data containing outliers and nonlinear trends [6]. Both methods are practically standard tools for trend analysis in the climatology. In the present study they are applied for every grid point time series individually. In the present work, as in many similar studies (e.g., [6, 9-12, 26]) the significance level is fixed at 5% (two-tail test).

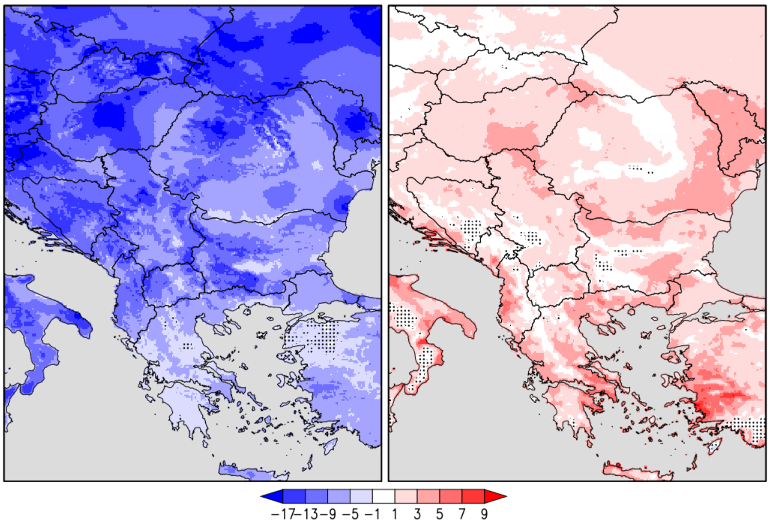

Fig. 3. Trend magnitude of the HDD and CDD in the first and second column respectively. The units are °D per 1 year. Stippling indicates grid points with changes that are **not** significant at the 5% significance level

The most apparent result from the analysis of Fig. 3 is the markedly expressed negative trend for the HDD and positive trend for the CDD. The trends magnitude of the HDD is, in absolute terms and as a whole, bigger than the trend magnitude of the CDD. The trends of the both indices are practically everywhere statistically significant at the 5% and their patterns are consistent over the domain, i.e., there are no mixed trends for both indices.

5. Conclusion

Based on the availability of up to date dataset [12] based on the primary data from the FP7 UERRA project, we provide an overview of the spatial patterns in very high resolution and the long term temporal evolution on annual basis of the HDD and CDD over CSE Europe in the period 1961-2018.

The study confirms the suitability of the considered dataset for index-based analysis of the near past and present climate in computationally feasible way as has been already shown in [13].

Although not fairly exhaustive, the study confirms the essential impact of the ongoing climate change on the heating, ventilating and air-conditioning industry over CSE Europe. Consistent with the long-term changes of the mean and extreme temperatures over the domain, documented in the most recent papers, the present study reveals strong evidences for the impact of the regional climate warming on the considered indices. As emphasized in [18], a decrease in the demand for public and domestic heating can significantly decrease overall energy use in Europe, but this gain can be offset in part or completely by an increase in cooling demand. Furthermore, heating is delivered to end users in different ways (individual boilers fuelled by oil, gas and coal, and electricity and district heating), whereas cooling is supplied currently almost exclusively through electricity. As a result, a given change in cooling needs is generally associated with larger costs, a larger change in primary energy demand and larger impacts on the peak capacity of supply networks than the same change in heating requirements.

The study could be extended and continued in many aspects. The logical next step is to accomplish the work assessing the future changes and trends based on (preferably regional) climate simulations. Hence, the temperatures in all CMIP5 scenarios are projected to rise further, it is reasonable to expect additional decrease of the HDD and increase of CDD. Our preliminary computations with the regional climate model RegCM confirm this assumption. The study could also be extended backwards in time as far as possible in order to capture more general and robust trends. A necessary prerequisite for such task, however, is, as for many other efforts in the regional climatology, the (free) availability of reliable data with proper spatial coverage and spatial-temporal resolution.

The data sets with the HDD and CDD, as well as the trend measures (TSE trend magnitude estimation and *p*-value from the MK test) are in standard form (GrADS binary/descriptor files) and could be supplied from the corresponding author upon request.

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Trend Analysis of CMIP5 Ensemble of Climate Indices over Southeast Europe with Focus on Agricultural Impacts

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Abstract: *Nowadays there is a strong degree of agreement that the climate change is the defining challenge of our time, which will exert influence on the ecosystems, on all branches of the international economy and on the quality of life. The analysis based on climate indices is widely used non-parametric approach for quantification of the mean state as well as extreme climate events. This study, which is continuation of our previous efforts, is dedicated to the assessment of the trend magnitude and the trend statistical significance of six temperature-based and three precipitation-based indices in projected future climate over Southeast Europe up to the end of the 21st century. The indices are computed from the bias-corrected output of five CMIP5 global models, reinforced with all four RCP emission scenarios. The model output is accessed from the section of the Inter Sectoral Impact Model Intercomparison Project in the Copernicus Data Store. The multi model ensemble medians of the temperature-based indices shows considerable increase which is consistent with the warming of the mean temperatures. These changes are statistically significant in most cases and intensify with the radiative forcing. The revealed tendencies of the precipitation-based indices are more complex when compared with temperature tendencies.*

Keywords: *Climate indices, RCP, CMIP5 Ensemble, future climate, trend analysis.*

1. Introduction

Nowadays there is a strong degree of agreement that the climate change is the defining challenge of our time, which will exert influence on the ecosystems, on all branches of the international economy and on the quality of life. However, as stated in [18], immediate damages to humans and ecosystems are not caused by gradual changes in the mean state but mainly by so-called extreme climate events. The extreme weather phenomena are discussed in all reports of the Intergovernmental Panel on Climate Change. There are various methods to investigate extreme events, but the computation and analysis of Climate Indices (CIs), derived from daily data (observations or model output) is probably the most widely used non-parametric approach. Subsequently, the literature is very large ([1-3, 18, 19] and many others). To detect changes in these extremes, it is important to apply sets of CIs that are statistically robust, cover a wide range of climate conditions, and have a high signal-to-noise ratio [1]. Such sets are used in several projects on climate change with a focus on different spatial scales and temporal extent.

The relevance of the trend assessment of climate extremes is frequently emphasized (see, for example, [1, 18] and references therein). The principal reason is that it is vital to discover the presence of long-term persistent tendencies as well as to quantify their magnitude.

Our working group has previous, partially project-driven, experience with CIs-based analysis [4-6]. The present study is a natural continuation of our recent efforts, documented in [7, 8]. These two studies are dedicated to the assessment of the future climate over SouthEast (SE) Europe, and are based on an ensemble of CIs with the main goal to compare the multiyear CIs-means for the present and the projected future climate. The main aim of the present work is to assess the trend magnitude and statistical significance of six temperature-based and three precipitation-based indices in projected future climate over the same domain up to the end of the 21st century in a consistent manner. The indices are computed from the bias-corrected output of five CMIP5 global models, reinforced with all four RCP emission scenarios. As in [18] and [19] and many other similar studies, the present one exploits the ensemble multi-model median, noted henceforth MMX50, rather than the output from the individual models.

The article is structured as follows: The used scenarios, models, and input data are concisely described in the second section. The theoretical background of the performed statistical analysis is placed in the third section. The core of the article is in the fourth section where the performed computations and the obtained results are described. The brief concluding remarks are in the last section.

2. Scenarios, models and input data

The Coupled Model Intercomparison Project (CMIP) is a standard experimental protocol for studying the output of Coupled Atmosphere-Ocean General Circulation Models (CAOGCMs). The main aim of the fifth phase of CMIP, CMIP5, is to study the climate and climate change in the past, present, and future, using a set of simulations with different climate simulators in various spatial and temporal scales [22]. The CMIP5 experiment uses a set of emission scenarios called Representative Concentration Pathways (RCP) [15] to assess the interactions between the human activities on the one hand and the environment on the other hand, and their evolution. In contrast to the previous generations of scenarios, the RCPs are mitigation scenarios that assume active policy actions directed to achieve certain emission targets. Four RCPs have been formulated: RCP2.6, RCP4.5, RCP6.0 and RCP8.5. They are based on a range of projections of future population growth, technological development, and societal responses. The labels for the RCPs provide a rough estimate of the radiative forcing in the year 2100 (relative to pre-industrial conditions).

The present study exploits the database whose creation is described in [7], whereas the primary data access point was the Copernicus Data Store. It is based on the collection of bias-corrected climate datasets provided through Inter Sectoral Impact Model Intercomparison Project (ISIMIP 1, **https://www.isimip.org/protocol/**), Fast Track simulation round. These climate datasets contain daily-resolution, bias-corrected climate data from five CMIP5 CAOGCMs according to Table 1 covering the period 1950-2099 (historical run – up to 2005 and CMIP5 simulations for 2011-2099), downscaled to a 0.5°×0.5° lat-lon grid. The main goal of ISIMIP is to offer reliable global climatological data for agro-climatic impact assessments but most of the included variables have universal applicability.

Table 1. CAOGCMs used in ISIMIP 1 Fast Track simulation round

Model Acronym	Institution, country	Spat. Res. (Lon.×Lat.×Lev.)
GFDL-ESM2M	Geophysical Fluid Dynamics Laboratory, USA	144×90×24
HadGEM2-ES	Met Office Hadley Centre, UK	192×145×40
IPSL-CM5A-LR	Institut Pierre-Simon Laplace, France	96×96×39
MIROC-ESM-CHEM	AORI, NIES, JAMSTEC, Japan	128×64×80
NorESM1-M	Norwegian Climate Centre, Norway	144×96×26

As emphasized in the introduction, the study is based entirely on the MMX50.

The selected CIs are the same as in [7] and [8] where the six temperature-based are: Minimum of the Minimum Temperatures, Maximum of the Maximum Temperatures, Frost Days, Tropical Nights, Cold and Warm Spell Duration Indices, noted traditionally as TNn, TXx, FD, TR, CSDI and WSDI. The three precipitation based indices are Annual Precipitation Sum, Heavy Precipitation Days and Consecutive Dry Days, noted RR, RR10mm and CDD, respectively. In the articles above-referenced, the reader could find the explanatory motivation of this selection as well as links to the definitions of these CIs.

3. Methods

The magnitude of the trend is estimated by means of the Theil-Sen Estimator (TSE). The method TSE is named after H. Theil and P. Sen, who published the pioneering papers ([12] and [17]). Conceptually, the method is very simple: If x_i, $i = 1, \dots, n$, and y_i, $i = 1, \dots, n$, are the independent (most frequently the time) and dependent variables correspondingly, the estimation of the model is done by calculating the slopes of all possible $\binom{n}{2} = \frac{n(n-1)}{2}$ combinations of pairs of points. The slope between every two points is equal to

(1) $$\beta = \frac{y_j - y_i}{x_j - x_i}, \ x_i \neq x_j.$$

The final non-parametric slope $\hat{\beta}_1$ is then defined as the spatial median of these slopes:

(2) $$\hat{\beta}_1 = \text{median}\left\{\tilde{B}\right\},\ \left\{\tilde{B} = b_{ij} \mid b_{ij} = \frac{y_j - y_i}{x_j - x_i},\ x_i \neq x_j,\ 1 \leq i < j \leq n\right\}.$$

Positive value of $\hat{\beta}_1$ reveals an increasing trend, negative value is sign of decreasing trend.

The TSE is essentially an estimator for the slope alone; the line has been constructed by means of different methods. In fact there are a large variety of ways to calculate the intercept $\hat{\beta}_0$. We apply the frequently used relation, proposed in [9]:

(3) $$\hat{\beta}_0 = Y_{\text{median}} - \hat{\beta}_1 X_{\text{median}},$$

where Y_{median} and X_{median} are the medians of the dependent and independent variables correspondingly.

The main strength of the TSE is its robustness. As stated by many authors (see [10] and references therein), the TSE, compared to the frequently used ordinary Least Squares Estimation (LSE), is much less sensitive to outliers. This conclusion could be explained intuitively so: A positive outlier will increase the sample mean in direct proportion to the size of the outlier. In fact, there is no upper limit on the effect that can be induced on the sample mean by an outlier. On the other hand, the effect of an outlier on the sample median is bounded; once the outlier becomes the largest observation in the sample it has no further influence on the median [20]. In fact, the breakdown point of TSE is $1 - 1/\sqrt{2} \approx 29.3\%$, meaning that it can tolerate arbitrary corruption of up to 29.3 % of the input data-points without degradation of its accuracy [23]. The performance of both regression methods, LSE and TSE, for trend estimation of meteorological data is assessed in [4]. Among other findings, it is revealed that in certain cases the LSE could produce trend slope even with wrong sign. The TSE produces for the same dataset reliable result.

Although $O(n^2)$ procedure, the TSE is still computationally feasible, keeping in mind that in the most geophysical and engineering applications $n < 1000$.

The statistical significance of the trend is estimated by means of the Mann-Kendall (MK) test [12, 13].

Like the TSE, the MK is non-parametric rank-based procedure. The null and the alternative hypothesis of the two-sided test, denoted traditionally H_0 and H_A of the MK test for trend in the random variable *x* are as follows:

(4) $$H_0:\ \Pr(y_j > y_i) = 0.5,\ \ j > i,$$
$$H_A:\ \Pr(y_j < y_i) \neq 0.5,\ \ j > i.$$

The MK statistic *S* is calculated as

(5) $$S = \sum_{k=1}^{n-1} \sum_{j=k+1}^{n} \text{sgn}(y_j - y_k),\ \ j > k,$$

where y_i and y_k are the values of the considered variable in the moments *j* and *k*, respectively, *n* is the total number of years and the sign function is defined as

(6) $$\operatorname{sgn}(y_j - y_k) = \begin{cases} 1 & \text{if } y_j - y_k > 0, \\ 0 & \text{if } y_j - y_k = 0, \\ -1 & \text{if } y_j - y_k < 0. \end{cases}$$

For large n (practically for $n \geq 8$), the distribution of S can be well approximated by a normal distribution with mean zero and variance computed as

(7) $$\mathrm{VAR}(S) = \frac{1}{18}\left[n(n-1)(2n+5) - \sum_{p-1}^{g} t_p(t_p - 1)(2t_p + 5) \right],$$

where g is the number of tied groups, and t_p is the amount of data with the same value in the group $p = 1, \ldots, g$. The normalised test statistic Z is given by:

(8) $$Z = \begin{cases} \dfrac{S-1}{\sqrt{\mathrm{VAR}(S)}} & \text{if } S > 0, \\ 0 & \text{if } S = 0, \\ \dfrac{S+1}{\sqrt{\mathrm{VAR}(S)}} & \text{if } S < 0. \end{cases}$$

If the normalised test statistic Z is equal to zero, the data are normally distributed, and the positive values of Z mean a rising trend and negative a decreasing trend [25]. The null hypothesis is rejected at significance level α if $|Z|> Z_{\alpha/2}$ (two-tail test), where $Z_{\alpha/2}$ is the value of the standard normal distribution with an exceedance probability $\alpha/2$ [3].

The probability value (p-value) of the MK test is computed as

(9) $$p(Z) = 0.5 - \Phi(|\mathrm{Z}|) kde \Phi(|\mathrm{Z}|) = \frac{1}{\sqrt{2\pi}} \int_0^{|\mathrm{Z}|} e^{-\frac{t^2}{2}} dt.$$

For a specific significance level $\alpha \in (0,1)$ the null hypothesis is rejected whenever $p(Z) < \alpha$.

Like the TSE, the MK test is a procedure, especially suitable for non-normally distributed data, data containing outliers and nonlinear trends. Consequently, it is widely used in many engineering and geophysical branches as hydrology (see, for example, [11, 25, 26]). They are recommended from the World Meteorological Organisation [24] and are practically standard tools for statistical assessment of trend in the meteorology ([1-6, 17-18] and many others).

4. Performed computations and obtained results

All calculations are performed by purposely written from the author's programs in FORTRAN90/95. The parameters of the TSE regression are computed also directly, using (2) and (3). The median slope is calculated exactly by computing all lines through pairs of points. Although quadratic in time, this approach is still feasible due to its simplicity and, as noted above, by the relatively small length of the time series (in case n=89, the number of years 2011-2099). The median itself is computed with the A. Miller's subroutine (freely-available repository at **http://jblevins.org/mirror/amiller/**), which implements the efficient truncated quicksort algorithm.

The p-value of the MK-test is also computed directly according to the sequence (5)-(8). The routine, based on Chebyshev fitting [21] is used for the computation of the error function in (9). In the present work, as in many similar studies (e.g., [3, 5, 18-19]), the significance level is fixed at 5%.

Unlike the LSE, benchmarks for the TSE and MK test are difficult to find. In the present study, we use for this goal the representative source [14] and the results are identical.

The magnitudes of the trend in time as well as its statistical significance are estimated individually for all grid cells and separately for each scenario.

Fig. 1 shows the results of the trend analysis for TNn and TXx.

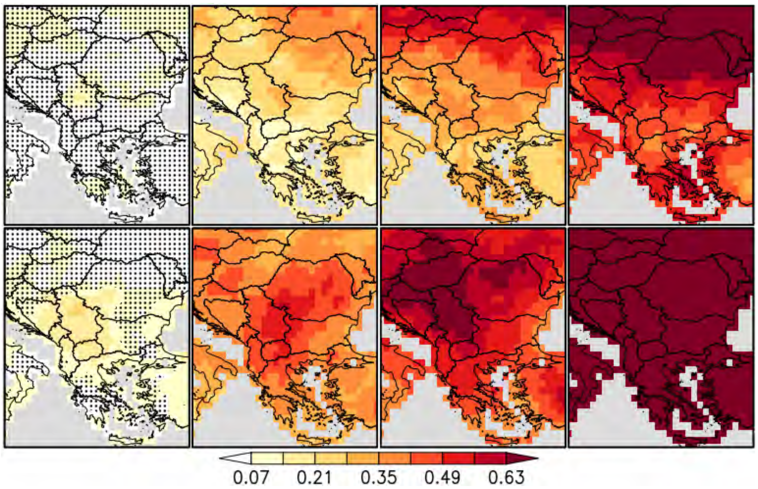

Fig. 1. Trend slopes (unit: ^{o}C per 10 years) of the MMX50 of the TNn (first row) and TXx (second row) for the RCP2.6, RCP4.5, RCP6.0 and RCP8.5 in the first, second third and fourth column correspondingly. Stippling indicates grid points with changes that are **not** significant at the 5% significance level

Fig. 1 shows a gradual increase of the overall slopes (i.e., the rate of the change, in case increase) of both indices from RCP2.6 to RCP8.5, i.e., proportional to the radiative forcing. The value of the trend magnitude of the TNn appears bigger over the northern part of the domain for RCP6.0 and RCP8.5 but as a whole, the spatial distributions do not shows clear systematic pattern. The most apparent difference between the trend magnitude fields of the TNn and TXx are the generally bigger values for the TXx for all four scenarios. This could be related to the documented in many articles (see, for example, [1]) warming asymmetry. It is worth emphasizing, however, that depending of the considered domain, spatial and temporal scales as well as the methodology applied, the reported results are different, even partially contradicting.

The results for the other temperature based CIs are shown in Fig. 2.

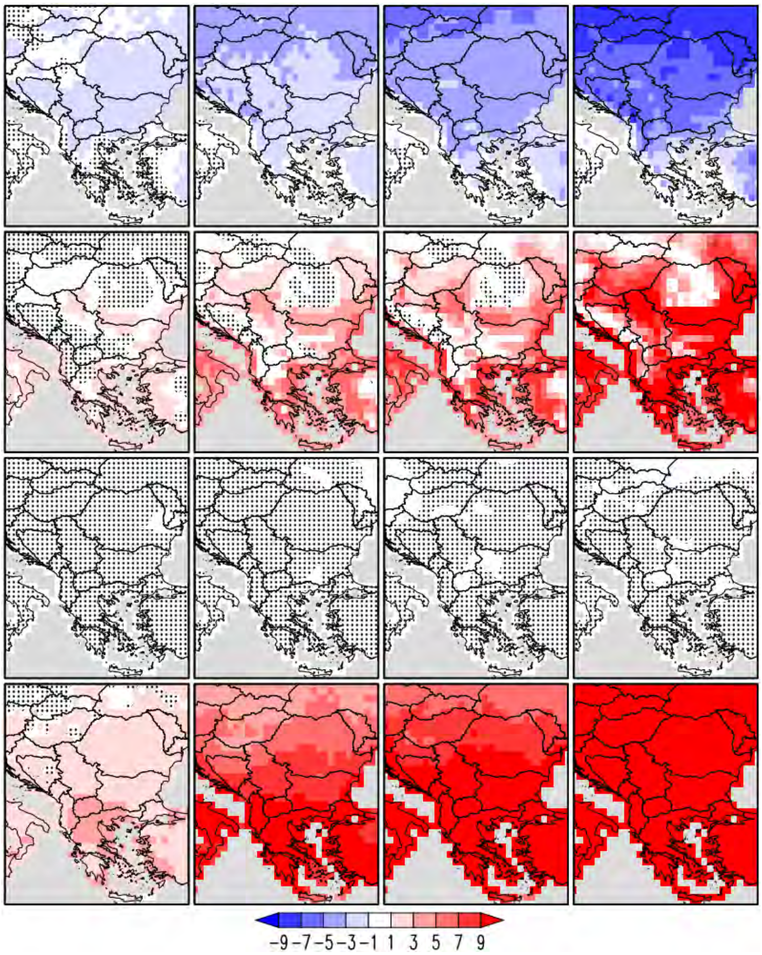

Fig. 2. Same as Fig. 1 but for the FD, TR, CSDI and WSDI on the first second third and fourth row correspondingly. The units are days per 10 years

Consistent with the changes in the mean and extreme temperatures, the overall picture shows progressive (i.e., from RCP2.6 to RCP8.5) decrease of the slope FD and increase of the TR and WSDI. The trends of these CIs are statistically significant over the bigger part of the domain in all scenarios. Somewhat surprising appears the fields of the CSDI: In contrast to the expectations, there is practically no trend under any scenario. The reason is rooted in the relatively small value of this index even in the reference period, as shown in [8]. Thus, under the conditions of the generally warmer climate, the CSDI drops close to zero (i.e., constant), causing the absence of a trend.

The vertical gradient of the trend magnitude is most apparent in the case of the tropical nights especially along the main Carpathian ridge. It is stated in [3] that the occurrence of TR is substantial only in low elevation areas (below 800 m), particularly exposed to persistent and intense warm spells in summer. Generally, tropical nights are not characteristic of the mountain climate of the Balkan Peninsula. It is worth to emphasize, however, that the zones with not essential trend increase become smaller with the rise of the radiative forcing, suggesting that even the mountains will be exposed in the future to excessive warmth.

As in many other places of the world, in contrast to the projected changes in the temperature indices, where there is a general agreement on the sign of change independent of the region considered, changes in the precipitation indices over the considered region are less consistent in this regard [8, 19].

As noted in [8], the considered precipitation-based indices are used as key parameters in many studies of present [18] and projected future climate [19].

Fig. 3 shows the results of the trend analysis for the annual precipitation sum RR that is probably the most important precipitation-based climate index.

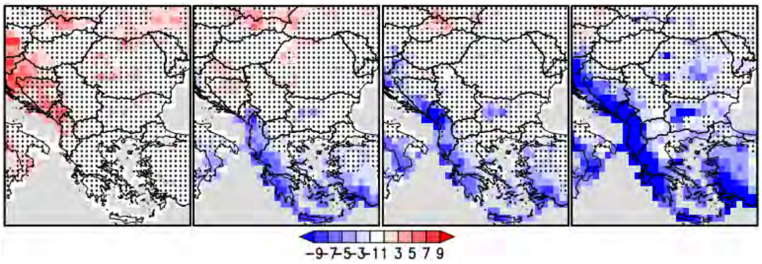

Fig. 3. Same as Fig. 1 but for the RR. The units are mm per 100 years

The most relevant result of the analysis of Fig. 3 is also most noticeable: Except relatively small areas along the Adriatic coast and Asia Minor, there is no statistically significant trend over the domain.

Finally, we present in Fig. 4 the trend analysis outcome for the Heavy Precipitation Days and Consecutive Dry Days.

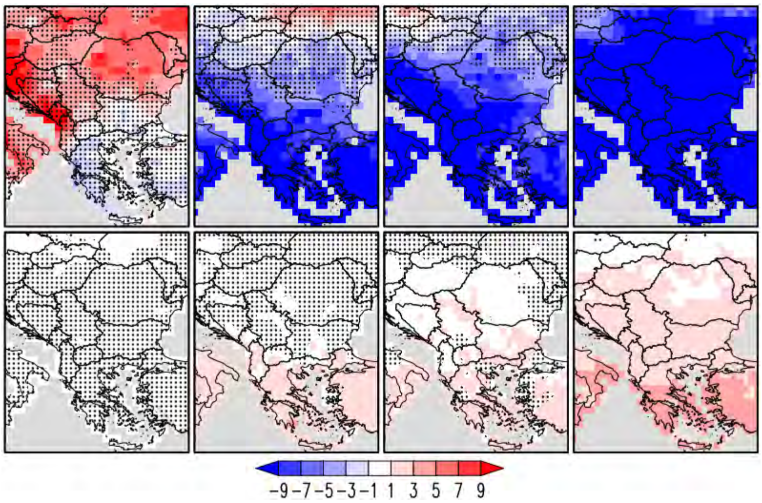

Fig. 4. Same as Fig. 1 but for the RR10 mm and CDD. The units are days per 10 years

The relatively big difference, even in sign, between the trend magnitude for RCP2.6 on one hand and all other three scenarios on the other, is the most notable outcome from the analysis of the RR10mm. The trend for RCP2.6 is prevailing positive (i.e., increase of the heavy precipitation days) and in the others – dominating negative. It should be kept in mind that RCP2.6 represents mitigation scenarios that aim to limit the increase of global mean temperature to less than 2 °C [15] and thus it is the only one RCP compatible with the goals of the Paris Agreement. It is worth emphasizing also that the long-term tendencies of some precipitation extremes could deviate from the course of evolution of the mean state [1].

The spatial distribution of the trend magnitude for CDD is consistent in all scenarios. The prevailing trend is positive (i.e., increase of the consecutive dry days) but, as a whole, is relatively weak and, subsequently, statistically significant over the bigger part of the domain only for RCP6.0 and RCP8.5.

5. Conclusion

Based on the availability of new sources of information representing the state of the art global climate change simulations in the frame of the CMIP5 project, which are freely accessible from the Copernicus Data Store, we present a trend analysis of key temperature and precipitation-based climate indices over Southeast Europe.

The study confirms the suitability of the database created from ISIMIP1 products for CIs-based analysis of the projected future climate in a computationally feasible way as has been already shown in [7, 8]. The most important outcome from the study is the notable expressed and spatially dominating positive trend (i.e., uprise tendency) of the warm-related indices and, vice versa, the negative trend of the cold-related indices. These tendencies are proportional to the radiative forcing and are, as a whole, statistically significant for the scenarios RCP4.5-8.5. The signal of the significant trends is spatially consistent as there are no areas of mixed trends within the considered domain. Generally, the revealed warming is, evidently, a continuation of already detected tendency in the historical records of the twentieth century over the region [3, 5, 18].

Concerning the precipitation-based indices, the study confirms the complexity of the expected precipitation-related changes and their inherent ambiguity. It is worth emphasizing also that the inter-model spread within the ensemble is bigger compared to the temperature-based CIs and has in some cases systematic character. Most essential in this regard is, however, the revealed absence of trend of the precipitation sum.

Finally, it has to be noticed that the projected increase of the CDD could amplify the negative impact of the expected hotter climate.

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HPC Simulations of the Present and Projected Future Climate of the Balkan Region

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Abstract. The forthcoming climate changes are the biggest challenge facing mankind today. They will exert influence on the ecosystems, on all branches of the international economy, and on the quality of life. The climate changes and their consequences have a great number of regional aspects, which global models cannot predict. That is why an operation plan for adaptation to climate changes has to be based on well-grounded scientific assessments, taking in consideration regional features of the climate changes and their consequences. The present work aims to give an overview of the high performance computing (HPC) facilities' implementation for studying of present and future regional climates of the Balkan region. Simulations were performed with the regional climate model RegCM on the supercomputer Avitohol of IICT – BAS. The global climate simulations, taken from HadGEM2 database were used as source for the initial and lateral boundary conditions. The simulations were performed for the following time slots: 1) 1975 – 2005 – reference period, 2) 2020 – 2050 – near future and 3) 2070 – 2099 – far future. The simulations for the future climate were carried out for 3 CMIP5 emission scenarios: RCP2.6 (optimistic scenario), RCP4.5 (realistic scenario) and RCP8.5 (pessimistic scenario). The simulation results for the reference period were compared with the independent, observation-based data set E-OBS. These preliminary simulation results reveal that the projected climate changes are strongest in the far future and RCP8.5. According to the temperature, the warming signal is spatially dominating with peak values the summer, when it is more than 4.5 °C. The projected precipitation change is more complex, both in time and space. It is worth emphasizing, however, that the expected summer months reduction, which could amplify the negative impact of the expected warmer climate.

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DEGREE-DAYS AND AGRO-METEOROLOGICAL INDICES IN PROJECTED FUTURE CLIMATE OVER SOUTHEAST EUROPE

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ABSTRACT

The present study analyzes the potential changes of residential heating and cooling degree-days as well as three stakeholder-relevant indices of agro-meteorological change (growing season length, sum of the active and sum of the effective temperatures) for Southeast Europe over near past (1975–2004), near (2021-2050) and far (2070–2099) future periods. All indicators were calculated from the output data of our simulations with the regional climate model RegCM driven by the ERA-Interim reanalysis for the near past and by the global circulation model HadGEM2-ES under RCP2.6 and RCP4.5 CMIP5 radiative forcing scenarios for the future periods. The validation of the model-based indices against their counterparts, computed from the observational dataset E-OBS, shows that the model reproduces the spatial variability and magnitude of the indices generally well. The study reveals a decrease of the heating degree days and considerable increase of the cooling degree days as well as increase of the agro-meteorological indices practically over the whole domain in the future. The detected changes, which agrees with most recent studies, are direct consequence of the expected general temperature tendencies in the region and intensify with the radiative forcing.

Keywords: Degree-days, Agro-meteorological indices, CMI5 RCPs, Regional Climate Simulations

INTRODUCTION

According to the high-level synthesis report of the United Nations, titled ’United In Science’ (https://public.wmo.int/en/resources/unitedinscience), the climate change is the defining challenge of our time. It will exert influence on the ecosystems, on all branches of the international economy, and on the quality of life. That is why an operation plan for adaptation to climate changes has to be based on scientifically well-grounded assessments, giving an account of regional features in the climate changes and their consequences [1]. The globally averaged surface temperature of the Earth increased 0.85°C over the 1880 to 2012 period. It is extremely likely that the observed warming of the climate system was caused by the increased anthropogenic emission of greenhouse gases [2]. The impacts of climate change are manifold and vary regionally, even locally,

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Sensitivity of the Simulated Heat Risk in Southeastern Europe to the RegCM Model Configuration—Preliminary Results

Vladimir Ivanov[1(✉)], Georgi Gadzhev[1], Kostadin Ganev[1], and Hristo Chervenkov[2]

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Abstract. The spatial distribution of the biometeorological conditions is a topic of many studies in different countries. One of the most important aspects of the weather adverse effect on the human beings is the consequences from too much exposure to the heat conditions. The human body can adapt to temperatures, but to some extent. If the air temperatures become too high, human beings at first feel uncomfortable, but the consequences can be a serious threat to health and even life. The main reasons for this threat are related to the lack of perspiration and cardiovascular problems. Atmospheric numerical models for simulating the heat stress is used in many studies. One of the most affected region in the near past, but also most likely in the future, is the Southeastern Europe, including Bulgaria. Global models are with too low resolution, but still they suggest very strong heat stress especially at the end of the 21th century. According to other studies, results from regional meteorological models suggest similar conclusions. The current research is about the heat stress conditions in the Balkan Peninsula, evaluated from ten–year simulations. They are performed with regional climate model RegCM. The model is run many times with different combinations of physics parameterization of some processes. The aim is to compare the heat stress simulated by different model configurations for the Balkan Peninsula and so to reveal the dependence of heat stress evaluation on the model configuration. That would answer the question of the sensitivity of the model to the parameterization schemes from a biometeorological point of view.

Keywords: Regional climate simulation · RegCM4.4 · Heat index · Heat stress · High performance computing

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Statistical Moments of the Vertical Distribution of Air Pollution over Bulgaria

Georgi Gadzhev(✉), Kostadin Ganev, and Plamen Mukhtarov

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Abstract. The air quality has a key impact on the quality of life and human health. The atmospheric composition fields are formed as a result of complex interaction of processes with different temporal and spatial scales from global to regional to a chain of local scales. The earth surface heterogeneities, including the complex terrain, have a very significant impact on the atmospheric dynamics, hence on the formation of air pollution pattern. The incredible diversity of dynamic processes, the complex chemical transformations of the compounds and complex emission configuration together lead to the formation of a complex vertical structure of the atmospheric composition. The detailed analysis of this vertical structure with its temporal/spatial variability jointly with the atmospheric dynamics characteristics can enrich significantly the knowledge about the processes and mechanisms, which form air pollution, including near earth surface. The present paper presents some results of a study, which aims at performing reliable, comprehensive and detailed analysis of the atmospheric composition fields 3D structure and its connection with the processes, which lead to their formation.

The numerical simulations of the vertical structure of atmospheric composition fields over Bulgaria have been performed using the US EPA Model–3 system as a modelling tool for 3D simulations and the system nesting capabilities were applied for downscaling the simulations from 81 km to 9 km grid resolution over Bulgaria. The national emission inventory was used as an emission input for Bulgaria, while outside the country the emissions are from the TNO high resolution inventory.

Keywords: Vertical structure · Air pollution · Atmospheric composition · Numerical simulation · High performance computing

1 Introduction

The parameters of the atmosphere have key impact on quality of life and human health. Because of this, quite naturally, the surface air quality is mostly studied. From the other hand the atmospheric composition fields are formed as a result

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HPC Simulations of the Atmospheric Composition Bulgaria's Climate (On the Example of Coarse Particulate Matter Pollution)

Georgi Gadzhev(✉), Kostadin Ganev, and Plamen Mukhtarov

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Abstract. The present work aims to provide an overall view of the HPC facilities implementation for studying the regional atmospheric pollution transport and transformation processes of Bulgaria. The study aims at revealing the main features of the atmospheric composition of Bulgaria climate and at tracking and characterizing the main pathways and processes that lead to atmospheric composition formation in the country.

The US EPA Models–3 system is chosen as a modeling tool. As NCEP Global Analysis Data with 1° resolution is used as a meteorological background, the nesting capacities of WRF and CMAQ are used to reduce simulations over Bulgaria to 9 km. The Bulgarian national inventory is applied within the territory of the country and the TNO emission inventory is used as emission input outside of Bulgaria. Special pre-processing procedures are created for introducing temporal profiles and speciation of the emissions.

The study is based on a large number of numerical simulations carried out day by day between 2007–2014. The simulations were performed on the supercomputer Avitohol of IICT–BAS. The following atmospheric composition characteristics will be demonstrated, on the example of the coarse particulate matter, and discussed in the Paper:

1) Seasonal and annual concentration field's pattern, with their typical diurnal course;
2) Evaluation of the contribution of different dynamic and transformation processes to the formation of the atmospheric composition of the country's climate;
3) Vertical structure of the atmospheric composition fields, considered from a point of view of dynamic and transformation processes interaction.

Keywords: Vertical structure · Air pollution · Atmospheric composition · Numerical simulation · High performance computing

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HPC Simulations of the Extreme Thermal Conditions in the Balkan Region with RegCM4

Vladimir Ivanov[1(✉)], Rilka Valcheva[2], and Georgi Gadzhev[1]

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Abstract. The outdoor environment influences human beings differently. If it is too cold for the organism, that could cause frostbite, freezing and other dangerous health conditions. On the other hand, if it is too hot, the heat stress could become too high, and consequences such as heat stroke, fainting, etc. could emerge. In either case, the outdoor environment could become deadly for humans. The climate changes impose an adaptation of the human individuals to the current and the future thermal conditions. The current research aims to study the risk of extreme heat and cold thermal stress on the Balkan Peninsula and some adjacent territories. For that purpose, we performed numerical simulations with the regional climate model RegCM4 for the period from 1975 to 2005. The initial and boundary conditions were taken from the HadGEM2 Earth System Model. The simulations were performed on the supercomputer Avitohol of IICT—BAS. We studied the extreme thermal conditions in the cold and the warm seasons with two different biometeorological indexes. The first one describes how cold the human individual feels in low temperatures and windy environment. The second one describes how hot the human being feels in high temperatures and humid conditions. The simulation results for the influence of the current climate on human beings are demonstrated in the paper.

Keywords: RegCM · Heat stress · Wind chill · Heat wave · HPC simulation · Climate

1 Introduction

The heat stress for human beings is one of the most important problems in modern society. There is a lot of research work addressing that problem and the need for mitigation activities towards decreasing the harmful impacts on the people. According to IPCC reports, the temperature is increasing at many locations in

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The Seasonal Recurrence of Air Quality Index for the Period 2008–2019 Over the Territory of Sofia City

Georgi Gadzhev

Abstract The impact of Air Quality (AQ) on human health and quality of life is an issue of great social significance. Evaluating this impact will provide a scientifically robust basis for elaborating efficient short term measures and long term strategies for mitigation of the harmful effects of air pollution on human health and quality of life. The AQ impact on human health and quality of life is evaluated in the terms of Air Quality Indices (AQI), which give an integrated assessment of the impact of pollutants and directly measuring the effects of AQ on human health. The objectives of the present work are evaluations in different years and for the different seasons in selected years, based on extensive computer simulations of the AQ for Sofia city carried out with good resolution using up-to-date modelling tools and detailed and reliable input data. Some extensive numerical simulations of the atmospheric composition fields have been performed recently. The US EPA Model-3 system was used as modelling tool. A fairly extensive data base was developed from simulations which were used for studies of the atmospheric composition and including the AQ climate. The simulations are for 12 years from 2008 to 2019 and calculated on five domains: Europe, Balkan Peninsula, Bulgaria, Sofia Municipality and Sofia City with increasing space resolution to 1 km for the territory of Sofia City.

Keywords Air quality indices · Air quality · Quality of life · Health risks

1 Introduction

The air is the living environment of human beings and, obviously, the atmospheric composition has a great importance for the quality of life and human health. Air Quality is a key element for the well-being and quality of life of European citizens. There is increasing evidence of adverse effects of air pollution on the respiratory

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Modelling of the Seasonal Sulphur and Nitrogen Depositions over the Balkan Peninsula by CMAQ and EMEP-MSC-W

Georgi Gadzhev and Vladimir Ivanov

Abstract The air quality US EPA models-3 system consisting of SMOKE—emission model and pre-processor, MM5—meteorological driver, and CMAQ—chemical-transport model, is used in many studies of the air quality in the Balkan Peninsula, and in particular Bulgaria. It runs in different model resolutions, depending on the domain, from European to city scale. The EMEP-MSC-W model is another chemical transport model, widely used in air quality modelling. Two of the processes involved in the concentration change of some pollutant are the dry and wet depositions. The air quality modelling capability depends on many factors, for example, meteorology and emissions. We study the differences in the simulation of the wet and dry depositions for Nitrogen and Sulphur compounds, between the CMAQ and the EMEP-MSC-W model for a period of 8 years.

Keywords Modelling · CMAQ · EMEP · Pollution · Composition · Air Quality

1 Introduction

The air pollution nowadays forces many countries to take actions for mitigating its adverse effects on human health. Therefore, we need a lot of information, which is increasing in recent years. There are already more direct and indirect data connected to the air quality from different surface-based and satellite-based observing systems. However, we need to understand the different processes involved in the creation, transportation, and transformation of the air pollutant species, which help us to understand their distribution at different spatial and temporal scales. The research community performs these tasks by air quality models systems, with chemical transport models as the main component [4–6]. We use one of these systems with the chemical transport model CMAQ, for modeling the air quality in the Balkan Peninsula. Previous results from air pollution modelling for the Balkan Peninsula and Bulgaria

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Environmental Protection and Disaster Risks

Selected Papers from the 1st International Conference on Environmental Protection and Disaster RISKs (EnviroRISKs)

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Assessment of the Joint Quantiles of Temperature and Precipitation in CMIP5 Future Climate Projections over Europe

Hristo Chervenkov, Georgi Gadzhev, Vladimir Ivanov, and Kostadin Ganev

Abstract The present study assesses the changes in the exceedances of the joint extremes of temperature and precipitation quantiles as well as the trend magnitude and statistical significance of these changes. Following the Beniston's idea, the combination of cool/dry, cool/wet, warm/dry and warm/wet modes in projected future climate over Europe up to the end of the twenty first century is investigated in consistent manner. These modes are defined as excedances of fixed quantile thresholds, the lower and the upper quartile respectively. The use of joint quantiles allows an exploration of climate statistics that in many instances would be overlooked by simply analyzing single thresholds of temperature or precipitation. The used for the computation of the quantiles data for the mean 10-day temperature and 10-day precipitation sum are obtained as ensemble multi-model median from the bias-corrected output of 5 CMIP5 global models, forced with all 4 RCP emission scenarios. The model output is accessed from the section of the Inter Sectoral Impact Model Intercomparison Project in the Copernicus Data Store. Generally, the obtained results are coherent with the consolidated outcomes of the most recent studies, considering the projected future changes of the mean temperature and the precipitation across Europe. Key finding is, however, the revealed steady and statistically significant increase of the number of the extreme warm and dry events over the whole Mediterranean basin.

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Degree-Days and Agro-meteorological Indices in CMIP5 RCP8.5 Future Climate—Results for Central and Southeast Europe

Hristo Chervenkov, Georgi Gadzhev, Vladimir Ivanov, and Kostadin Ganev

Abstract The present paper is continuation of our recent study and analyzes the potential changes of residential heating and cooling degree-days as well as three stakeholder-relevant indices of agro-meteorological change (growing season length, sum of the active and sum of the effective temperatures) for Central and Southeast Europe over near past (1975–2004), near (2021–2050) and far (2070–2099) future periods. All indicators were calculated from the output data of our simulations with the regional climate model RegCM driven by the ERA-Interim reanalysis for the near past and by the global circulation model HadGEM2-ES under RCP8.5 CMIP5 radiative forcing scenario for the future periods. The validation of the model-based indices against their counterparts, computed from the observational dataset E-OBS, shows that the model reproduces their spatial variability and magnitude generally well. A linear bias correction of the considered indices is also demonstrated. Consistent with the general trend of the mean and extreme temperatures over the region, the study reveals a decrease of the heating degree days and considerable increase of the cooling degree days and the agro-meteorological indices practically over the whole domain in the future. The detected changes are fairly not symmetrical - the relative increase of the cooling degree days is significantly bigger than the decrease of the heating degree-days.

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MODELLING OF DRY AND WET DEPOSITION PROCESSES FOR THE SULPHUR AND NITROGEN COMPOUNDS OVER BULGARIA

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***Abstract**: The quality of life is of big importance for human society. Atmospheric composition is one of the most important environmental components, which have a profound influence on human health and quality of life. That is why it is quite natural the surface air pollution concentrations to be most studied. The atmospheric pollution has great impact not only on quality of life, but on the environment as a whole. Therefore, it is important to study the atmospheric compounds dry and wet deposition. The present work is focused on the computer simulations of the dry and wet deposition of the Nx and Sx pollutants. The simulations are performed with the US EPA Models-3 System: Meteorological model WRF; Emission model SMOKE; Atmosphere Composition Model CMAQ for the period 2008 – 2014. The provided model simulations are with horizontal resolution 9 kilometers for the territory of Bulgaria. The NCEP Global Analysis Data meteorological background with 1°x 1°resolution is used as a meteorological background. The models nesting capabilities were applied to downscale the simulations to 9 km resolution. The TNO emission database for year 2005 is used as an input for the Models – 3 System. The model results are compared with the database computed from the EMEP MSC-W model, using a procedure for nudging the results of the 9 km CMAQ simulations, into the EMEP grid with 0.1° x 0.1° resolution.*

***Key words:** CMAQ, air quality, WRF, EMEP-MSC-W, EMEP, SMOKE, high-resolution, emission*

INTRODUCTION

The understanding of the air pollution distribution helps us to involve and improve mitigation measures for the human health. The Nitrogen and Sulphur compounds are the ones with adverse health effect on the living beings (Georgieva, 2014). Each of them is a subject on processes of transformation, creation and transportation, which affect their distribution in one or another territory, spatial and temporal scales. There are many observation data acquired by different kind of surface, elevated and satellite measurements. However, to understand their distribution in different spatial and temporal scales, we need to model them with the chemical-transport models. The research community uses different models for studying the air quality in Europe. Two of the most common ones are the CMAQ (Byun and Ching, 1999, Byun and Schere, 2006) and EMEP-MSC-W (Simpson, 2012), run in different temporal and spatial scales, as well as meteorological drivers. The air pollution modelling depends also on the specific emission sources used in the model configurations. The study deals with the air quality features over the territory of Bulgaria. Previous studies on that topic examine the surface concentrations (Chervenkov et al., 2005, 2006, 2008, Chervenkov, 2007) as well as their adverse effect on the human individuals in the country and the surrounding area. Different process determine the concentrations on different height levels - dry deposition, wet deposition, horizontal and vertical advection, horizontal and vertical diffusion, emission, chemical transformation, aerosol processes, and aqueous chemistry. The objective of that research is to study the differences in the high-resolution simulations with the CMAQ and the EMEP-MSC-W models of the Nitrogen (N) and Sulphur (S) dry and wet deposition processes for the territory of Bulgaria over the period 2008 - 2014.

METHODS

The processes accounting to the different contribution of the concentration field changes for each pollutant in the CMAQ model are: horizontal diffusion (HDIF); horizontal advection (HADV); vertical diffusion (VDIF); vertical advection (VADV); dry deposition (DRYDEP); emissions (EMISS); chemical transformations (CHEM); aerosol processes (AERO); cloud processes (CLOUD):

$$\Delta c_i^1 = (\Delta c_i^1)_{hdif} + (\Delta c_i^1)_{vdif} + (\Delta c_i^1)_{hadv} + (\Delta c_i^1)_{vadv} + (\Delta c_i^1)_{drydep} + +(\Delta c_i^1)_{emiss} + (\Delta c_i^1)_{chem} + (\Delta c_i^1)_{cloud} + (\Delta c_i^1)_{aero} \quad (1)$$

The mean concentration change of i^{th} pollutant in for the specific model layer from time t to time $t + \Delta t$ The solution of the transport and transformation equations gives (2)

$$\Delta c_i^1 = \frac{1}{h_1}\int_0^{h_1}\left(c_i(t+\Delta t) - c_i(t)\right)dz \quad (2)$$

The nitrogen depositions contains the contributions from NO_2 (Nitrogen dioxide), NO (Nitrogen oxide), NO_3 (Nitrogen trioxide), N_2O_5 (Dinitrogen pentoxide), HNO_3 (Nitric acid), HONO (Nitrous acid), ANH_4J (Accumulation-mode ammonium mass), ANH_4I (Aitken-mode ammonium mass), ANO_3J (Accumulation-mode nitrate mass), ANO_3I (Aitken-mode aerosol nitrate mass) and NH_3 (Ammonia). The S depositions contains the contribution from SO_2 (Sulphur dioxide), SULF (Sulphate aerosols), ASO_4J (Accumulation-mode aerosol Sulphate mass), and ASO_4I (Aitken-mode aerosol Sulphate mass).

The present work is focused on the computer simulations of the daily dry and wet deposition of the Nx and Sx pollutants with two chemical-transport model systems. The first one is the US EPA Models-3 System. It uses the meteorological model WRF as a driver (Shamarock et al., 2008), the emission preprocessor SMOKE (CEP, 2003, Houyoux and Vukovich, 2009), and MCIP3 as a Meteorology - Chemistry Interface Processor, and the CMAQ as a chemical-transport model. The provided model simulations have hourly time step with horizontal resolution 9 kilometers for the territory of Bulgaria for 2008 – 2014. The NCEP Global Analysis Data meteorological background with 1°x 1°resolution is used as a meteorological background. The models nesting capabilities were applied to downscale the simulations to 9 km resolution. The TNO emission database (Denier 2010) for year 2010 is used as an input for the Models – 3 System for the emission preprocessor. The second model system used for comparison with the previous one is with the Meteorological Synthesizing Centre-West (MSC-W) of the European Monitoring and Evaluation Programme (EMEP). It is a chemical transport model (Simpson et al., 2012), a key tool involving in the European air pollution policy assessments. The model has changed over the years, adding different features, and currently, his horizontal resolution ranging from 5 km to 1 degree with 20 vertical levels. In our study, we use a grid size 0.1° x 0.1°. The EMEP-MSC-W model runs with meteorological fields from the numerical weather prediction system ECMWF-IFS Cycle36r1. The model output is with daily frequency, so we do not need to do further post-processing. For comparison of the models, we use the Normalised Mean Bias noted in the text as NMB (5):

$$NMB = 100 * (\sum_I CMAQ - \sum_I EMEP)/(\sum_I EMEP) \quad (3)$$

RESULTS

The average winter dry nitrogen (N) depositions modelled by the CMAQ are higher and with more heterogeneous spatial structure than by the EMEP (fig. 1). The dry depositions from CMAQ have higher values on the mountain areas. The spatial distribution of the CMAQ total depositions has a structure with characteristics more similar to the dry depositions. The results show that the NMB has a spatial structure follow the topography. The lower terrain parts have lower NMB than the areas with higher elevation. We can see also, that there are three spots of the western part of the domain with a negative NMB. The NMB of the total depositions has similar spatial distribution as for the dry one, but the biases on the mountain and northeastern areas are smaller.

The CMAQ simulates higher average summer N dry as well as wet depositions than the EMEP_MSC_W (fig 2). The dry ones from the CMAQ output are relatively lower in the mountain areas. The wet depositions distribution is opposite. The spatial structure of the EMEP depositions is more homogeneous, as in the winter case. The NMB of the dry and total depositions have not distinctive patterns. The NMB of the wet deposition is negative in the lower terrain forms, and positive in the areas with higher elevation. The values are in the same range as in the winter depositions, except for the wet ones.

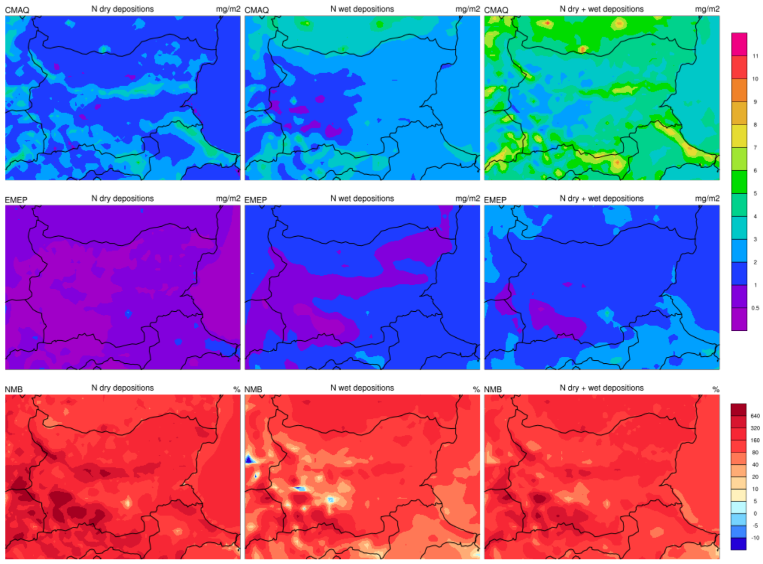

Fig. 1. Average daily dry CMAQ (first column, first row) and EMEP-MSC-W (first column, second row) Nitrogen winter depositions. Average daily wet CMAQ (second column, first row) and EMEP-MSC-W (second column, second row) Nitrogen winter depositions. Average daily total CMAQ (third column, first row) and EMEP-MSC-W (third column, second row) Nitrogen winter depositions. Normalized mean bias (third row) of the dry (first column), wet (second column) and total (third column) depositions.

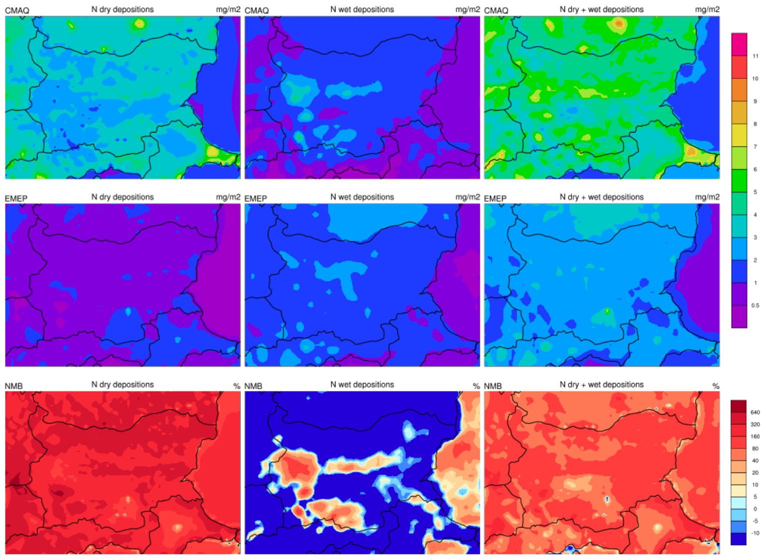

Fig. 2. Average daily dry CMAQ (first column, first row) and EMEP-MSC-W (first column, second row) Nitrogen summer depositions. Average daily wet CMAQ (second column, first row) and EMEP-MSC-W (second column, second row) Nitrogen summer depositions. Average daily total CMAQ (third column, first row) and EMEP-MSC-W (third column, second row) Nitrogen summer depositions. Normalized mean bias (third row) of the dry (first column), wet (second column) and total (third column) depositions.

The spatial distribution of the winter Sulphur (S) depositions is given in the fig. 3. The CMAQ dry S depositions are higher in the mountain and eastern areas, with four spots with values above 9 mg/m^2. The the winter S wet depositions are higher in the southeast. The CMAQ total depositions are distinctively higher in the southeast and the most northern areas. The NMB is mostly positive, with spots of negative values with bigger areas for the wet depositions.
The results for the summer S depositions are given in the fig. 4. The dry ones from the CMAQ are smaller than in the winter, and the EMEP ones do not change so much for that season. The CMAQ wet depositions are higher in the mountain areas. The spots with distinctively higher values are modelled in the western parts of the country by the CMAQ, and in the central by the EMEP-MSC-W. The total

emissions repeat and combine these patterns. The NMB does not follow the topography. There are more areas of NMB with negative values, than in the winter, especially for the wet S depositions.

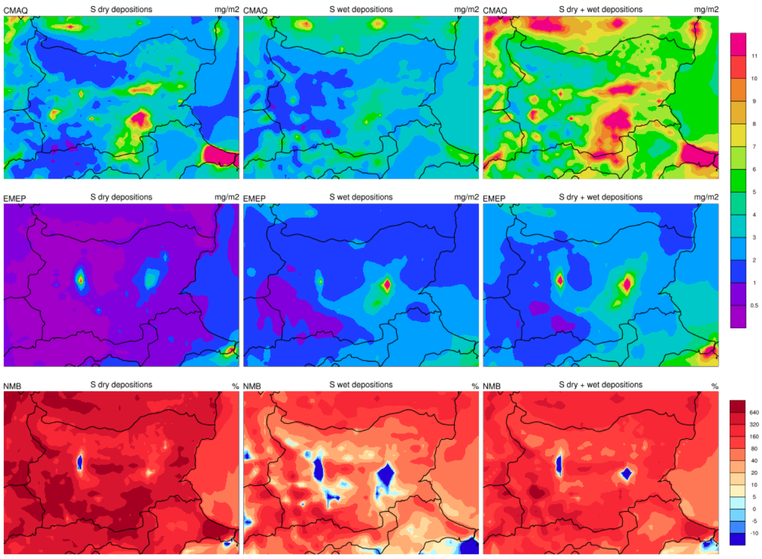

Fig. 3. Average daily dry CMAQ (first column, first row) and EMEP-MSC-W (first column, second row) Sulphur winter depositions. Average daily wet CMAQ (second column, first row) and EMEP-MSC-W (second column, second row) Sulphur winter depositions. Average daily total CMAQ (third column, first row) and EMEP-MSC-W (third column, second row) Sulphur winter depositions. Normalized mean bias (third row) of the dry (first column), wet (second column) and total (third column) depositions.

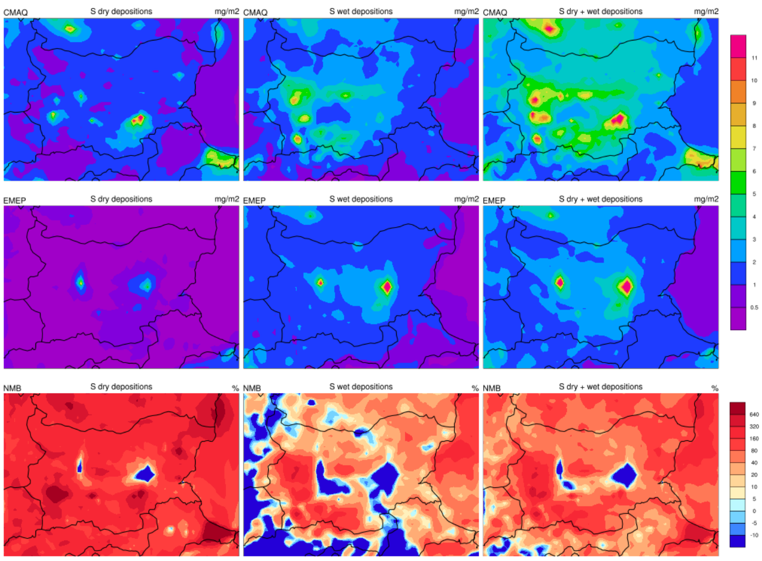

Fig. 4. Average daily dry CMAQ (first column, first row) and EMEP-MSC-W (first column, second row) Sulphur winter depositions. Average daily wet CMAQ (second column, first row) and EMEP-MSC-W (second column, second row) Sulphur winter depositions. Average daily total CMAQ (third column, first row) and EMEP-MSC-W (third column, second row) Sulphur winter depositions. Normalized mean bias (third row) of the dry (first column), wet (second column) and total (third column) depositions.

CONCLUSION

The results show that the output Nitrogen and Sulphur dry depositions of the WRF-MCIP3-CMAQ configuration are higher than the ones from the EMEP-MSC-W model configuration. That statement is valid also for the wet depositions, but to a lesser extent. Three factors determine the simulated differences. The first one is the topography, as we the results shows. The second one is the emission inventory. It implies a difference in the initial conditions for the dry and wet depositions between the two systems. The other main factor is the different meteorology drivers used in the CMAQ and EMEP-MSC-W, which together with the topography features increase or decrease the wet depositions on more or less areas.

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Computer Simulations of Air Quality and Bio-Climatic Indices for the City of Sofia

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Abstract: Air pollution is responsible for many adverse effects on human beings. Thermal discomfort, on the other hand, is able to overload the human body and eventually provoke health implications due to the heat imbalance. Methods: The aim of the presented work is to study the behavior of two bio-climatic indices and statistical characteristics of the air quality index for Sofia city—the capital of Bulgaria for the period 2008–2014. The study is based on the WRF-CMAQ model system simulations with a spatial resolution of 1 km. The air quality is estimated by the air quality index, taking into account the influence of different pollutants and the thermal conditions by two indices, respectively, for hot and cold weather. It was found that the recurrence of both the heat and cold index categories and of the air quality categories have heterogeneous space distribution and well manifested diurnal and seasonal variability. For all of the situations, only O_3 and PM_{10} are the dominant pollutants—these which determine the AQI category. It was found that AQI1, AQI2, and AQI3, which fall in the "Low" band, have the highest recurrence during the different seasons, up to more than 70% in some places and situations. The recurrence of AQI10 (very high) is rather small—no more than 5% and concentrated in small areas, mostly in the city center. The Heat index of category "Danger" never appears, and the Heat index of category "Extreme caution" appears only in the spring and summer with the highest recurrence of less than 5% in the city center. For the Wind-chill index category, "Very High Risk" never appears, and the category "High Risk" appears with a frequency of about 1–2%. The above leads to the conclusion that both from a point of view of bioclimatic and air quality indices, the human health risks in the city of Sofia are not as high.

Keywords: air quality; outdoor thermal comfort; air quality index; heat index; wind chill; Bulgaria; Europe

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1. Introduction

The air is the living environment of human beings, and obviously, a number of atmospheric parameters, have great importance for the quality of life and human health. Some of the most important groups of characteristics of the atmosphere directly affect quality of life and human health.

The air quality (AQ) is a key element for the well-being and quality of life of European citizens. According to the WHO, air pollution severely affects the health of European citizens [1] (between 2.5 and 11% of the total number of annual deaths are due to air pollution [2]). There is considerable concern about impaired and detrimental air quality conditions over many areas in Europe, especially in urbanized areas, in spite of about 30 years of legislation and emission reduction. Current legislation (e.g., ozone daughter directive 2002/3/EC and the recent directive 2008/50/EC for AQ and clean air for Europe [3,4]) requires informing the public on AQ, assessing air pollutant concentrations throughout the whole territory of Member States and indicating an exceedance of limit and target values, forecasting potential exceedance, and assessing possible emergency measures to abate exceedance using modelling tools.

Despite international—including European—agreements and protocols regarding different constituents of air pollutants (sulfur dioxides, nitrogen dioxides, organic compounds, heavy metals, etc.), decreasing pollution and accumulated knowledge have only a partial effect. The situation is especially severe regarding ozone in urban areas. The main reasons for this are the increased emissions of ozone precursors (basically nitrogen dioxide and organic compounds).

Special attention is paid to primary emitted or secondary formed particulate matter. They have the property to adsorb various chemical compounds on their surface, including some toxic substance (heavy metals, black carbon, and organic hydrocarbons), NH_3, NO_x and VOCs, mutagens, DNA modulators, etc., and interacting with them or catalyzing the processes taking place between these compounds, contribute to the formation of secondary atmospheric pollutants—other aerosol components that are difficult for quantitative determination. The particulate matter classification is based on aerodynamic diameters. Since 1990 began, the separation of particulates in several major fractions: PM_{10} (Particulate matter with a diameter < 10 μm), $PM_{2.5}$ (Particulate matter with a diameter < 2.5 μm), and ultrafine particulate matter with a diameter < 0.1 μm (PM_{01}). Particulate matters enter the body by the respiratory system and, depending on their size, are fractionalized in its different sections. The particles with a diameter below 2.5 μm reach pulmonary alveolus, where, along with the adsorbed compounds on their surface, they may fall in pulmonary macrophages, respectively, in the whole body, and generate harmful effects on human health. The established strong association between the increased incidence of respiratory, cardiovascular, and neoplastic diseases, the reduced life expectancy, and air pollution, on the other hand, define the latter as a significant public health issue. [5–8]. A number of studies conducted in Bulgaria also confirm the link between air pollution and human health, mostly in regions having serious environmental problems [9–12].

A number of parameters of the near-surface atmosphere (temperature, humidity, radiation, wind speed, pressure) jointly form an important bioclimatic characteristic of the habitable human environment. The condition when there is no strain on the human thermoregulatory system is called thermal comfort. When the air temperatures are high, the person should take additional precautions because of the emergence of dangerous health conditions as hyperthermia, cramps, sunburn, sunstroke, and even death [13]. Higher humidity could decrease or stop perspiration, and it is the main additional factor impeding the human thermoregulatory system from reaching balance. In cold weather, there is a possibility of hypothermia. In that case, the main additional factor for worsening the health conditions is the stronger wind, which increases the convection from the human body, hence its cooling. The temperature of the uncovered parts in particular, and eventually, the body's core temperature decrease. A number of studies [14–17] present different methods for the calculation of the discomfort index and evaluating the role of thermal comfort on the quality of life and human health. More extensive reviews of the existing discomfort indices can be found in [18–23]

More sophisticated methods for the calculation of Discomfort Indices, taking into account additional factors, such as wind speed and solar radiation, are also available. Predicted Mean Vote—PMV [24] and Physiologic Equivalent Temperature—PET [25] are based on the human heat balance model [26–30]. These methods account for the total heat effect due to all the physical factors that affect the human body's thermal sensation using the human heat balance equation. This equation uses, as an input, the ambient temperature, wind speed, relative humidity, and mean radiant body temperature under different man actions and clothes. For the purpose of our study, we choose two indexes—heat index [31–33] and wind chill index [34,35]. They are relatively simple, and do not require using many meteorological and physiological parameters that could be not readily available, and that add some uncertainty. They are numerical values in several intervals, called categories, each of which correspond to a different degree of deviation from comfort. They are used to study the extreme heat and cold conditions in Bulgaria from observations [36–38] and southwestern Europe from model simulations [39]. One of the aims of that research is to study the recurrence of the hot and cold conditions with different degrees of severity in the Sofia city region—the capital of Bulgaria—by two indices—heat index and wind chill.

It has been found that extremely high temperatures cause a bigger morbidity risk and higher mortality. Urban areas are especially at risk because the urban microclimate is relatively warmer than the surrounding non-urban environment, a phenomenon called "Urban heat island".

The motivation of the present study is that Sofia is the largest city in Bulgaria with a large population and intensive urban transport and a large number of industrial and other sources of pollution; therefore, the study of the influence of atmospheric parameters on the quality of life in the city is of particular importance. Estimates of the AQI have been made before, but never with this resolution and they have never been combined with estimates of bioclimatic indices.

The objectives of the present study are to perform reliable, comprehensive, and detailed studies of the impact of lower atmosphere parameters and characteristics on the quality of life and health risks for the population in the city of Sofia by applying an appropriate and up to date methodology. Thus, the formulated study objectives contain several keywords, which have to be explained.

Methodology: This is the totality of metrics for the evaluation of the atmospheric parameters' impact on the quality of life and health risks for the population; a set of properly chosen, well verified, and validated models of atmospheric dynamics and chemical composition; databases; and a set of appropriately defined scenarios for extensive computer simulation experiments.

Reliable and comprehensive studies: This means carrying out extensive and appropriately enough defined numerical experiments to form statistically significant ensembles of output data, which reflect the diversity of meteorological conditions with their typical recurrence and that allow reliable conclusions to be made for the atmospheric characteristics' impact on population quality of life and health risks.

Detailed studies: This means a high enough spatial/temporal resolution of the computer simulations, which reflects the multi-scale nature of the processes. This makes it possible to detect the interactions of different scale phenomena and track the basic mechanisms and pathways through which low atmosphere characteristics are formed, respectively, that impact on population quality of life and health risks.

2. Materials and Methods

The AQI evaluations are based on extensive computer simulations of the AQ in Sofia, carried out with good resolution, using up-to-date modeling tools, and detailed and reliable input data [40–49].

All the simulations are based on the US EPA Model-3 system:

WRF v.3.4.1 [50]—Weather Research and Forecasting Model, used as a meteorological pre-processor. The large scale (background) meteorological data used in the present study are the NCEP global analysis data with $1^\circ \times 1^\circ$ resolution—in Grib2 format every six hours [51]. The configuration set uses the WSM 6-class graupel microphysical parameterization scheme [52], and CAM schemes for parameterization of the longwave and shortwave radiation [53]. The land-surface parameterization scheme is Pleim-Xiu [54]. The planetary boundary layer parameterization scheme is ACM2 (Pleim) [55]. The model uses USGS 24-category land cover (Figure 1b), with one category describing the surface properties of urbanized areas.

CMAQ v.4.6—Community Multi-scale Air Quality model [56,57], the Chemical Transport Model (CTM).

SMOKE—the Sparse Matrix Operator Kernel Emissions Modelling System [58], the emission pre-processor of Models-3 system.

TNO inventory [59] is exploited for the territories outside Bulgaria in the mother CMAQs domain. For the Bulgarian domains, the National inventory, as provided by Bulgarian Executive Environmental Agency, is used.

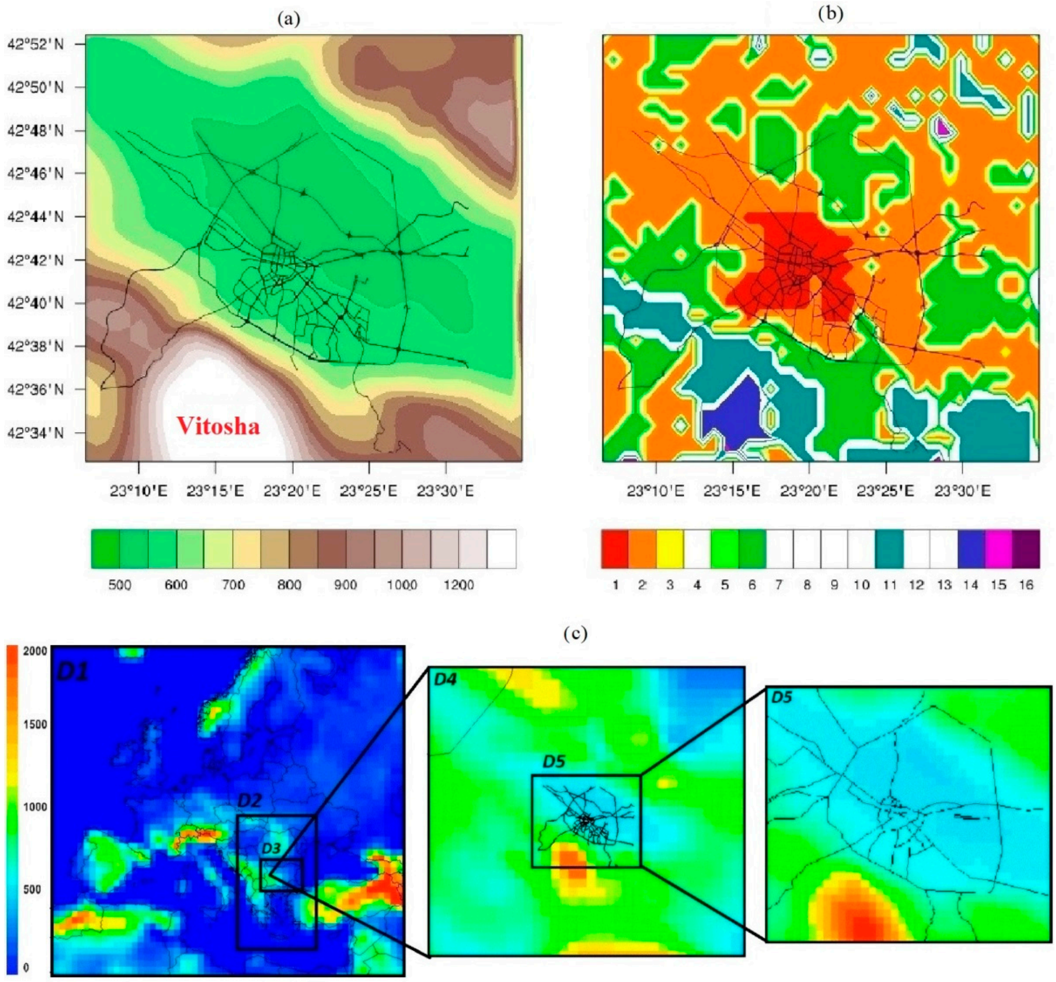

Figure 1. Domain elevation in (m) (**a**). Land cover (**b**) categories: 1—Urban and Built-up Land; 2—Dryland Cropland and Pasture; 3—Irrigated Cropland and Pasture; 5—Cropland/Grassland Mosaic; 6—Cropland/Woodland Mosaic; 11—Deciduous Broadleaf Forest; 14—Evergreen Needleleaf; 15—Mixed Forest; 16—Water Bodies. Elevation (m) of five nested domains (**c**).

The simulations are carried out for the following five nested domains: D1 (Europe)—81 × 81 km, D2 (Balkan peninsula)—27 × 27 km, D3 (Bulgaria)—9 × 9 km, D4 (Sofia municipality)—3 × 3 km, and D5 (Sofia city)—1 × 1 km (Figure 1c). WRF nesting capabilities are applied for downscaling the simulations to a 1-kilometer step for the innermost domain (Sofia). The simulations are performed with Two-Way Nesting mode on.

CMAQ meteorological input is created from the WRF output, exploiting the CMAQ meteorology-chemistry interface—MCIP, v3.6. CMAQ simulations were performed in D2, D3, D4, and D5 domains. The CMAQ pre-defined (default) concentration profiles are used as boundary conditions for (the coarsest domain) D2. The boundary conditions for the inner domains are determined through the nesting capabilities of CMAQ.

The validation of WRF model and the Models 3 system was previously performed. The validation of WRF is presented in [60] and the validation of the whole system in [61].

The WRF and CMAQ output are recorded each hour; therefore, all frequencies (recurrences) considered below are calculated on an hourly basis.

For calculation of the bio-climatic indices, we use the air temperature and relative humidity at 2- and 10-meter wind speed from numerical simulations of the bio-meteorological conditions with the WRF-ARW model for the Sofia city for the 2008–2014 period with a spatial resolution of 1000 m.

One of the most commonly used indices is the UK Daily Air Quality Index [62], also used in Bulgaria [40–42,63]. According to [63], 4 main pollutants—O_3, NO_2, SO_2, and

PM_{10}—are used to calculate the AQI. The further considerations in the paper are made on the basis of long-term AQ simulations, which make it possible to reveal the climate of AQI spatial/temporal distribution and behavior. The AQI is defined in several segments, different for each considered pollutant. Different averaging periods are used for different pollutants. The breakpoints between index values are defined for each pollutant separately (Table 1). For each particular case, the concentration of each pollutant falls into one of the bands shown in Table 1. Thus, the AQI for each pollutant is determined. The overall AQI, which describes the impact of the ambient pollutant mix, is defined as the AQI for the pollutant with maximum value of the index.

Table 1. Boundaries Between Index Points for Each Pollutant.

INDEX	O_3	NO_2	SO_2	PM_{10}
	μg/m³	μg/m³	μg/m³	μg/m³
1	0–32	0–95	0–88	0–21
2	33–66	96–190	89–176	22–42
3	67–99	191–286	177–265	43–64
4	100–126	287–381	266–354	65–74
5	127–152	382–477	355–442	75–86
6	153–179	478–572	443–531	87–96
7	180–239	573–635	532–708	97–107
8	240–299	636–700	709–886	108–118
9	300–359	701–763	887–1063	119–129
10	>360	>764	>1064	>130

Each of the AQI bands comes with advice for at-risk groups and the general population (Table 2). The reference levels and Health Descriptor used are based on health-protection-related limits, targets, or guideline values set by the EU, at a national or local level, or by the WHO [1].

Table 2. Air Quality Indices and health effect description.

Banding	Value	Health Descriptor
Low	1–3	Effects are unlikely to be noticed even by individuals who know they are sensitive to air pollutants
Moderate	4–6	Mild effects, unlikely to require action, may be noticed amongst sensitive individuals.
High	7–9	Significant effects may be noticed by sensitive individuals and action to avoid or reduce these effects may be needed. Asthmatics will find that their "reliever" inhaler is likely to reverse the effects on the lung.
Very High	10	The effects on sensitive individuals described for "High" levels of pollution may worsen

The spatial and temporal behavior of the air quality index for the city of Sofia is defined as all simulations are presented as the sum of each index in each band—Low, Moderate, High, and Very High. The AQI from the "Low" band indicate the cleanest air. Therefore, high values of the recurrence of AQI from the "Low" band mean more hours with clean air. Small values of the recurrence of AQI from the "Low" band, respectively, mean more hours with not so clean air. In the other Moderate, High, and Very High categories, high values indicate more cases with polluted air, and low—more cases with clean air.

The heat index is defined as the temperature a human individual in a real environment would feel in a reference one having certain values of the effective wind speed (2.57 m/s, vapor pressure (1.6 kPa), and barometric pressure (101.3 kPa), as well as zero extra radiation and no clothing [32]. There are other indices such as Universal Thermal Climate Index and Physiological Equivalent Temperature, that allow the solar and terrestrial radiation, and other clothing and physiological parameters to be taken into consideration, but the dependence of the calculation on mean radiant temperature from diffuse radiation, and dependence on other types of parameters such as metabolic rate, bring an additional uncertainty in their calculation. Additionally, the heat index and wind chill index are used in forecasts in many countries including Switzerland, USA, Canada, and Bulgaria, and people became used to them by changing their behavior for adaptation, which, in turn, influences the potential for heat and cold stress. The heat index is composed of a multiple regression formula, valid in air temperatures of at least 26.6 °C and relative humidity above 40%. The results of the heat index (HI) are split for the spring, summer, and autumn, because of the possibility of hot conditions even in the transition seasons. It is in temperature units. It is calculated and presented in categories shown in Table 3. Due to their low recurrence, the Danger and Extreme Danger conditions are combined in one category —Danger. It is calculated according to [31–33] with the following regression formula:

$$HI = -42.379 + 2.04901523 * T + 10.14333127 * RH - 0.22475541 * T * RH$$
$$- 0.00683783 * T^2 - 0.05481717 * RH^2 + 0.00122874 * T^2 * RH$$
$$+ 0.00085282 * T * RH^2 - 0.00000199 * T^2 * RH^2$$

where temperature and heat index are in °F, and the RH is in %. As Fahrenheit scale is not very popular in Bulgaria, all the temperature values are converted to degree C.

If the air temperature is below 26.6 °C and the relative humidity is below 40%, we use the air temperature as a heat index. The wind chill index [34] is studied for winter, spring, and autumn because these are the times when it is possible for these categories to be observed. It is reported in temperature units and is used as a wind chill temperature (WCT) with categories given in Table 4 [35]. The categories Very High Risk, Severe Risk, and Extreme Risk are combined in one category—"Very High Risk", for the same reasons as in for the Danger and Extreme Danger heat index.

Table 3. Heat index categories and health effects.

Heat Index Category	Numerical Interval	Health Precautions
Caution	26.7–32.2 °C	Fatigue is possible with prolonged exposure and activity. Continuing activity could result in heat cramps.
Extreme Caution	32.2–40.5 °C	Heat cramps and heat exhaustion are possible. Continuing activity could result in heat stroke.
Danger	40.5–54.4 °C	Heat cramps and heat exhaustion are likely; heat stroke is probable with continued activity
Extreme Danger	≥ 54.4 °C	Heat stroke is imminent

The wind chill index is defined in temperatures lower than or equal to 4.4 °C and wind speeds of at least 1.34 m/s. The wind chill index is calculated with the following formula [34]:

$$WCT = 13.12 + 0.6215 * T\alpha - 11.37 * V^{0.16} + 0.3965 * T\alpha * V^{0.16}$$

where *Ta* is the air temperatures in °C, and *V* is the wind speed in km/h. It is valid for temperatures below 4.4 °C (40 °F) and a wind speed equal to or above 1.34 m/s (3 mph). If the values of the air temperature and wind speed are outside the valid intervals, we accept that the WCT is equal to the air temperature.

Table 4. Wind chill index categories and health effects.

Wind Chill Category	Numerical Interval	Health Precautions
Light Risk	0–−9 °C	Slight increase in discomfort.
Moderate Risk	−10–−27 °C	Uncomfortable. Risk of hypothermia and frostbite if outside for long periods without adequate protection.
High Risk	−28–−39 °C	High risk of frostnip or frostbite. Exposed skin can freeze in 10 to 30 min; Check face and extremities for numbness or whiteness; High risk of hypothermia if outside for long periods without adequate clothing or shelter from wind and cold.
Very High Risk	−40–−47 °C	Very high risk of frostbite; Exposed skin can freeze in 5 to 10 min; Check face and extremities for numbness or whiteness; Very high risk of hypothermia if outside for long periods without adequate clothing or shelter from wind and cold.
Severe Risk	−48–−54 °C	Severe risk of frostbite; Exposed skin can freeze in 2 to 5 min; Check face and extremities frequently for numbness or whiteness; Severe risk of hypothermia if outside for long periods without adequate clothing or shelter from wind and cold.
Extreme Risk	≤−55 °C	DANGER! Exposed skin can freeze in less than 2 min; Outdoor conditions are hazardous.

3. Results

3.1. Air Quality Indices

The annually averaged fields of recurrence of days with a certain air quality index are presented in Figure 2. In the "Low" category, the areas with a low air quality status are mainly the city's ring road and busier transport routes, as well as the central parts, and they occur most in the morning hours. It is also observed in the "Moderate" band, early in the morning, with about a 20–30% recurrence of days with polluted air. In the afternoon in this category, there is pollution over Vitosha Mountain, which is probably due to the turbulent transport of ozone from higher levels in a turbulent atmosphere. The ozone in Bulgaria is largely due to transport from abroad [64]. This is one of the reasons, together with the ozone photochemistry reactions, why the ozone concentrations early in the morning are smaller than at noon (less intensive transport from higher levels) [40–42].

The graphs present the diurnal course and seasonal distribution of the average recurrences (in %) for the different pollution indices (from 1 to 10) for the territory of Sofia (Figure 3), as well as for different selected points of the city—Orlov Most (the city center) and Bistrica (a village in the surroundings of Sofia) (Figures 4 and 5).

Figure 3 shows that the indices AQI1, AQI2, and AQI3, which fall in the "Low" band, have the highest recurrence during the different seasons. The diurnal course of these indices is well defined. In the morning, AQI1 and AQI2 have a recurrence of about 40–50%, and, at that time, AQI3 has a minimum recurrence. In the spring and summer, in the afternoon, AQI4 has a peak with a recurrence of about 10%. In all the seasons, the other indices have an insignificant recurrence with about 5% repeatability.

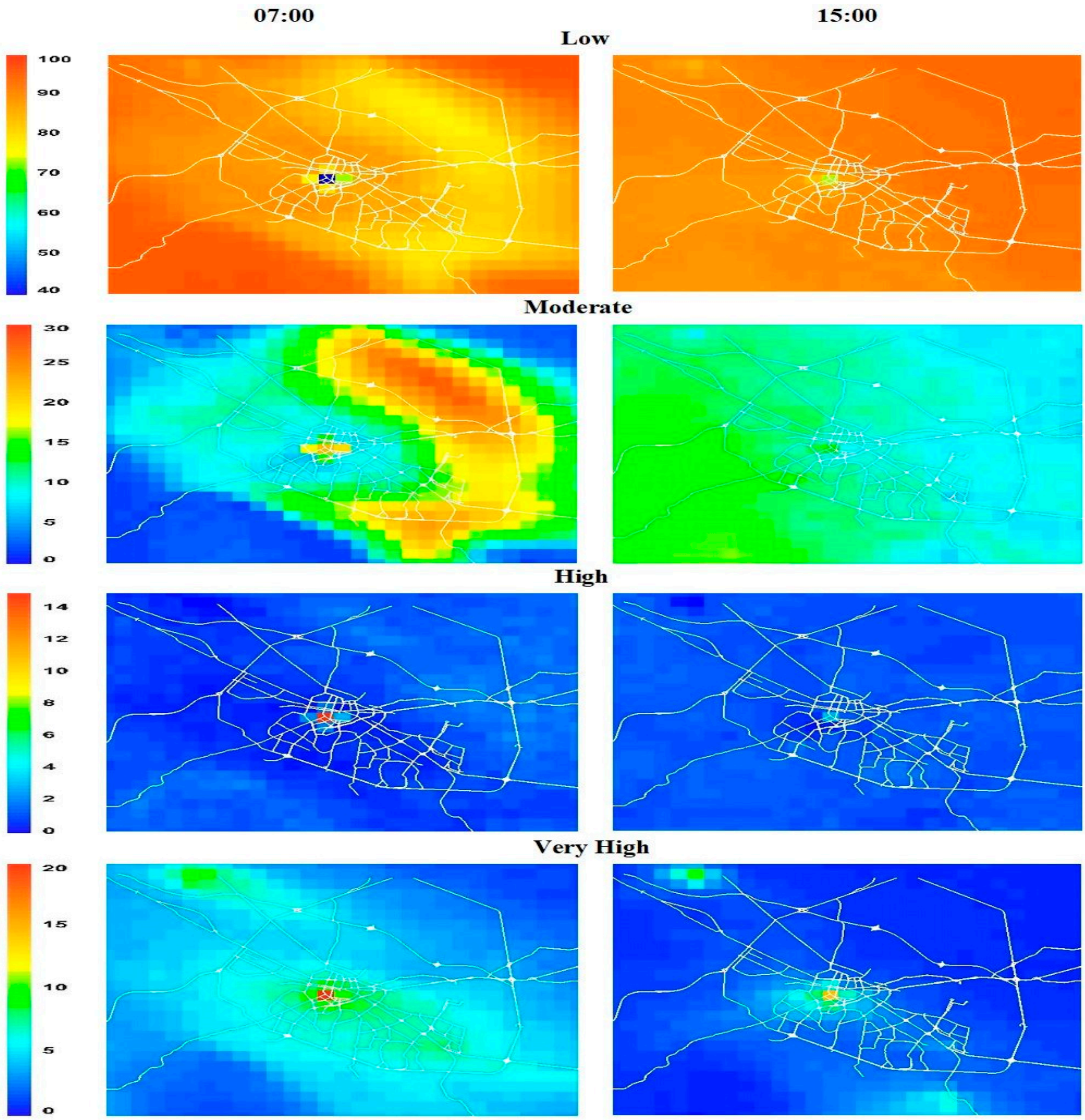

Figure 2. Annual recurrences (in %) of the AQI for the band Low, Moderate, High, and Very High for the territory of Sofia city.

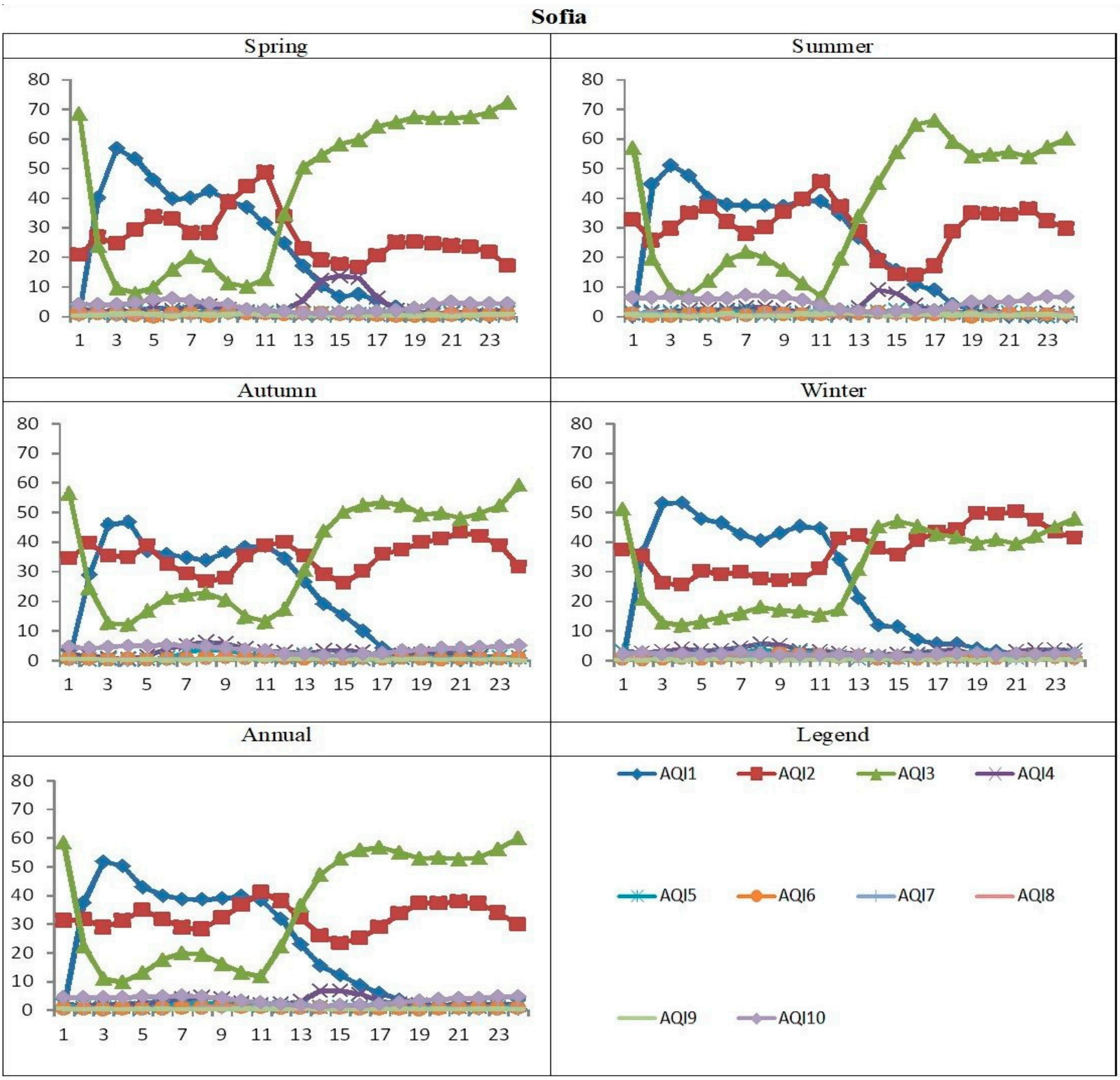

Figure 3. Average recurrence (in %) of the different indices (from 1 to 10) for the territory of the city of Sofia.

Figure 4 for the Orlov Most point shows that the indices AQI1, AQI2, and AQI3, which fall in the "Low" interval, have the greatest recurrence during the different seasons. The diurnal course of these indices is well defined. In the morning, AQI1 and AQI2 have a recurrence of about 40%, and in the afternoon, it drops to about 20%. At this time, AQI3 has a minimum recurrence in the morning and a maximum in the afternoon of about 50%. AQI4 has an afternoon maximum of about 10% in the spring and summer. In all the seasons, AQI10 stands out, which corresponds to the "Very High" category and, for this point, has a high repeatability of about 10%.

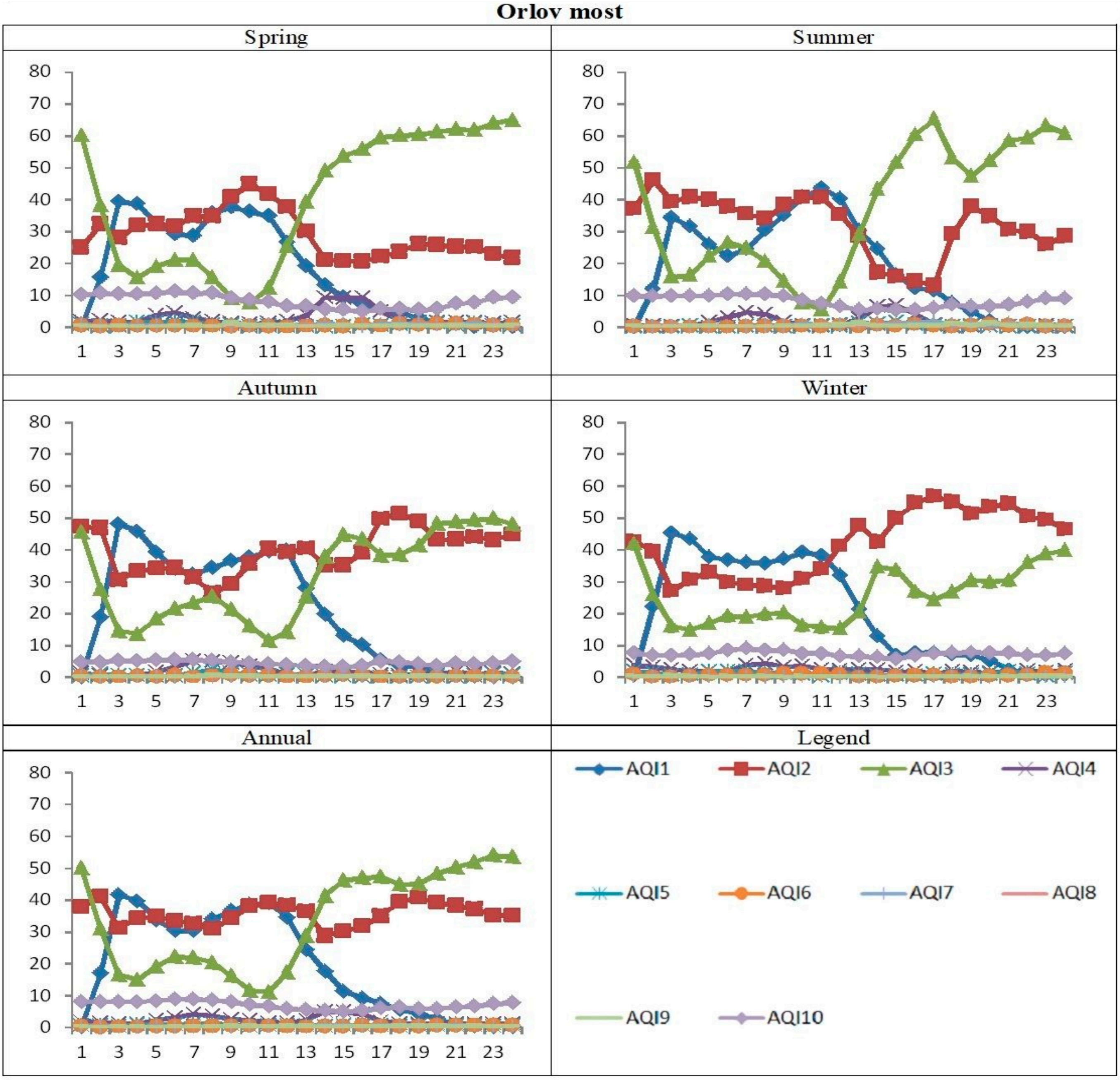

Figure 4. Average recurrence (in %) of the different indices (from 1 to 10) for the Orlov Most (Sofia).

Figure 5, for the Bistritsa point, shows that the indices AQI1, AQI2, and AQI3, which fall in the "Low" interval, have the greatest recurrence during the different seasons. The diurnal course of these indices is well defined. In the morning, AQI1 and AQI2 have a recurrence of about 40%, and in the afternoon, it drops to about 20% during the warm months and back distribution during the cold months. At this time, AQI3 has a minimum recurrence in the morning and a maximum in the afternoon of about 50%. AQI4 has an afternoon high of about 10% in the spring. In all the seasons, AQI10 stands out, which corresponds to the "Very High" category and, for this point, has a recurrence of about 5% in the morning in all the seasons.

The diurnal and seasonal variability of the AQI is obviously due to both diurnal and seasonal changes of traffic and heating, as well as of the boundary layer dynamics (see for example [65]).

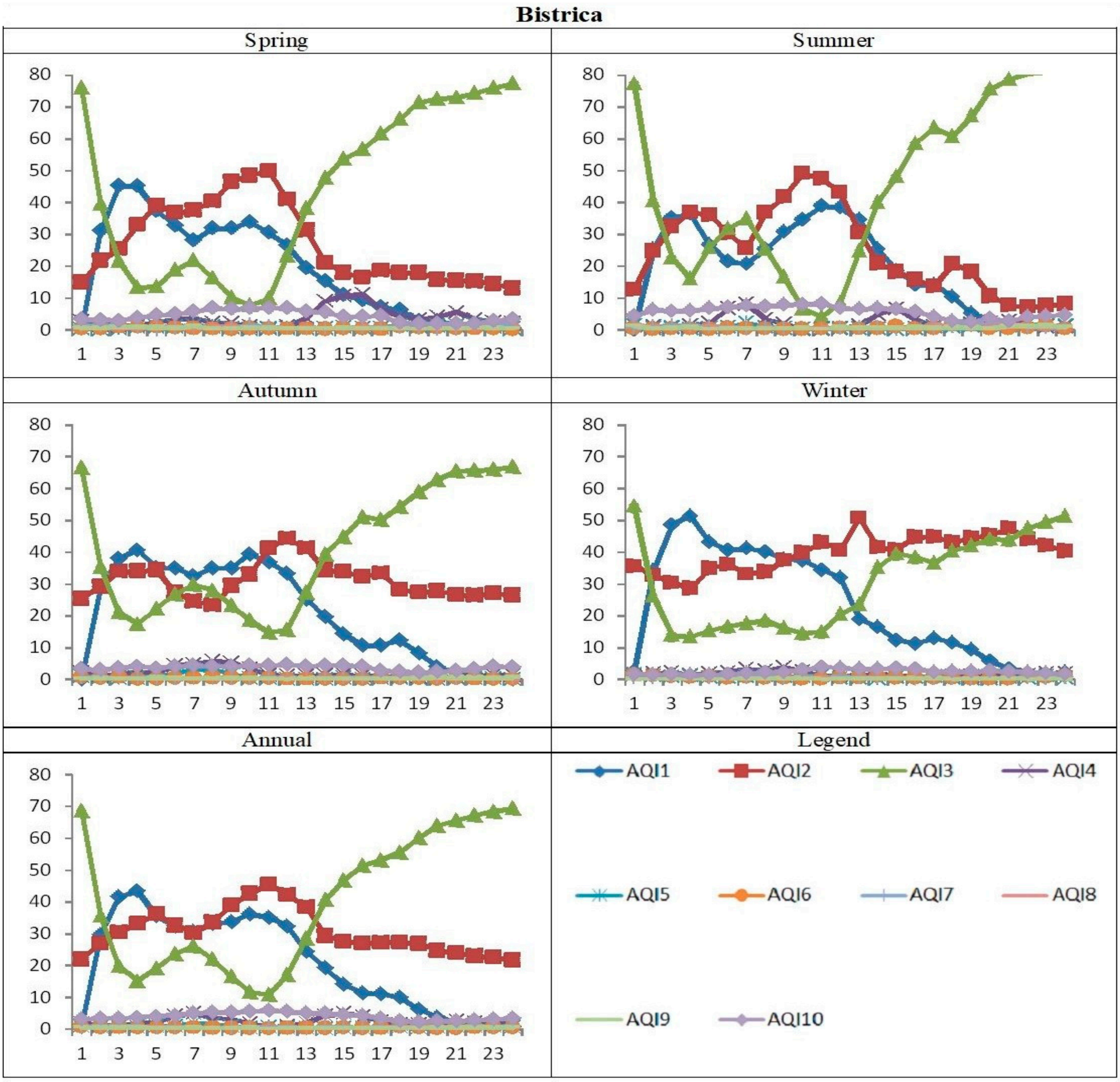

Figure 5. Average recurrence (in %) of the different indices (from 1 to 10) for the Bistrica.

3.2. Bio-Climatic Indices

The simulation results show that the distribution of the frequency of different HI categories is more diverse only in summer (Figure 6). The Caution cases were mostly between 0 and 1% and 1 to 2% in part of the more populated city area. There was no Extreme Caution in the autumn. That season, however, is characterized by more areas with Caution cases between 1 and 2%. During the summer, the probability of the health index "Caution" conditions is higher and has a more complex horizontal distribution. The central city parts had 10 to 15%. The percentages are between 5 and 10 in the other territories of the city limits and Sofia Valley as a whole and decrease with an increasing altitude. The spatial distribution of the Extreme Caution conditions in that season is more homogeneous, similar to the spring and autumn ones. There are no cases of Danger and Extreme Danger conditions over the three seasons, and the Extreme Caution conditions absent in the autumn. Therefore, the weather was not as extreme in the autumn as in the spring.

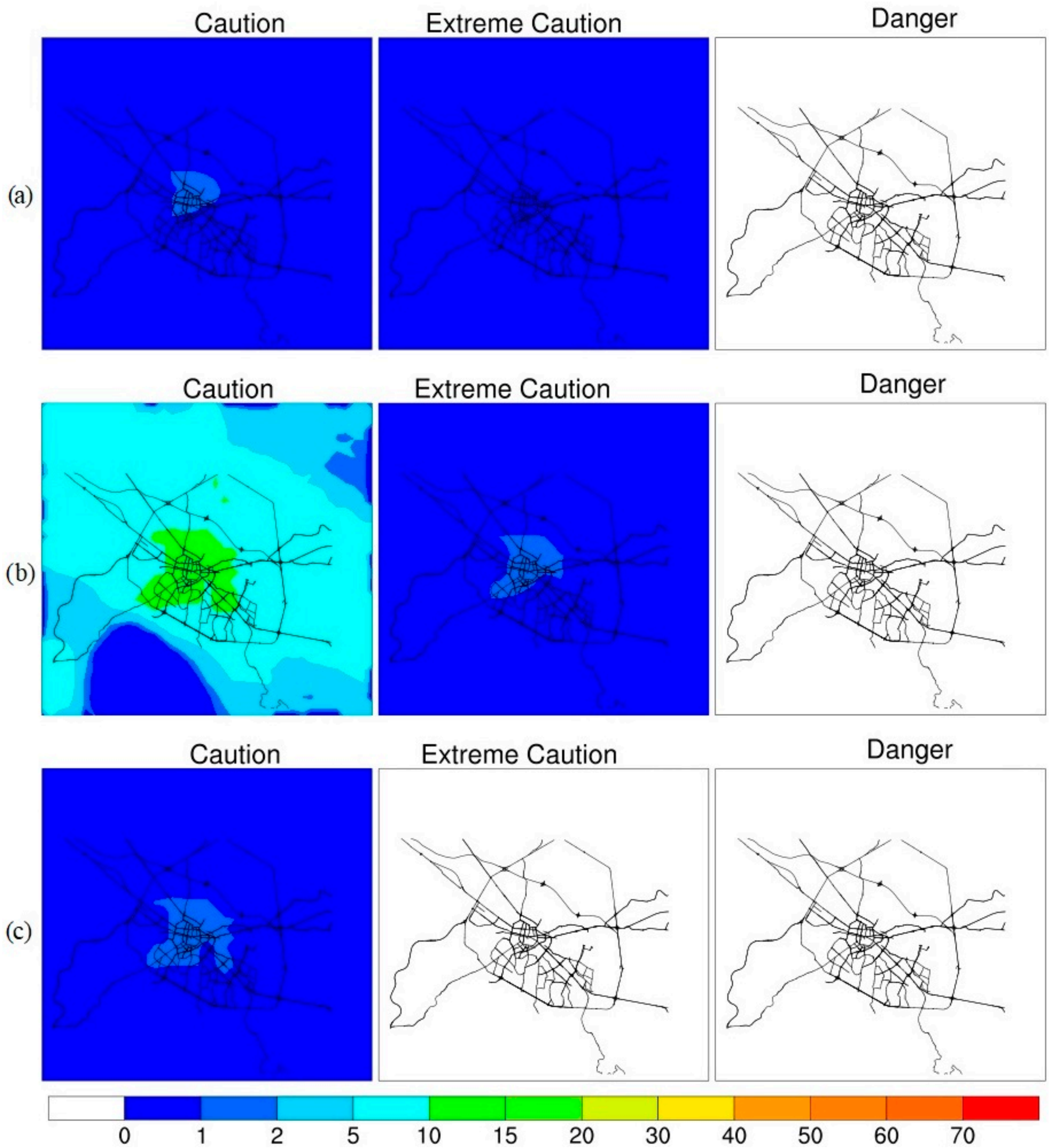

Figure 6. Frequency (in %) for (**a**) spring, (**b**) summer, and (**c**) autumn of the Heat index categories in the Sofia region during the spring (first row), summer (second row), and autumn (third row).

The simulated wind chill categories over the winter and spring are Light Risk, Moderate Risk, and High Risk, and only Light Risk and Moderate Risk in the autumn (Figure 7). In most of the domain, 5 to 10% of cases were categorized as Light Risk, and this increased up to 40% in higher altitudes. The winter Moderate Risk cases were mostly between 1 and 2%, up to 10% at Vitosha Mountain. The winter Light Risk percentages were from 50 to 60, with some spots below 50%. The Moderate Risk cases follow the terrain height with 10 to 15% in the Sofia Valley, increasing up to 30% in the mountainous areas and 50% at Vitosha Mountain. The spatial distribution of the percentages with Light Risk during the spring has almost the same pattern. The Moderate Risk cases in the spring also follow the terrain height. The percentages are between 1 and 2% in the Sofia Valley, increasing to 5% in higher altitudes and 20% at Vitosha Mountain. The autumn Moderate Risk is up to 1%, except at Vitosha Mountain. There are High Risk cases only in the winter and spring.

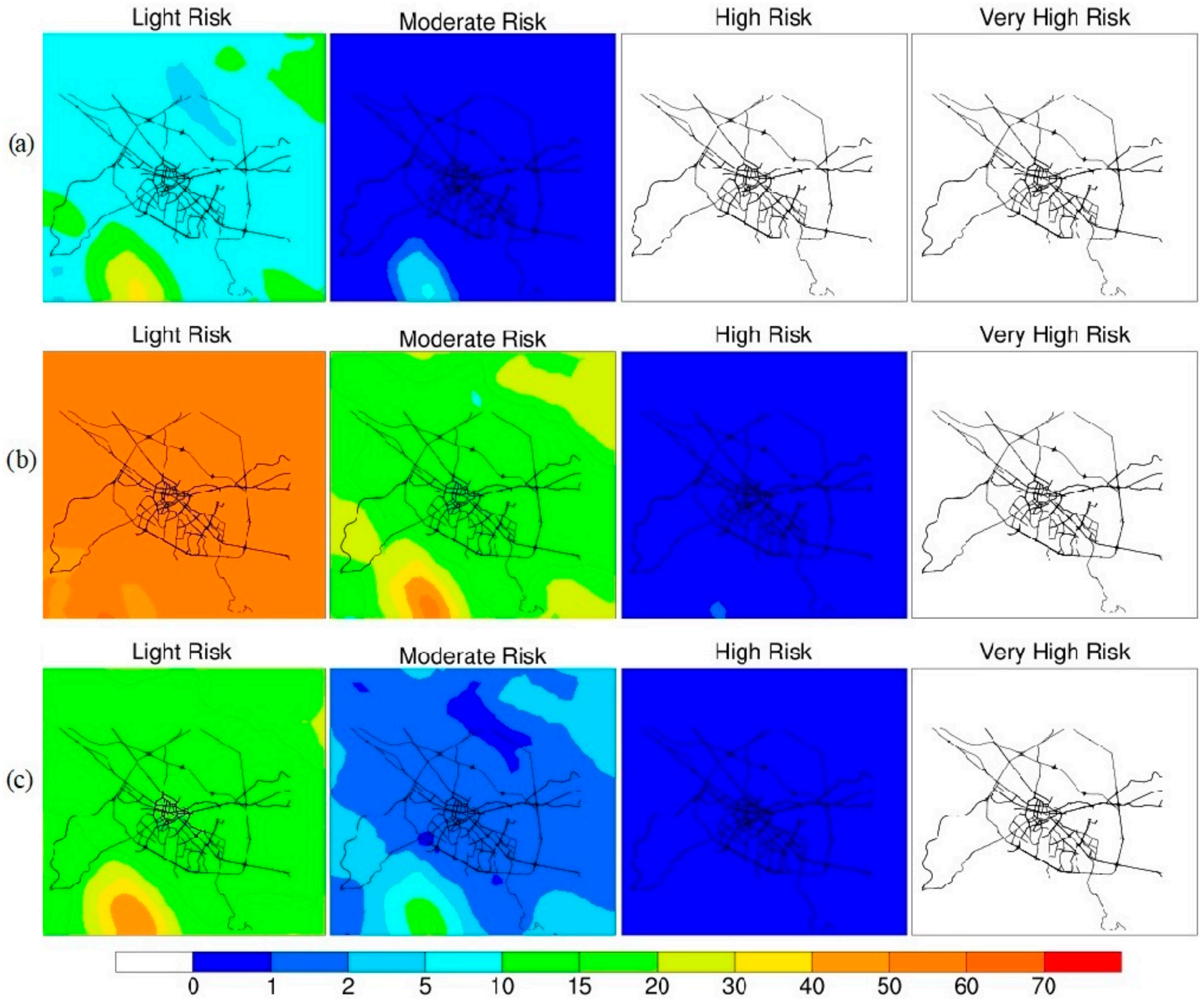

Figure 7. Frequency (in %) for (**a**) autumn, (**b**) winter, and (**c**) spring of the Wind chill categories in the Sofia region during the spring (first row), summer (second row), and autumn (third row).

Usually, the air temperatures in the warm and cool seasons are highest at or after noon, which draws our interest to study the frequency of the HI categories at 12 UTC (14 EET or 15 EEST). Their spatial distribution, shown in Figure 8, implies the following inferences. The summer, as the hottest season, has the highest number of Caution cases and is the only one with Extreme Caution cases. The frequency of Caution conditions is up to 20% in the mountainous areas, between 20 and 30% in the Sofia Valley, and between 40 and 50% in most of the Sofia city limits. The Extreme Caution category is presented only during that season, with below 1% in most of the domain and 5 to 10% in the more populated area of the city. The autumn percentages are between 5 and 10% in the central city parts, from 2 to 5% in the outer ones, and below 2% in the mountainous areas. The spatial distribution during the spring is kind of similar, but the percentages are smaller with 1 to 5%.

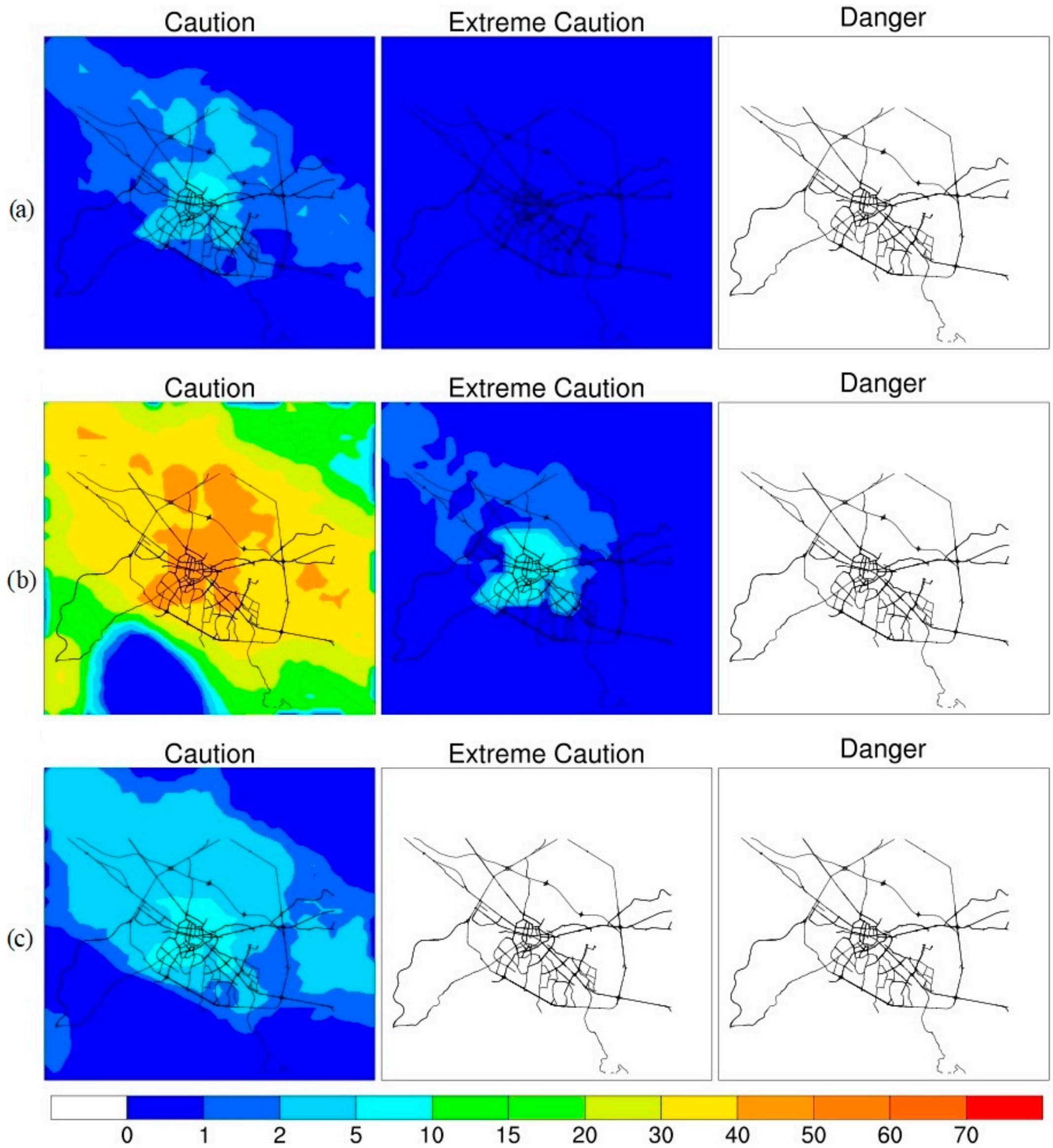

Figure 8. Frequency (in %) for (**a**) spring, (**b**) summer, and (**c**) autumn of the Heat index categories "Caution" (first column), "Extreme caution" (second column), and "Danger" (third column) in the Sofia region at 12 UTC during the spring (first row), summer (second row), and autumn (third row).

The human's daily life regime implies that it is interesting to study the wind chill index during the early morning and evening hours. The simulated WCT categories at 06 UTC are presented in Figure 9. Only the first two categories are presented in the autumn. The percentages of Light Risk are between 10 and 15% in the central city and mountainous areas. The Sofia Valley ones are smaller, with 5 to 10%. The Moderate Risk conditions are bigger than 1% only at Vitosha Mountain. The winter Light Risk percentages are from 50 to 70%, higher in the Sofia Valley. The Moderate Risk conditions in that season are between 20 and 30% in part of the city limits and mountainous areas, and lower in the other parts of Sofia Valley. Vitosha Mountain, as the highest terrain, is above 50%. The spring Light Risk frequency distribution is similar to the winter Moderate Risk, but the percentages are about 5% smaller, and there are only three little city spots with higher ones. The spring Moderate Risk percentages are 2 to 5% in most of the domains, except Vitosha Mountain and some places around the city. The winter and spring Moderate Risk conditions are below 1%.

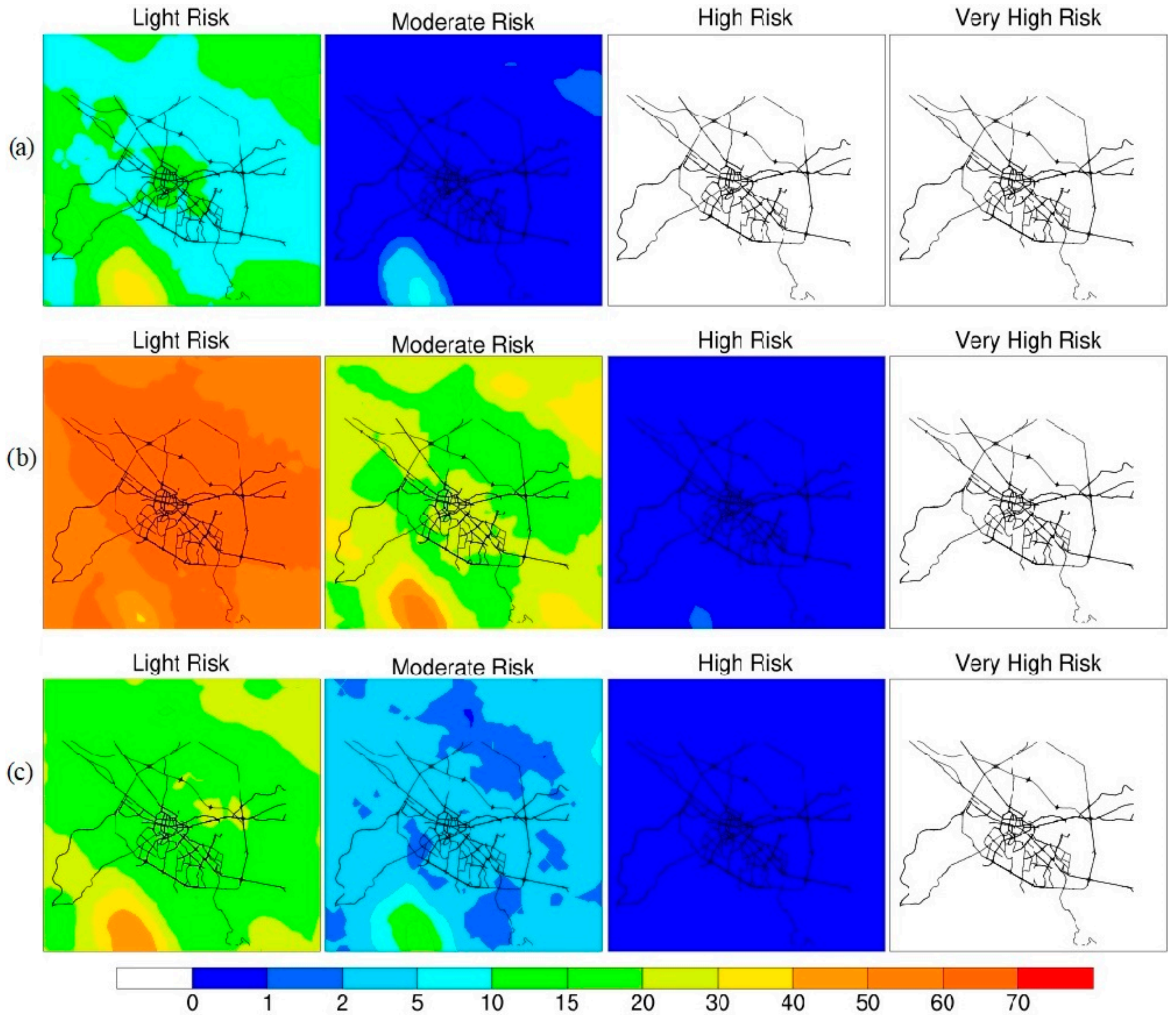

Figure 9. Frequency (in %) for (**a**) autumn, (**b**) winter, and (**c**) spring of the Wind-chill index categories "Low risk" (first column), "Moderate risk" (second column), and "High risk" (third column) in the Sofia region at 06 UTC during the autumn (first row), winter (second row), and spring (third row).

The spatial distribution of the frequencies of the wind chill categories at 15 UTC is shown in Figure 10. The Light Risk conditions in the three seasons are smaller than the ones in the 06 UTC. The autumn Light Risk frequencies are between 1 and 2% in most areas of the city limits, increase to between 2 and 5% in the Sofia Valley, and are higher in the mountainous areas. The winter percentages are mostly between 40 and 50, and the spring ones between 5 and 10%, except at Vitosha Mountain. The Moderate Risk during the transition seasons is mostly below 1% and up to 15% at Vitosha Mountain. The winter ones are 2 to 10% in the Sofia Valley and higher in the higher altitudes around, especially, the Vitosha mountain, where they reach up to 50%. The High-Risk cases are simulated only in the winter and spring.

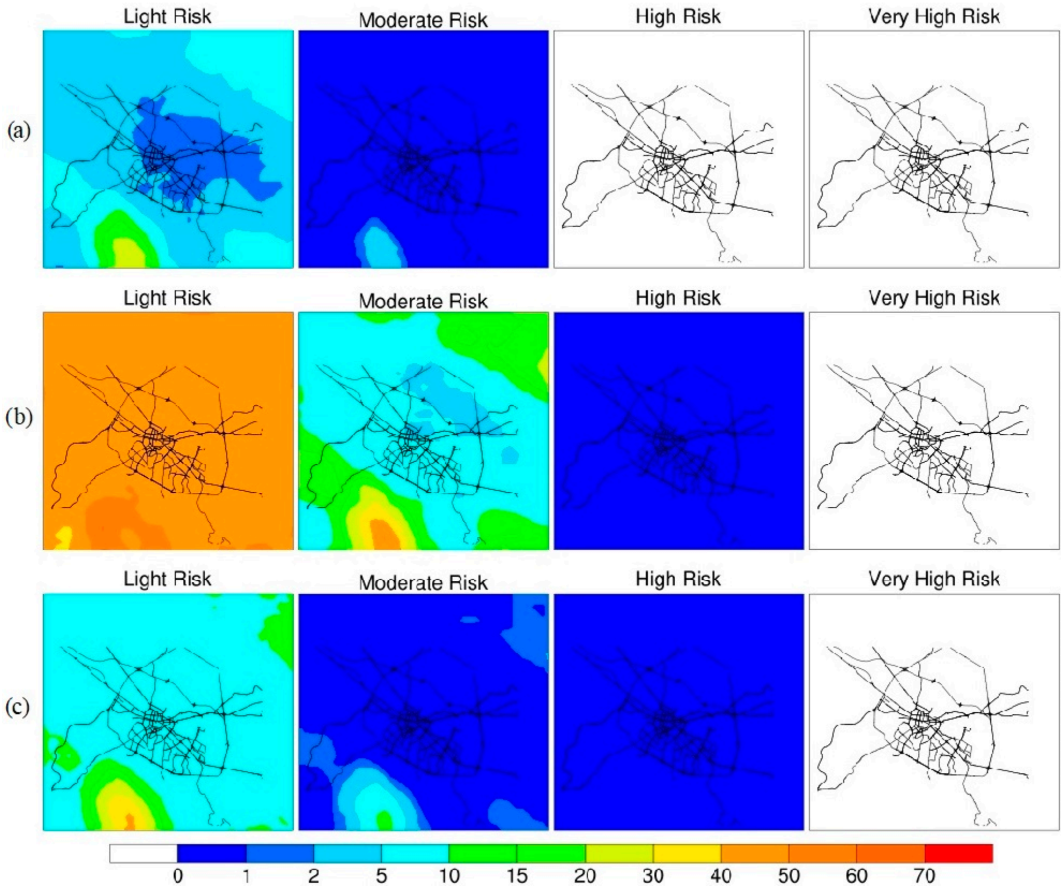

Figure 10. Frequency (in %) for (**a**) autumn, (**b**) winter, and (**c**) spring of the Wind-chill index categories "Low risk" (first column), "Moderate risk" (second column), and "High risk" (third column) in the Sofia region at 15 UTC during the autumn (first row), winter (second row), and spring (third row).

4. Discussion

The Sofia city simulations show that Sofia's air quality status (evaluated with a spatial resolution of 1 km) falls mostly in the Low and Moderate bands, but the recurrence of cases with High pollution is close to 10%, mostly at the city center. The recurrence of indices AQI2 and AQ3 (Low range) is different during the day, and it reaches 40% over the whole city territory. The recurrence of AQI2 is about 40% in the morning hours and cold months and about 50% at noon and in the afternoon. A high AQI3 recurrence can be seen in afternoon hours, at about 60% in hot months, and 20% in cold months. The AQI4 has a high recurrence at noon. The cases with bad AQ reach 10% over the selected points. The AQI10, which presents the Very High band, shows a recurrence of about 5–10% during the whole day, all the seasons, and for all points.

The pollution in the city is probably due to the surface sources such as road transport and the TPPs in the city [66]. Apart from these general features, the climatic behavior of the AQI probabilities is rather complex, with significant spatial, seasonal, and diurnal variability. The areas with a slightly worse AQ status are not necessarily linked to the big pollution sources. Wide rural and even mountainous regions can also have a significant probability for AQI from the Moderate range.

The hot spot in Sofia city, where the high-value indices have a higher recurrence, is in the city center. That is quite natural, because the dense population and street network and most intensive road transport in the city center generate very high pollution emissions. The Very High band recurrence is relatively high—about 10%, especially in cold months, where the atmosphere is usually stable and the turbulence transport of aloft pollution is hampered.

Generally, the adverse heat conditions in the Sofia city region reach up to 15% of cases. The summer frequency of conditions for fatigue decreases gradually with the increasing altitude from the city center to the Sofia Valley and mountainous areas. On the other hand, the transition seasons simulations show a more homogeneous distribution of the possibility for that health effect, with more cases in the most urbanized parts (Figure 1). The possibility for heat cramps and heat exhaustion is higher, mainly in the city during the summer. The spatial distributions for 12 UTC are more complex, and the differences between the lower and higher altitudes are more emphasized, possibly due to the higher temperatures at that time. The higher frequencies for fatigue, heat cramps, and heat exhaustion in the urban territories (Figure 1), in comparison to the other ones, are also more pronounced. Generally, the results from the simulation show higher frequencies in the most urbanized territories (Figure 1) and lower ones in higher altitudes. It should be kept in mind that the USGS land use categorization does not account for the urban trees; therefore, the strong cooling effect of urban trees [67] is not simulated in the present study.

The winter slight discomfort is almost the same in the whole domain. It changes with the elevation (Figure 1) in the transition seasons, with a higher frequency in the higher altitude areas. The risk of hypothermia in winter and spring also shows the increasing frequency with altitude. The risk of hypothermia during the autumn, as well as the risk of freezing in the winter and spring, are almost in the same frequency interval. The slight discomfort conditions in the 06 UTC show a little more complex picture, expressing a higher similarity with the changing of the elevation (Figure 1). The spatial distribution of the frequency of the risk of hypothermia, however, shows an opposite behavior—the distribution in 06 UTC is not as complex and similar to the elevation changes (Figure 1) as the whole one. The wind chill severity is highest in the 06 UTC than in the 15 UTC.

5. Conclusions

The areas with a low and partly those with a moderate air quality index are mainly the city's ring road and busier transport routes, as well as the central parts, and they occur most in the morning hours. The Moderate pollution in the afternoon over Vitosha Mountain is due to ozone, the origin of which can be the photochemical reactions of nitrogen oxides from sources in the city and also the turbulent transport of ozone from higher levels in a turbulent atmosphere. The air quality index bands for locations in Sofia city and Bistritsa with the greatest contribution recurrence are AQI1, AQI2, and AQI3. The AQI3 index recurrence has a maximum in the afternoon hours in the spring and summer, and morning ones for other seasons and annually. The AQI1 and AQI2 recurrences are higher in the morning hours.

We suggest that at least two factors could play a role in these features of the bioclimatic indices. The first one is the normal changing of the temperatures with the changes in altitude. The second one is the urban heat island effect, manifested as higher temperatures in the urban area (Figure 1) than in the rural and suburban ones, due to the higher absorption and re-emitting radiation because of smaller green and water body areas. The conditions of slight windchill discomfort and risk of hypothermia during 2008–2014 for transition seasons and winter increase their frequencies in mountainous areas. Still, it is not always valid for the city limits and the Sofia Valley.

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BULGARIAN EMERGENCY RESPONSE SYSTEM FOR RELEASE OF HAZARDOUS POLLUTANTS - DESIGN AND FIRST TESTS

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Abstract

The present paper demonstrates some preliminary results of the set up and testing of a system for modelling of toxic air pollution due to possible accidents in industrial sites. The study is carried out in the frame of the NATO SfP N 981393 project, which aims at providing means for efficient control and protection of population exposure in case of accidental release of hazardous chemicals due to a terrorist attack or an industrial accident.

Risk assessment for the region of „Vereja Him" factory, Jambol, Bulgaria is performed. The modelling tool used for this study is US EPA Models-3 System: WRF, CMAQ and SMOKE (partly). The CB05 toxic chemical mechanism, including chlorine reactions, is used. The "regular" emission input exploits the high-resolution TNO emission inventory with tendency to make use of local data.

The meteorological pre-processor WRF is driven by NCAR Final Reanalysis data. Applying the nesting abilities of the Models-3 System the problem is downascaled to a resolution of 1km for the area surrounding the„ Vereja Him" site, where 25 tons of chlorine are released two times daily (03 and 15 UTC), and separate calculations are performed for every release.

The shown numerical results very well demonstrate the good performance of the models and the practical value of the preparedness mode of the planned emergency response system.

Key words: *air pollution modelling, US EPA models-3 system, toxic gases, emergency response, grid computing*

1. INTRODUCTION

Governmental agencies and institutions that are responsible for emergency management have always been concerned about accidental releases from industrial facilities and nuclear power plants. During the past few years there is also a growing concern that future terrorist activities may involve the release of chemical, biological and/or nuclear (C/B/N) material.

The Balkan region is economically the least developed part of Europe, which, for a significant part of the population, results in poverty. Some of the countries in the region are also fields of serious ethnic and/or religious confrontation. Additionally, there are a lot of industrial enterprises in the region (chemical or power plants), which may turn into powerful sources of toxic pollutants after an industrial accident or a terrorist attack. They may cause significant damages to human health and environment in the region.

For emergency management, the adage "It's better to do something than nothing" is not true since the wrong response can be very costly and potentially as dangerous as the threat itself. Scientific and technical information is critical for helping emergency managers to make sound decisions with regards to response to critical threats (National Research Council, 2005). The Balkan Peninsula is a region with complex topography, which causes significant disturbances of the air flows. These mesoscale disturbances may have a great influence not only on the local pollution transport and hence on the detailed pollution pattern, but also on the trans-boundary transport of harmful substances. Using simplified approaches and tools for the calculation of the atmospheric dispersion would inevitably lead to inappropriate response to the threat.

The present work expected results of course could not prevent such events, but will supply the authorities, the relevant international organisations and the public with information, which will make possible proper measures for diminishing the damages, caused by accidental harmful releases in the atmosphere, to be planned.

As stated above the planned modelling system will have the potential to assist emergency managers in three stages:

- In preparedness mode, "risk analysis" will be performed. It will result in a set of risk assessments for different emergency scenarios for selected "hot spots". These assessments can be of a direct use for the relevant national bodies in the Partner countries for developing strategies for immediate emergency response (for example evacuation of people from the pollution exposed regions, proper assignment of medical teams) in order to minimize the pollution impact on human health. They will give valuable information for optimisation of the air quality monitoring network.
- In the operational mode the system will produce an approximate evaluation of the location and amount of the harmful releases in the atmosphere and make a fast short-term forecast of the pollutant propagation in local and regional scale. This information will help the authority decisions about the immediate measures and activities (for example evacuation of people from the pollution exposed regions, proper assignment of medical teams) to be carried out in order to minimize the pollution impact on human health. This information will also warn the international community of possible trans-boundary harmful pollutant transport.
- In the off-line mode the modelling system will produce a more detailed and comprehensive analysis of the possible longer-term impact of the harmful releases on the environment and human health in local to regional scales, including the whole Balkan region. This information, made available to the authorities and the public will help the formulation of long-term strategic measures and activities for abatement of the caused damages and gradual restoration of the environment.

The development of an emergency response modelling system certainly is not a novelty. Such systems exist in many countries, including some of the partner countries participating in the present consortium. However, the modelling systems currently employed are simplified and/or the model realization is based on a very coarse resolution. Thus, the novel aspects in the proposed project are mainly in the intension to elaborate a system based on the most up-to date and complex meteorological and pollution transport models with proved high-quality simulation performance, high-spatial resolution and options for two way nesting. These requirements come from the very complex terrain of the Balkan Peninsula and will give the possibility to follow the accidentally released harmful gases from local to regional and to European scale, accounting for the mesoscale dynamic phenomena, to 'zoom-in' and obtain a very detailed air pollution evaluation in the particularly damaged regions. The application of the functions of influence methodology for specifying the accidental release location and power is another novelty in the proposed project.

Although the modelling effort will mainly focus on the calculation of dispersion in local and regional scale of C/B/N agents, it should be noted that the modelling system to be developed will also be applicable to tracking other hazardous materials, such as air pollutants and smoke from forest fires.

The system is not fully developed yet, so only some examples, demonstrating the preparedness (risk assessment) mode of the system will be given in the current paper.

2. ABOUT THE NATO ESP.EAP.SFPP 981393 "MODELLING SYSTEM FOR EMERGENCY RESPONSE TO THE RELEASE OF HARMFUL SUBSTANCES IN THE ATMOSPHERE" PROJECT

The project aims at developing of a unified Balkan region oriented modelling system for operational response to accidental releases of harmful gases in the atmosphere (as a result of terrorist attack or industrial accident), which would be able to:

- Perform highly accurate and reliable risk analysis and assessment for selected "hot spots";
- At a warning signal from the measuring network, by using the functions of influence technique, to detect (if not known) the harmful release location and evaluate the nature and the amount of the released harmful gases;
- Provide the national authorities and the international community with short-term regional scale forecast of the propagation of harmful gases;
- Perform, in an off-line mode, a more detailed and comprehensive analysis of the possible longer-term impacts on the environment and human health in the Balkan region and make the results available to the authorities and the public.

The project coordinates the joint efforts of several institutions in four Balkan countries – Albania, Bulgaria, Greece and Romania.

In addition to the main project outcome – the planned modelling system for operational response to accidental releases of harmful gases in the atmosphere, the project enabled a significant enrichment of the computer facilities of the participating countries. For example a 64-node cluster, purchased in the framework of the project, was installed in the Geophysical Institute, BAS. A significant part of the efforts in the project is devoted to training of young scientists in atmospheric dispersion modelling for supporting emergency response.

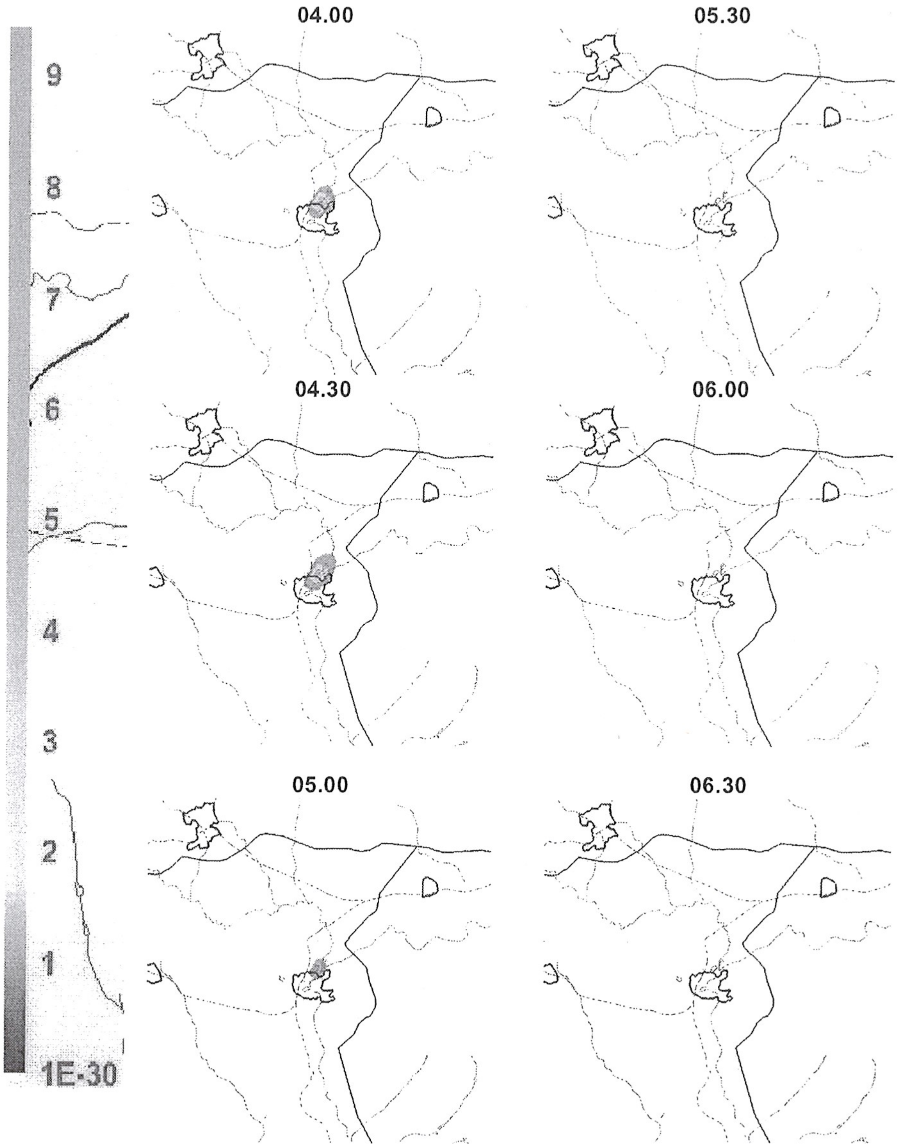

Fig. 1. Averaged concentration fields [*ppb*] for Cl_2, January 2008, release time 3 UTC.

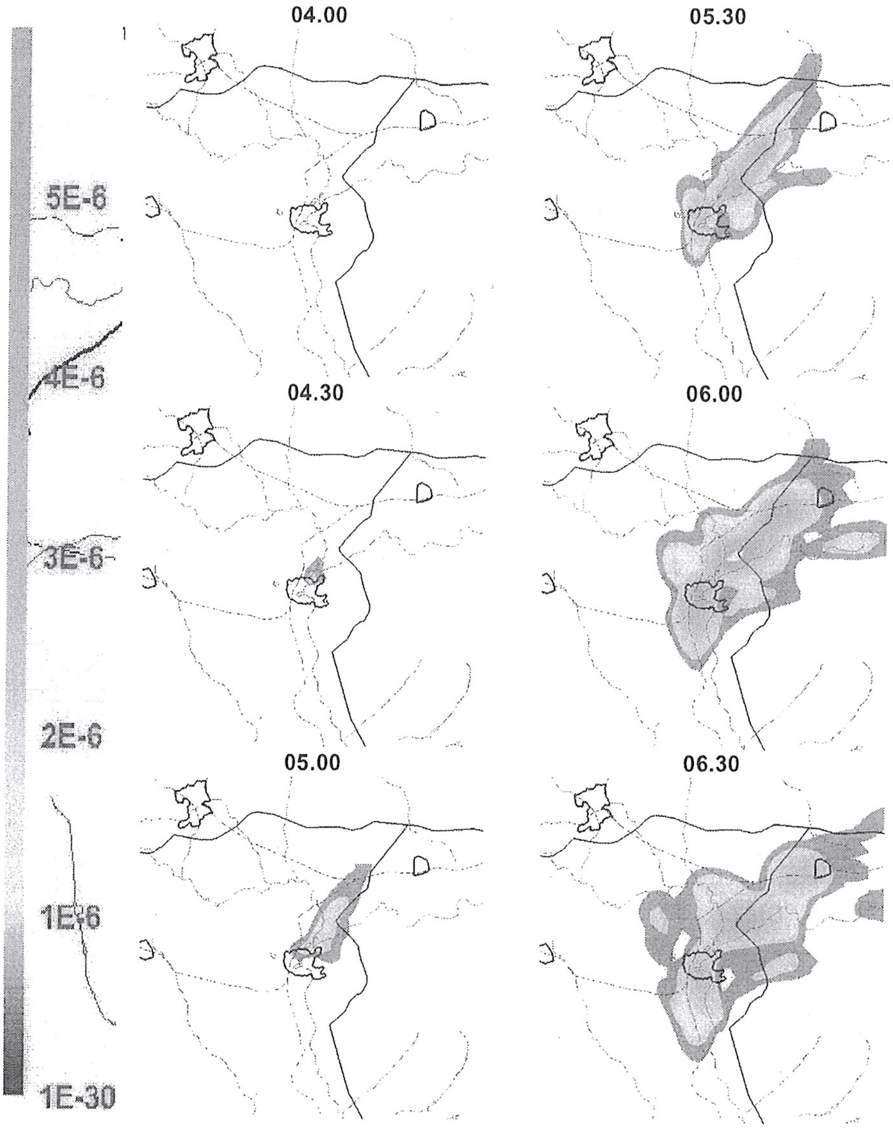

Fig. 2. Averaged concentration fields [*ppb*] for atomic Cl, January 2008, release time 3 UTC.

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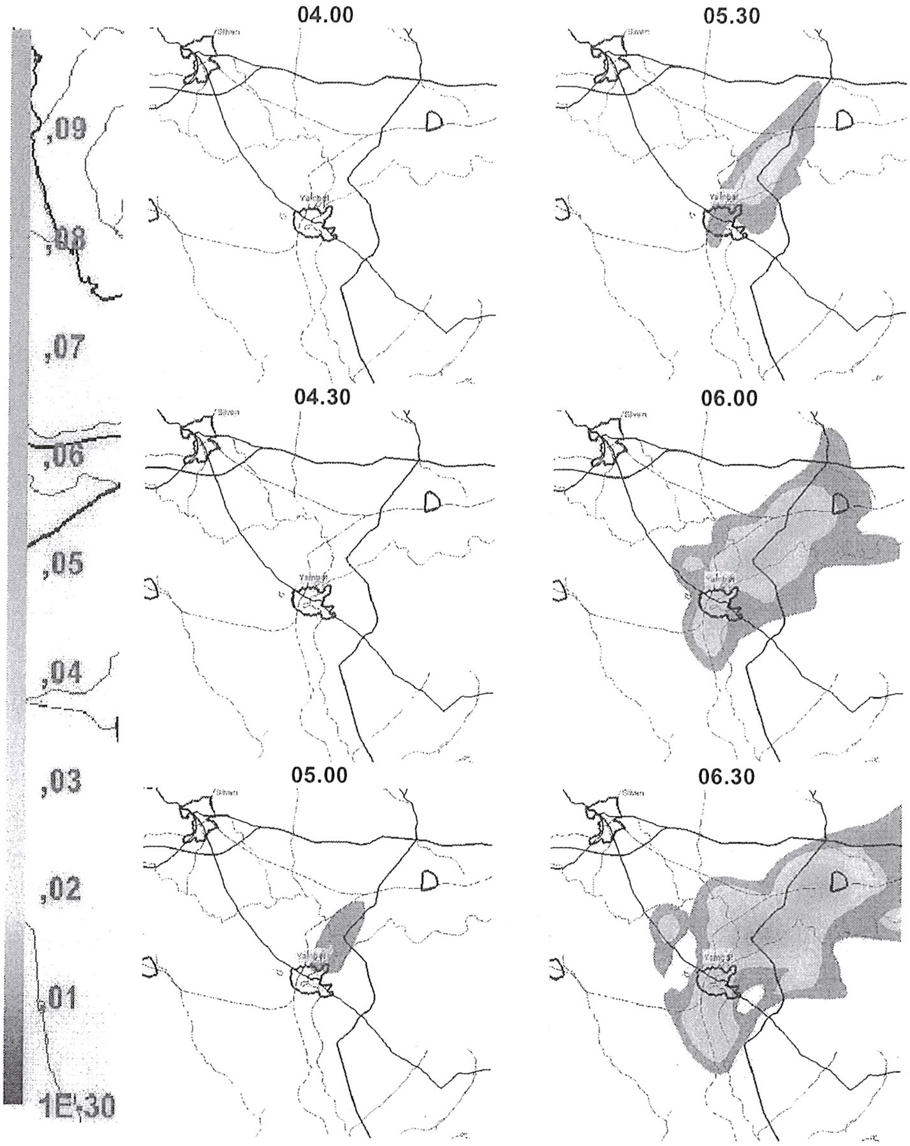

Fig. 3. Averaged concentration fields [*ppb*] for HCl, January 2008, release time 3 UTC.

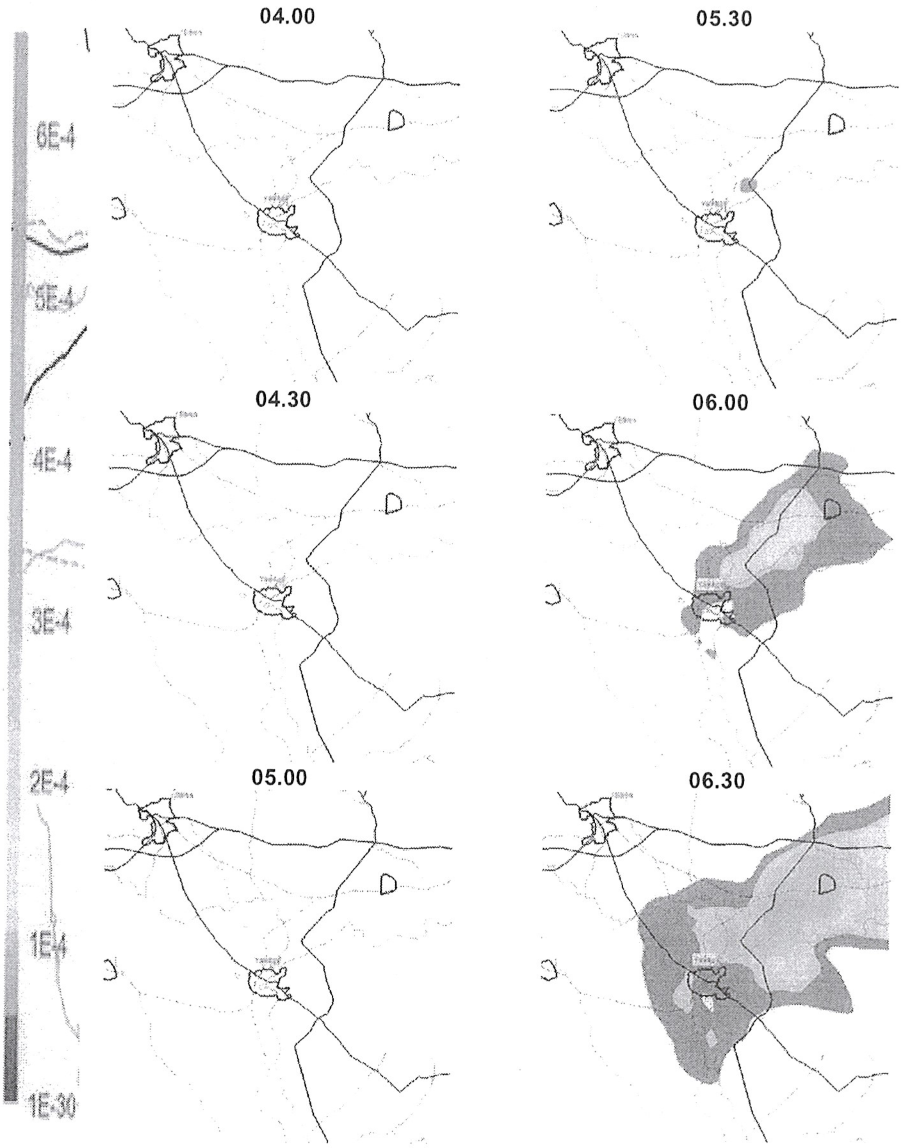

Fig. 4. Averaged concentration fields [*ppb*] for HOCl, January 2008, release time 3 UTC.

3. MODELING TOOLS

It was decided the system to be based on the US EPA Model-3 system, which was chosen as a modelling tool because it appears to be one of the most widely used models with proved simulation abilities. In the same time, this is a modelling tool of large flexibility with a range of options and possibilities to be used for different applications/purposes. Many research groups in Europe already use the Model-3 system or some of its elements and this number is going to increase rapidly.

The system consists of three components:

- MM5 - the 5th generation PSU/NCAR Meso-meteorological Model MM5 (Dudhia, 1993, Grell et al., 1994) used as meteorological pre-processor. This model is pretty often replaced by the next generation model WRF (Shamarock et al., 2007);
- CMAQ - the Community Multiscale Air Quality System (Byun et al., 1998, Byun and Ching, 1999), being the Chemical Transport Model (CTM) of the system. A chlorine chemical mechanism has been added to CMAQ based on Tanaka et al. (2003). 20 gas phase reactions were combined with the CB05V mechanism and incorporated into the model. CB05CLTX mechanism contains additional species and reactions not included in SAPRC99TX3. Six species track emissions from anthropogenic and biogenic sources. Other species allow simulating the fate and transport of molecular chlorine and hydrogen chloride emissions. The additional reactions not only simulate the photochemical destruction of these eight compounds but also simulate how the chlorine compounds affect ozone photochemistry. To simulate the effect, CB05CLTX includes species representing the daughter products of molecular chlorine and hydrogen chloride.
- SMOKE - the Sparse Matrix Operator Kernel Emissions Modelling System (CEP, 2003) – the emission pre-processor of Models-3 system. SMOKE currently supports BEIS (Biogenic Emissions Inventory System) mechanism, versions 3.13 (Schwede et al., 2005). The model is fed with girded land use data. It computes the normalized emissions for each grid cell and land use category. The final step is adjusting the normalized emissions based on girded, hourly meteorology data as produced by MCIP and output a model-ready biogenic emissions file. For preparing the girded land use file GIS technology is applied to USGS (US Geological Survey) data base with resolution 1 km.

Each of these models consists of number of programs that can be run in different schedules depending of the task to be solved. The output of one module is input to others. Taking into account that they had to be run for multiple days it occurred that very complicated LINUX scripts were necessary to be created. The obtained results has been visualized by several graphical packages – GRAPH, GRADS, PAVE, SURFER – supplemented by meta-languages for automation of drawing. All this presumes high experience in Linux and other programming languages.

Quite a large experience in using these models is already achieved in our country (Ganev et al., 2008a, 2008b, 2009a, 2009b, Syrakov et al. 2009a, 2009b, 2009c, 2009d), which is by all means an advantage in developing the emergency response system. In its fast decision mode the system can be organised as a part of the Bulgarian national chemical weather fully automatic system (Syrakov et al. 2009a, 2009d).

As the simulation, especially in the risk analysis and assessment mode of the system require huge amount of computer resources, the grid computing technology is applied. The Computational Grid, or shortly, the Grid, is a computing environment which enables the unification of widely geographically distributed computing resources into one big (super)-computer (Atanassov et all., 2006, Foster and Kesselmann, 1998). The individual computing resources commonly consist mostly of computer clusters and several individual computers, which are interconnected by a high-speed very wide area network. The Grid is a computer system which is, at this moment, primarily intended for supporting e-Science, however the technology itself is very adaptable to the whole area of present and future computer usage. As the Grid was perceived as a viable solution for supporting e-Science, the modern

Grid development was started and is pushed by the scientific community. The major goal of the Grid is to enable the clustering and unification of distributed computing and data processing resources, as to collect as much computing power usable to applications necessitating high computer strength as possible. Some of scientific application examples necessitating the Grid are applications from the fields of particle physics, climate analysis, biomedical research, meteorology etc

4. SOME EXAMPLES OF THE SYSTEM RISK ASSESSMENT SIMULATIONS

4.1. What is risk analysis?

Risk (*R*) may generally be defined by the terms of probability (recurrence) of happening of a given event (*P*) and the impact of the same event (in the particular case on human health) (*I*) in the following way:

$R = P \times I.$

Applying this definition to the problem of air pollution impact this means that an event occurring with high probability, even with relatively low impact, may result in higher risk than a rare event with stronger impact. For the needs of the emergency response preparedness mode - developing strategies for immediate emergency response (for example evacuation of people from the pollution exposed regions, proper assignment of medical teams) in order to minimize the pollution impact on human health this means that a map of the risk (the product of probability and impact) around potential sources of emergency toxic gas releases should be constructed.

The impact should be evaluated by some metrics directly giving the effect of toxic gas on human health (a kind of regulatory threshold value), but it is clear that if the pollutant concentrations are taken as an impact it would be a matter of simple arithmetic operations to evaluate the health impact, possibly separately for different target groups of the population.

4.2. Brief description of the numerical experiments

Following the above definition of risk it is clear that a large number of simulations of the toxic gases (primary as well as secondary) dispersion around the potentially dangerous site should be made under comprehensive set of meteorological conditions and for different accidental release times. The averaged over this ensemble concentration fields should be treated as an assessment of the potential risk.

The simulations that will be demonstrated below are made for January 2008 for an instantaneous release of 25 t chlorine (Cl_2) released at the site of "VEREJA-HIM" Jambol in 3 o'clock in the morning and in the afternoon respectively.

The **NCEP Global Analysis Data** with 1°×1° resolution was used as meteorological forcing and the WRF and CMAQ nesting capabilities were used (the simulations are carried out in three nested domains with resolutions 25, 5, 1km, covering respectively the regions of South-Eastern Europe, Bulgaria, and the area surrounding the particular site) for downscaling the problem to a horizontal resolution of 1 km around the site. It should be noted that the "regular" emissions are also taken into account not only in the innermost domain, but also in the domain with spatial resolution of 5 km (Bulgaria) thus providing appropriate boundary conditions for the innermost domain.

4.3. Brief discussion of the numerical results

The time averaged surface concentration fields of Cl_2 (the primary pollutant), Cl, HCl and HOCl (secondary pollutants) for the two release times - 3 o'clock in the morning and 3 o'clock in the afternoon are shown on Figs. 1-8. There are several things about the concentration fields that should be mentioned:

1.) The surface concentrations from the release in 3 o'clock in the morning are much larger and for the secondary pollutants wide spread in comparison to those from the release in 3 o'clock in the afternoon. The explanation is quite obvious – the inversions in the morning hours keep the admixtures near ground, while the more unstable conditions in the afternoon facilitate the vertical transport and thus less of the pollutants remain near earths surface.

2.) The primary pollutant (Cl_2) disappears pretty fast due to chemical transformations which produce the secondary pollutants.

3.) The secondary pollutant fields pattern is pretty complex and for the morning release they cover a big domain around the "VEREJA-HIM" site. The concentration fields, especially in the morning, are a good demonstration why the risk assessment is necessary. It can be seen that the maximal risk could happen far from the site and with several hours delay, that some of the roads (evacuation of the population) at certain time could be rather risky, etc.

4. CONCLUSIONS

The shown results are very preliminary. In order to achieve a real assessment of the risk simulations should be made for a much larger set of meteorological conditions (probably several years in order to account for the seasonal variability) and for much more release times in order to account for diurnal variability. At this stage of the system development, however, it can be concluded that:

1.) The chosen modelling tools are probably suitable for this particular task and the obtained preliminary results are quite realistic and promising;

2.) The Grid computing technologies are a very appropriate for approaching tasks like risk assessment, which require performing of a very large number of simulations;

3.) The shown numerical results very well demonstrate the practical value of the preparedness mode of the system.

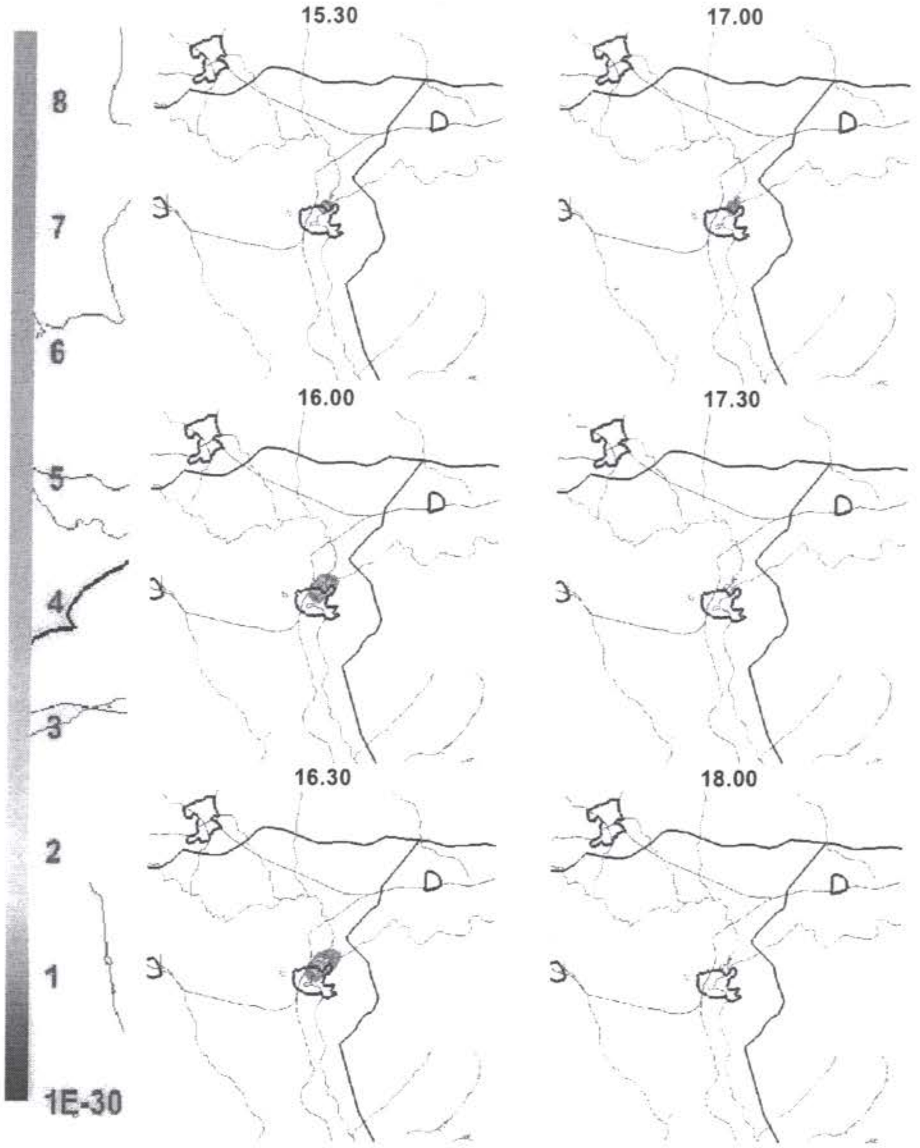

Fig. 5. Averaged concentration fields [*ppb*] for Cl_2, January 2008, release time 15 UTC.

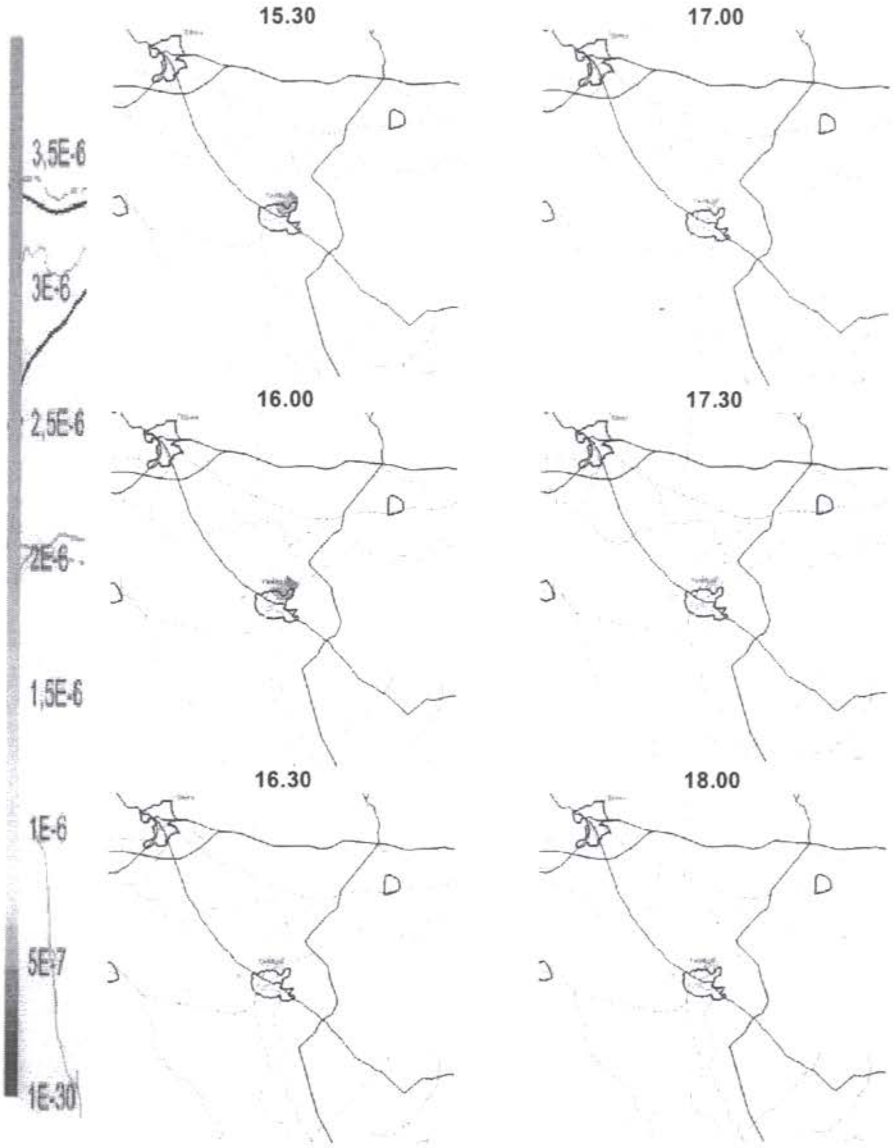

Fig. 6. Averaged concentration fields *[ppb]* for atomic Cl, January 2008, release time 15 UTC.

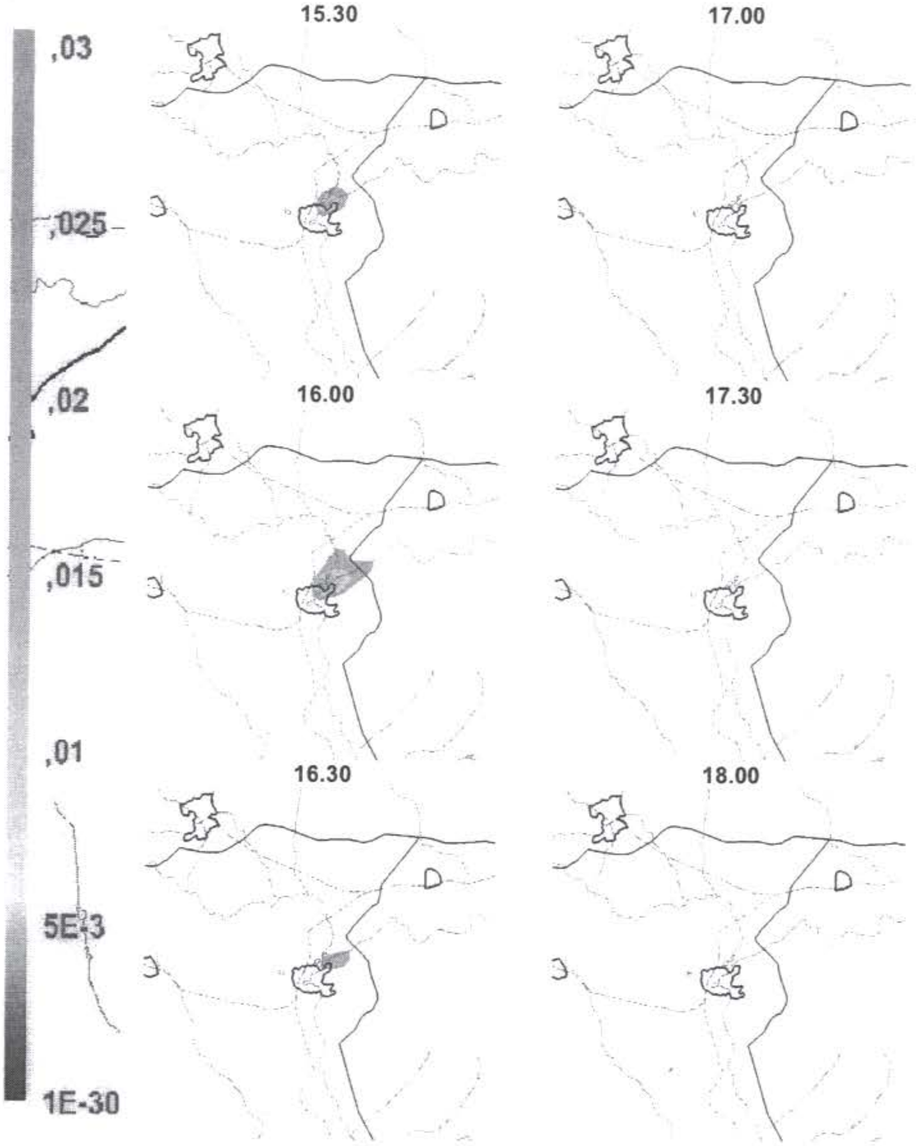

Fig. 7. Averaged concentration fields [*ppb*] for HCl, January 2008, release time 15 UTC.

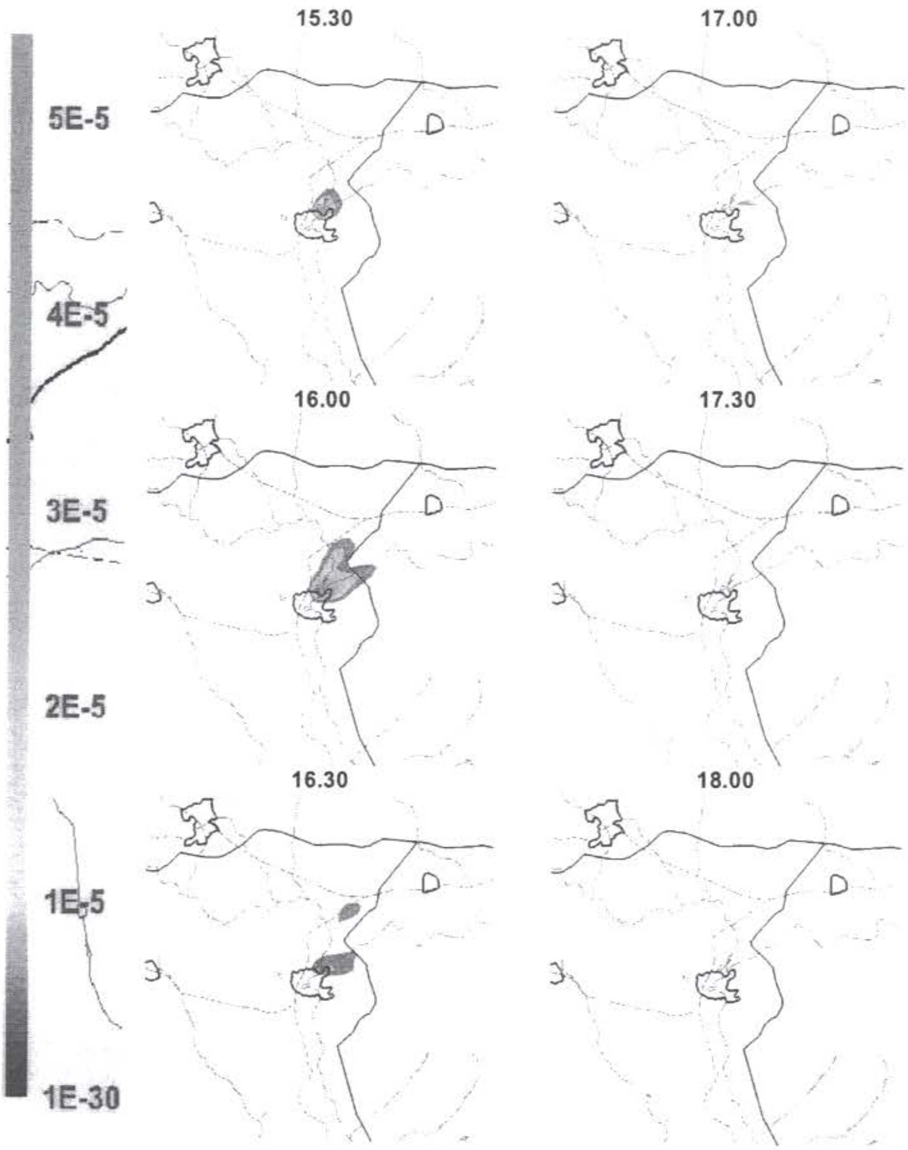

Fig. 8. Averaged concentration fields [*ppb*] for HOCl, January 2008, release time 15 UTC.

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Deep gratitude is due to US EPA, US NCEP and EMEP for providing free-of-charge data and software. Special thanks to the Netherlands Organization for Applied Scientific research (TNO) for providing us with the high-resolution European anthropogenic emission inventory.

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G. Gadzhev is World Federation of Scientists grant holder.

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PREFACE

This book contains extended abstracts (short communications) of some of the presented papers during the International Conference on "Numerical Methods for Scientific Computations and Advanced Applications" (NMSCAA'14), May 19-22, 2014, Bansko, Bulgaria. The conference was organized by the Institute of Information and Communication Technologies, Bulgarian Academy of Sciences in cooperation with Society for Industrial and Applied Mathematics (SIAM) and devoted to the 60th anniversary of Svetozar Margenov.

His main fields of research include: Large-Scale Scientific Computing and Parallel Algorithms; Numerical Methods for Partial Differential Equations (Finite Difference Schemes and Finite Element Method); Computational Linear Algebra (Iterative Methods and Algorithms, Preconditioning, Sparse Matrices); Large-Scale Computing of Environmental Problems; Biomedical and Engineering Problems; Supercomputing applications, etc. Svetozar Margenov receive his PhD in 1984 and the degree of Doctor of Science in 2002. From 2003 he was promoted to Full Professor in 2003. Currently, prof. Margenov is Director of the Institute of Information and Communication Technologies of the Bulgarian academy of sciences and Head of the Department of Scientific computing in the the same institute. He is an eminent scientists and university lecturer. Svetozar Margenov is an author of two monographs and more than 140 papers published in high ranked international journals and proceedings of conferences. He is a member of the Editorial Boards of

- *Numerical Linear Algebra with Applications* (NLAA),
- *Scalable Computing: Practice and Experience* (SCPE),
- *International Journal of Numerical Analysis and Modelling*, Series B.

During his very successful carrier he was a scientific advisor and mentor of many Ph.D. and MSc students.

The Conference Specific topics of interest are as follows:

- Multiscale and multiphysics problems;
- Robust preconditioning;
- Monte Carlo methods;
- Optimization and control systems;
- Scalable parallel algorithms;
- Advanced computing for innovations.

The list of plenary invited speakers includes: Peter Arbenz (ETH Zurich, CH); Owe Axelsson (Institute of Geonics, ASCR, CR); Radim Blaheta (Institute of Geonics, ASCR, CR); Oleg Iliev (ITWM, Kaiserslautern, Germany); Johannes Kraus (RICAM, Linz, AT); Raytcho Lazarov (TA&MU, College Station, USA); Peter Minev (University of Alberta, CA); Panayot Vassilevski (LLNL, Livermore, USA); Vladimir Veliov (TU-Vienna, AT and IMI BAS, BG) and Lyudmil Zikatanov (The Pennsylvania State University, USA).

Krassimir Georgiev

May 2014

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same burning time and ignition time. On Figure 1c the wind force is the same as on Figure 1a only the direction is different. The same is on Figure 1b and Figure 1d. We observe that the achieved by our model front of the fire is almost similar when the force of the wind is the same.

4 Conclusion

On this paper we apply GMM on wild fire modeling. In our model we take in to account the presence of the wind and it influence on closer cells. We run various tests and verify that the fire spread looks realistic.

Acknowledgment

This work has been partially supported by the European Commission project ACOMIN and by the Bulgarian National Scientific Fund under the grant I01/0006- "Simulation of wild-land fire behavior".

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Computer Simulations of the Atmospheric Composition Climate of Bulgaria - Some Basic Results

Georgi Gadzhev, Kostadin Ganev, Maria Prodanova, Dimiter Syrakov, Nikolai Miloshev

1 Introduction

Recently extensive studies for long enough simulation periods and good resolution of the atmospheric composition status in Bulgaria have been carried out using up-to-date modeling tools and detailed and reliable input data [1, 2, 3, 4].
The simulations aimed at constructing of ensemble, comprehensive enough as to provide statistically reliable assessment of the atmospheric composition climate of Bulgaria - typical and extreme features of the special/temporal behavior, annual means and seasonal variations, etc.
The present paper, in which a brief review of the studies, will focus on some important characteristics of the atmospheric composition climate of Bulgaria

2 Modeling tools and input data

All the simulations are based on the US EPA Model-3 system [5]The large scale (background) meteorological data used by the study is the NCEP Global Analysis Data with 1x1 degree resolution. The MM5 and CMAQ nesting capabilities are used to downscale the problem to a 3 km horizontal resolution for the innermost domain (Bulgaria).
The TNO high resolution emission inventory [6] is exploited. A detailed description of the emission modeling is given in [4]

3 Some illustrations

As already explained, the 8-year simulated fields ensemble is large enough to allow statistical treatment. In particular the probability density functions for each of the atmospheric compounds can be calculated, with the respective seasonal and diurnal variations, for each of the points of the simulation grid or averaged over the territory of the country. Knowing the probability function we know everything about the climate of the different compound concentrations (see Figure 1).
Another important characteristic of the atmospheric composition climate of the country is the contribution of the emission of different categories to the overall atmospheric composition pattern (see Figure 2).

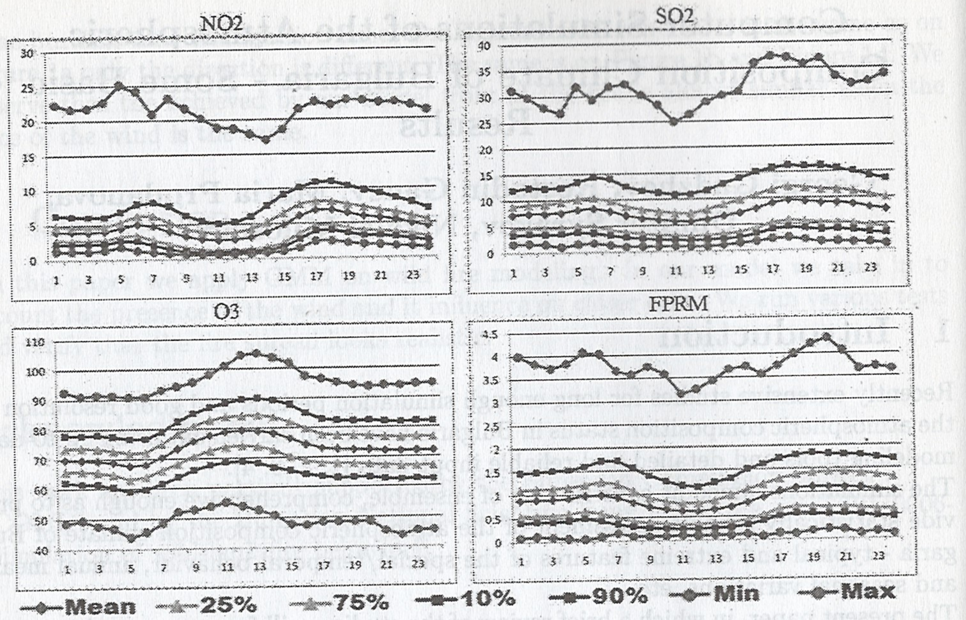

Figure 1: Annually mean diurnal variations of the averaged for the country NO2, SO2, O3 and fine PM surface concentrations [ug/m3]: curves of mean, maximal and minimal values as well as curves show the imaginary concentrations for which the probability of the simulated ones to be smaller is respectively 0.25, 0.75, 0.1 and 0.9.

4 Some basic facts about the atmospheric composition climate of Bulgaria

Some of the major findings about the atmospheric composition climate of Bulgaria are as follows:

- the behavior of the surface concentrations, averaged over the ensemble annually, or for the four seasons and over the territory of the country is reasonable and demonstrates effects which for most of the compounds can be explained from a point of view of the generally accepted schemes of dynamic influences (in particular the role of turbulent transport and its dependence on atmospheric stability) and/or chemical transformations;
- the SNAP 1 contribution to the surface SO2 concentrations is smaller than one should expect, having in mind that the 'Maritza' power plants are among the biggest sulfur sources in Europe. Probably, a significant amount of SO2 from these sources becomes a subject of larger scale transport and so is moved outside the country;

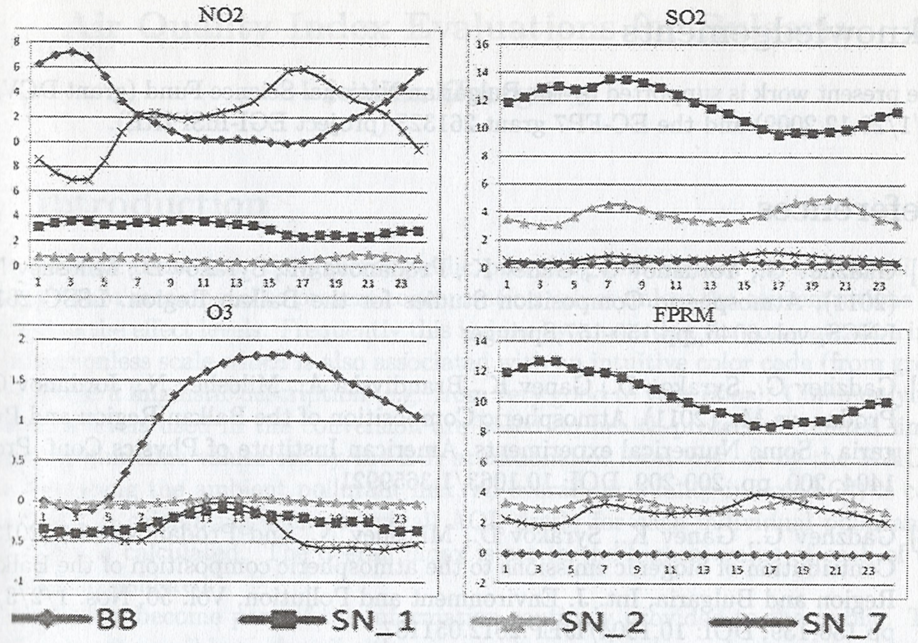

Figure 2: Annually mean diurnal variations of the averaged for the country contribution [%] of different emission categories on NO2, SO2, O3 and fine PM surface concentrations.

- the contribution of biogenic emissions to surface ozone in the country is relatively small. This indicates that local O3 production rate is limited by the availability of NOx concentration, a regime which is called NOx-limited. Obviously from a point of view of atmospheric composition climate the Balkan Peninsula and Bulgaria are predominantly 'rural' environment which explains the ozone photochemistry specifics in the region.;
- the contribution of the emission from categories 1 and 7, which are the major sources of the other ozone precursor - nitrogen oxides, is also small. This, once again is an indirect indicator, that the surface ozone in Bulgaria is to a small extend due to domestic sources, but is mostly imported;
- the results produced by the CMAQ - Integrated Process Rate Analysi s- demonstrate the very complex behavior and interaction of the different processes. The analysis of the behavior of different processes does not give simple answer of the question how the air pollution in a given point or region is formed.

Aknowledgements

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Air Quality Index Evaluations for Bulgaria

Ivelina Georgieva

1 Introduction

In communication with the general public providing information on the actual air quality is not meaningful to present concentration values unless the concentrations are related to the effect levels. Frequently this is done by converting the concentration into a dimensionless scale which is also associated with an intuitive color code (from green to red) and a linguistic description (e.g. from very good to very poor). Commonly the reference levels used in the conversion are based on health-protection related limit, target or guideline values set by the EU, at national or local level or by the WHO. For describing the ambient pollutant mix, an overall air quality index (AQI) is constructed. In calculating such an overall AQI, firstly for each individual pollutant a sub-index is calculated. The overall index is set to the highest value of each of the pollutant considered.

The AQI has become part of the information routinely provided to the public. The AQI makes it possible to describe the air quality in a simple, understandable way.

2 Computer simulated atmospheric composition

Recently extensive studies for long enough simulation periods and good resolution of the atmospheric composition status in Bulgaria have been carried out using up-to-date modeling tools and detailed and reliable input data [1, 2, 3, 4, 5, 6, 7, 8, 9].

The simulations aimed at constructing of ensemble, comprehensive enough as to provide statistically reliable assessment of the atmospheric composition climate of Bulgaria - typical and extreme features of the special/temporal behavior, annual means and seasonal variations, etc.

3 Some AQI examples

Utilization of the ensemble for studying the AQI climate in Bulgaria is the goal of the present work.

The AQI, calculated in the frame of Bulgarian Chemical Weather Forecast System [10, 11], ver.3, which follows the UK Air Quality Index [12] is used in the present work as well. Due to the limited volume of the present abstract only few examples, illustrating the AQI climate in Bulgaria will be demonstrated.

Figure 1, for example, demonstrates the seasonal and diurnal variation of the recurrence of different AQI categories, averaged for the territory of Bulgaria. As it can be seen AQI2 and 3 are with highest recurrence, while all other AQI are much less

RECURRENCE OF AIR QUALITY FOR THE CITY OF SOFIA FOR 2013 AND 2014

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Abstract. The air is the living environment of human beings and obviously the atmospheric composition has a great importance for the quality of life and human health. Air Quality (AQ) is a key element for the well-being and quality of life of European citizens. The objectives of the present work is performing reliable, comprehensive and detailed studies of the impact of lower atmosphere composition on the quality of life and health risks for the population in Sofia city. Lately, together with the numerical weather forecast, in many European countries Systems for Chemical Weather Forecast operate, Chemical Weather being understood as concentration distribution of key pollutants in a particular area and its changes during some forecast period. In Bulgaria, a prototype of such a system was built in the frame of a project with the National Science Fund. It covers a relatively small domain including Bulgaria that requires using chemical boundary conditions from similar foreign systems. As far as this data is prepared abroad and transferred by Internet, many failures took place during the operation of the system. To avoid this problem, a new version of the system was built on the base of the nesting approach. This version is realized on five domains: Europe, Balkan Peninsula, Bulgaria, Sofia Municipality and Sofia City with increasing space resolution - from 81 km (Europe) to 1 km (Sofia City). For the Mother domain (Europe) climatic boundary conditions are applied. All other domains take their boundary conditions from the senior one. Computations start automatically at 00 UTC every day and the forecast period is 3 days. The System is based on the well-known models WRF (Meso-meteorological Model) and US EPA dispersion model CMAQ (Chemical Transport Model). As emission input the TNO data is used for the two biggest domains. For the 3 Bulgarian domains the current emission inventory prepared by Bulgarian environmental authorities is exploited.

Key words: Air Quality Indices, air quality, quality of life, health risks.

Introduction

The Air Quality is a key element for the well-being and quality of life of European citizens. According to the World Health Organization, air pollution severely affects the health of European citizens. There is increasing evidence for adverse effects of air pollution on the respiratory and the cardiovascular system as a result of both acute and chronic exposure. In particular, a significant reduction of life expectancy by a year or more is assumed to be linked to long-term exposure to high air concentrations of particulate matter (PM). There is considerable concern about impaired and detrimental air quality conditions over many areas in Europe, especially in urbanized areas, in spite of about 30 years of legislation and emission reduction. Current legislation, e.g. the Ozone daughter directive 2002/3/EC (European Parliament, 2002), requires informing the public on AQ, assessing air pollutant concentrations throughout the whole territory of Member States and indicating exceedances of limit and target values, forecasting potential exceedances and assessing possible emergency measures to abate exceedances. For the purpose, modeling tools must be used in parallel with air pollution measurements. The goals of reliable air quality forecasts are the efficient control and protection of population exposure as well as possible emission abatement measures. In last years the concept of "chemical weather" arises and in many countries respective forecast systems are being developed along with the usual meteorological weather forecasts (see, for instance, Sofiev at al., 2006, Poupkou et al., 2008, Monteiro et al., 2005, San Jose et al., 2006, and others).

Air pollution easily crosses national borders. It would be cost-effective and beneficial for citizens, society and decision-makers that national chemical weather forecast and information systems were networked across Europe. For the purpose several projects in the European Framework Programs (GEMS, PROMOTE, MEGAPOLI, MACC, PASODOBLE etc.) as well as the COST Action ES0602 "Towards a European Network on Chemical Weather Forecasting and Information Systems") were launched aiming at providing a forum for harmonizing, standardizing and benchmarking approaches and practices in data exchange and multi-model capabilities for air quality forecast and (near) real-time information systems in Europe. It is supposed to examine existing, and work out new solutions for integrating the development efforts at national and international levels. One can find several CW systems' (performance and descriptions) in the Action's web-portal (http://www.chemicalweather.eu/Domains).

Modeling tools

BgCWFIS is designed in a way to fit the real-time constraints and to deliver forecasts for the next days on an hourly basis. US EPA Models-3 air quality modeling system is used, consisting of:

• CMAQ v.4.6 - Community Multi-scale Air Quality model, http://www.cmaq-model.org/, Denis et al. (1996), Byun and Ching (1999), Byun and Schere (2006), the Chemical Transport Model (CTM);

• WRF v.3.2.1 - Weather Research and Forecasting Model, http://www.wrf-model.org/, Skamarock et al. (2007), the meteorological pre-processor to CMAQ. The Weather Research and Forecasting (WRF) Model is a next generation meso-scale numerical weather prediction system designed to serve both operational forecasting and atmospheric research needs. It is an evolutionary successor to the MM5 model. The creation and further development of WRF is due to the collaborative efforts of several US institutions like NCAR, NOAA, NCEP and others. The WRF is a fully compressible and non-hydrostatic model with terrain-following hydrostatic pressure coordinate. The grid staggering is the Arakawa-C type. One can find more info on http://www.wrf-model.org/index.php;

• SMOKE v.2.4 - Sparse Matrix Operator Kernel Emissions Modelling System, http://www.smoke-model.org/, Coats and Houyoux (1996), Houyoux and Vukovich (1999), CEP (2003), the emission pre-processor to CMAQ. CMAQ demands its emission input in specific format reflecting the time evolution of all pollutants accounted for by the chemical mechanism used (CB-IV in this case). Emission inventories are used as row data for anthropogenic emission processing. The inventories are made on annual basis for big territories; many pollutants are estimated as groups (VOC and PM2.5 for instance). Preparation of emission input to a Chemical Transport Model requires emission processing. Such emission processing component in EPA Models-3 system is SMOKE but it is partly used, here, because it's quite strong relation to US emission sources specifics. In BgCWFIS, SMOKE is used only for calculating BgS emissions and for merging AS-, LPS- and BgS-files into a CMAQ emission input file. The area source emissions and the large point source emissions are prepared by the interface programs AEmis and PEmis.

In the System, WRF is driven by the NCEP GFS (Global Forecast System) data that can be accessed freely from http://www.ftp.ncep.noaa.gov/data/nccf/com/gfs/prod/. This data is global weather forecast in GRIB-2 format with space resolution of 1°×1° and 6-hour time resolution. The downloading of this data is invoked automatically every day at 00:00Z. 84-hour runs starting at 12:00Z of the previous day are used; the first 12 hours of the period being spinning-up followed by a 3-day weather forecast. The chemical weather forecast duration is from 00:00Z of the current day to 00:00Z of the fourth day after (3-day forecast).

TNO inventory for 2005 (Denier van der Gon et al., 2010) is exploited partly for Bulgaria domain, TNO being the Netherlands's Organization for Applied Scientific Research. For Bulgaria itself and for the other Bulgarian domains, the National inventory for 2010 as provided by Bulgarian Executive Environmental Agency is used. That means TNO inventory is used only for the territories outside Bulgaria in the mother CMAQ's domain.

The TNO produced several sets of inventories for different years. The anthropogenic sources in this inventories are distributed over 10 SNAPs (Selected Nomenclature for Air Pollution) classifying them according to the processes leading to harmful material release into the atmosphere (EMEP/CORINAIR, 2002). The 2010 TNO inventory has resolution of 0.125°×0.0625° (about 7×8 km). It is distributed as a comma- or tab-delimited text-file. Each line of the file contains data for a single box, namely the center of mesh coordinates, the country, the type of source (A/P), the SNAP, and the yearly emissions of

8 pollutants. The SNAP 7 (road transport) is presented as 5 sub-SNAPs. The pollutants are: methane (CH4), carbon oxide (CO), nitric oxides (NOx), sulfur oxides (SOx), non-methane volatile organic compounds (NMVOC), ammonia (NH3), Particulate Matter with d<10μm (PM10) and Particulate Matter with d<2.5μm (PM2.5).

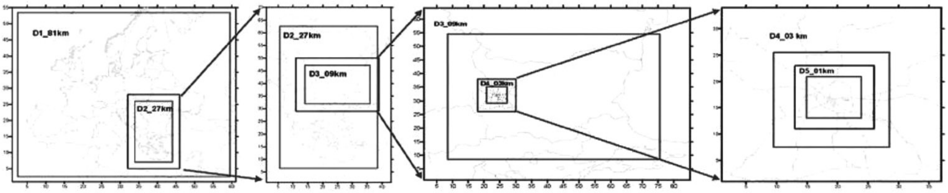

Fig. 1. Five computational domains of BgCWFIS, (CMAQ domain nested in WRF one)

The nesting capabilities of WRF and CMAQ are used to downscale the forecasts from European region to Sofia city area. The resolution of the mother domain (Europe) is 81 km, big enough as to correspond to the GFS met-data space resolution. Four other domains are nested in it and in each other – Balkan Peninsula (27km resolution), Bulgaria (9 km), Sofia municipality (3 km) and Sofia city (1 km) as shown in Fig. 1.

In BgCWFIS, climatic data is used for chemical boundary conditions following the presumption that the errors introduced by this assumption will decrease quickly to the center of the domain due to the continuous acting of the pollution sources. All other domains receive their boundary conditions from the previous domain in the hierarchy.

Operational Performance of BgCWFIS

Fourteen σ-levels with varying thickness determine the vertical structure of CMAQ model. The Planetary Boundary Layer (PBL) is presented by the lowest 8 of these levels.

The CMAQ v.4.6 input consists of various files containing concentration, deposition, visibility and other variables. The concentration output is a NetCDF file with 3-D hourly data for 78 pollutants - gases and aerosols.

The post-processing program XtrCON extracts part of the pollutants for archiving and further handling. Only surface values of the most important pollutants are saved - 8 gases and 11 aerosols (including PM10 and PM2.5). Part of these pollutants is more or less monitored and they are referred in the European legislation with the respective thresholds.

For the moment it presents 4 main pollutants - Ozone, NO_2, SO_2 and PM10 which are used to calculate the Air Quality Indices (AQI).

Calculation of the Air Quality (AQ) impact on human health and quality of life in Sofia city is the objective of the present study. The impact is calculated in the terms of the so called AQI – an integral characteristic directly measuring the effects of AQ on human health. The calculations are made on the basis of long term AQ simulations, which make it possible to reveal the climate of AQI spatial/temporal distribution and behavior.

The AQI is defined as a measure of air pollution seen in the context of its impact on human health. It provides an integrated assessment of the impact of the whole range of pollutants on human health and is calculated based on the concentration of various pollutants obtained from measurements or numerical modeling. The index is defined in several segments (EPA, 2009), each of which is a linear function of the concentration of each considered pollutant:

$$I = ((I\ high - I\ low) / (C\ high - C\ low))(C - C\ low) \quad (1)$$

where:

I = the AQI,

C = the pollutant concentration,

C low - the concentration breakpoint that is ≤ C,

C high - the concentration breakpoint that is ≥ C,

I low - the index breakpoint corresponding to C low ,

I high - the index breakpoint corresponding to C high.

In that calculation the index falls in one of the ranges of the dimensionless scale. In each range index values are associated with an intuitive color code, a linguistic description and a health description.

Pretty often in order to evaluate the air quality situation in European cities, all detailed measurements are transformed into a single relative figure: the Common Air Quality Index (CAQI) and this index have 5 levels using a scale from 0 (very low) to > 100 (very high). The index is based on 3 pollutants of major concern in Europe: PM10, NO_2, O_3 and will be able to take into account to 3 additional pollutants (CO, PM2.5 and SO_2).

One of the most commonly used air quality index is the UK Daily Air Quality Index (Leeuw, F. de, Mol, W., 2005), also used in Bulgaria (Etropolska et al. 2010), (Syrakov et al, 2012, 2013, 2014a, 2014b, 2015), (Georgieva, I., 2014), (Georgieva et al. 2015), (Georgieva, I. and Ivanov, V., 2017, 2018) and (Ivanov, V. and Georgieva, I., 2017).

Compute the AQI

To calculate the AQI requires several steps:

- Air pollutant concentrations (from measurements or model)
- Convert this air pollutant concentration to a AQI. The index is defined for each pollutant in a different way converting the concentrations into a dimensionless scale, associated with an intuitive color code (green to purple) and a linguistic description (Low to Very High).
- AQI values are divided into ranges, and each range is assigned a color code and health descriptor.

- An overall air AQI is constructed to describe the ambient pollutant mix – It's set to the highest value of each of the pollutant considered.

The breakpoints between index values are defined for each pollutant separately and the overall index is defined as the maximum value of the index. Different averaging periods are used for different pollutants. Each of the bands comes with advice for at-risk groups and the general population (Table 1).

Table 1 Boundaries Between Index Points for Each Pollutant

Index	O_3 Running 8 hourly mean (μg/m^3)	NO_2 Hourly mean (μg/m^3)	SO_2 15 minute mean (μg/m^3)	PM10 Particles, 24 hour mean (μg/m^3)	PM2.5 Particles, 24 hour mean (μg/m^3)
1 (Low)	0-33	0-66	0-88	0-11	0-16
2 (Low)	34-65	67-133	89-176	12-23	17-33
3 (Low)	66-99	134-199	177-265	24-34	34-49
4 (Moderate)	100-120	200-267	266-354	35-41	50-58
5 (Moderate)	121-140	268-334	355-442	42-46	59-66
6 (Moderate)	141-159	335-399	443-531	47-52	67-74
7 (High)	160-187	400-467	530-708	53-58	75-83
8 (High)	188-213	468-534	709-886	59-64	84-91
9 (High)	214-239	535-599	887-1063	65-69	92-99
10 (Very High)	≥240	≥600	≥1064	≥70	≥100

The reference levels and Health Descriptor used in the Table 2 are based on health-protection related limit, target or guideline values set by the EU, at national or local level or by the WHO.

Table 2. Air quality indices and their health impact (de Leeuw and Mol, 2005).

Banding	Value	Health Descriptor
Low	1-3	Effects are unlikely to be noticed even by individuals who know they are sensitive to air pollutants
Moderate	4-6	Mild effects, unlikely to require action, may be noticed amongst sensitive individuals.
High	7-9	Significant effects may be noticed by sensitive individuals and action to avoid or reduce these effects may be needed (e.g. reducing exposure by spending less time in polluted areas outdoors). Asthmatics will find that their 'reliever' inhaler is likely to reverse the effects on the lung.
Very High	10	The effects on sensitive individuals described for 'High' levels of pollution may worsen.

Results

Annual recurrence of AQI in "Low", "Moderate", "High" and "Very High" bands over territory of Sofia city for 2013 and 2014: Figures 2 and 3 demonstrate the spatial and diurnal variation of the annual recurrence of different AQI categories for the chosen hours 06:00 and 18:00GMT for 2013 and 2014. The picture shows the sum of recurrences of the AQI in each range - Low, Moderate and High range. What can be also noticed is: the recurrence in Low and Moderate range is different for both years, as in 2013 the recurrence in Low band is smaller than 2014, and reverse in Moderate range. In High range there is no any difference between both years.

In the Low range the air is most clean, so high recurrence values mean more cases with clean air and lower recurrence values mean, less cases with clean air (worse AQ status). In the other 2 plots (Moderate and High ranges) - high recurrence values means less favorable and respectively bad AQ status. It can be seen that most areas with high recurrence of cases with lower AQI status are in the city center and over the Vitosha Mountain early in the morning due to the weather conditions, higher NO_2 concentrations from the road transport and higher O_3 concentration in the mountain. This could be seen at Low and Moderate range maps in the morning hours. The major NO_2 sources in the city are the surface sources (road transport) and the surface NO_2 concentrations are higher early in the morning and much smaller at noon (the atmosphere is mostly unstable, and so the turbulence transports the NO_2 aloft more intensively). The maximal concentrations which are directly linked to the worse AQI status are formed in the city center and along the boulevard with most busy traffic.

In Moderate band at 18:00 GMT it can be also noticed about 20% recurrence with not so good AQI status over Vitosha mountain. Higher values over the Vitosha Mountain in the afternoon are due to the higher concentration of O_3 in mountain areas and intensive ozone transport from higher levels (intensive turbulence during midday). The behavior of the surface ozone is complex. The O_3 in Bulgaria is to a great extent due to transport from abroad (Gadzhev et al. 2013), (Kaleyna et al. 2013a, 2013b, 2014) and (Tcherkezova et al. 2013). This is the reason why the O_3 concentrations early in the morning are smaller (less intensive transport from higher levels), and higher at noon and afternoon (turbulence atmosphere and O_3 photochemistry)

High recurrence of cases with most polluted air (High band) appears again in the city center. In the city center can be observed about 20% "High" pollution in the morning and 10% in the afternoon. Bad AQI status from the High band never disappears.

Conclusions

The simulations for Sofia city show that the air quality status of Sofia is not so good (evaluated with a spatial resolution of 1km).

AQI status falls mostly in Low and Moderate bands, but the recurrence of cases with High pollution is close to 20% mostly at the city center.

The recurrence of Low band for 2013 is smaller than 2014, which means that in 2014 almost 90% the days have been with cleaner air.

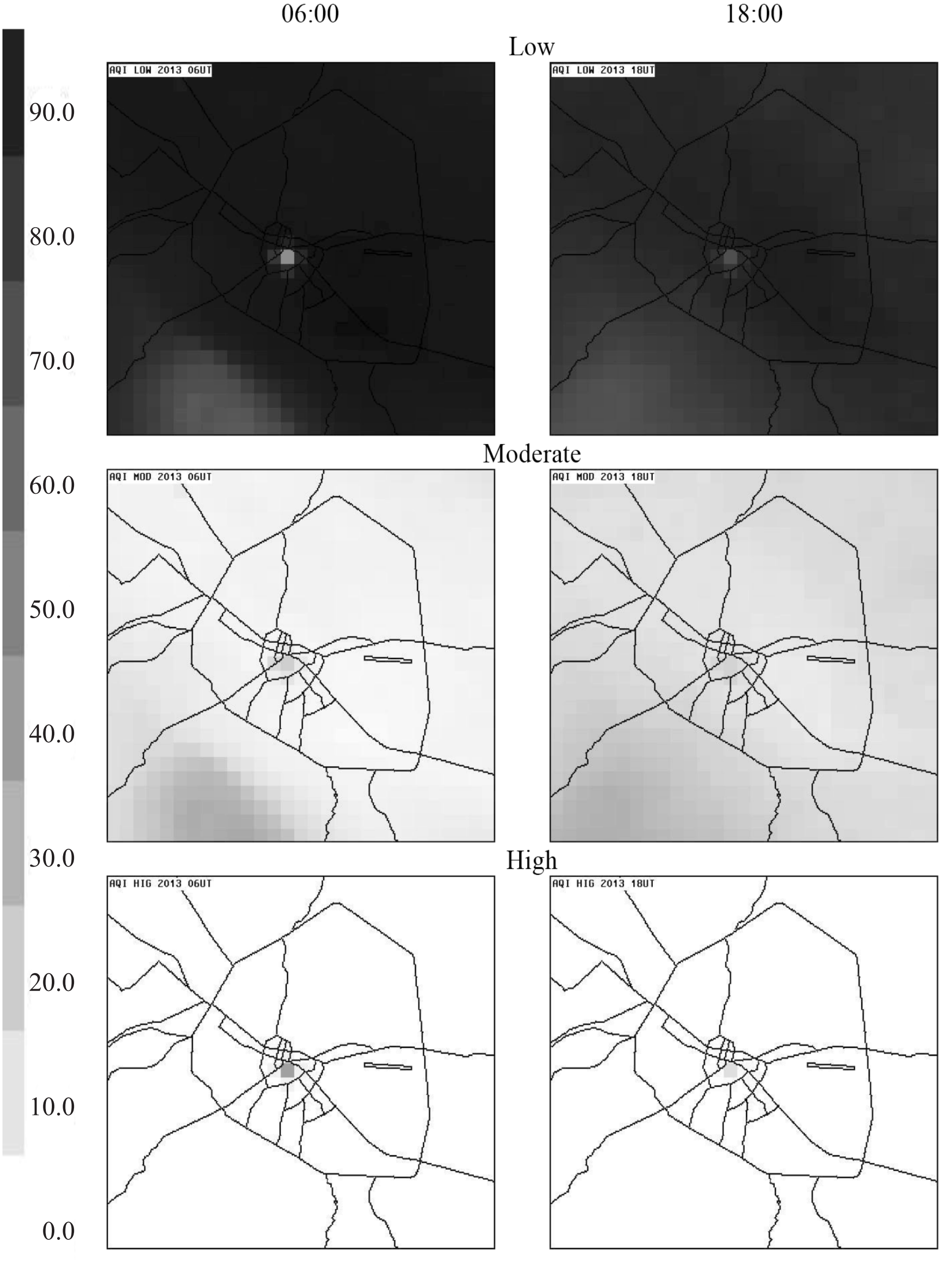

Fig. 2. Annual plots of the recurrence [%] of the AQI - Low, Moderate, and High bands in Sofia for 2013.

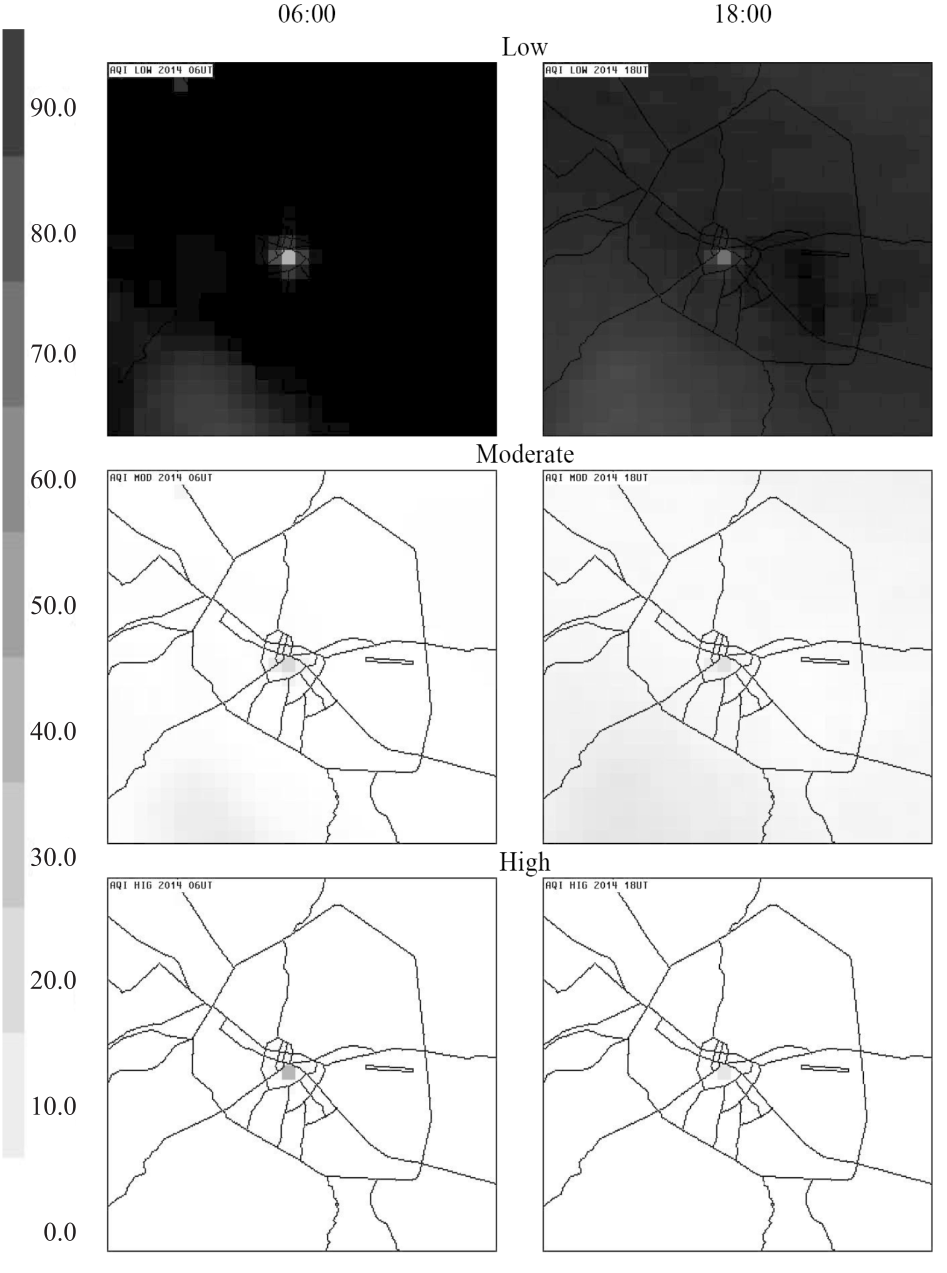

Fig. 3. Annual plots of the recurrence [%] of the AQI - Low, Moderate, and High bands in Sofia for 2014.

The pollution in the city is probably due to the surface sources like road transport and also the TPPs in the city.

Apart from these general features the climatic behavior of the AQI probabilities is rather complex with significant spatial, seasonal and diurnal variability. The areas with slightly worse AQ status are not necessarily linked to the big pollution sources. Wide rural and even mountain regions can also have significant probability for AQI from the Moderate range.

The hot spot in Sofia city, where index with higher impact (High band) is in the city center. The (High band) is relatively high - about 20 % in the morning and 10% in the afternoon.

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Оценка на качеството на въздуха за град София за 2013 и 2014

Г. Гаджев

Резюме: В настоящето изследване са представени средногодишните Индекси за качеството на въздуха през 2013 и 2014 за територията на град София. Използвани са данни за приземните концентрации на някои замърсители, моделирани от Българската система за прогноза на химическото време за изчисление на индексите. Чрез използването на математически апарат са определени индексите за качеството на въздуха, а от там и съответните повторяемости в трите категории „Ниско“, „Средно“ и „Високо“за двете години 2013 и 2014. Установяват се т.н. горещи точки, в които категория „Високо“ достига до 20%. Изказано е предположение за високите концентрации в центъра на града, че най-вероятно се дължат на приземните източници и ТЕЦ-те в града.

Proceeding of 1st International Conference on Environmental Protection and Disaster RISKs

Part One

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Air Pollution, Climate and Health

PRELIMINARY RESULTS FOR THE RECURRENCE OF AIR QUALITY INDEX FOR THE CITY OF SOFIA FROM 2008 TO 2019

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Abstract: The living environment of human beings and, obviously, the atmospheric composition has a great impact for the quality of life and human health. Air Quality (AQ) is a key element of European citizens' wellbeing and quality of life. The objectives of the present work are to conduct reliable, comprehensive and detailed studies of the impact of lower atmosphere composition on the quality of life and health risks for the population in the city of Sofia. The performed numerical simulations with the US EPA Models-3 system are for 12 years from 2008-2019 and calculated on five domains: Europe, Balkan Peninsula, Bulgaria, Sofia Municipality and Sofia City with increasing space resolution - from 81 km (Europe) to 1 km (Sofia City). The System is based on the well-known models WRF (Meso-Meteorological Model) and US EPA dispersion model CMAQ (Chemical Transport Model). As emission input the TNO data is used for the two biggest domains. For the 3 Bulgarian domains the current emission inventory prepared by Bulgarian environmental authorities is exploited.

Keywords: Air Quality Indices, air quality, quality of life, health risks.

INTRODUCTION

The Air Quality is a key element for the well-being and quality of life of human beings. According to the World Health Organization, air pollution severely affects the health of European citizens. There is increasing evidence of adverse effects of air pollution on the respiratory and the cardiovascular system as a result of both acute and chronic exposure. In particular, a significant reduction of life expectancy by a year or more is assumed to be linked to long-term exposure to high air concentrations of particulate matter (PM). There is considerable concern about impaired and detrimental air quality conditions over many areas in Europe, especially in urbanized areas, despite 30 years of legislation and emission reductions. Current legislation, e.g. the Ozone daughter directive

2002/3/EC (European Parliament, 2002), requires informing the public on AQ, assessing air pollutant concentrations throughout the whole territory of Member States and indicating exceedances of limit and target values, forecasting potential exceedances and assessing possible emergency measures to abate exceedances. For this purpose, modeling tools must be used in parallel with air pollution measurements. There are also different kind indexes for the well-being and quality of life of the humans, such as UV, Heat and Wind chill -Indexes, but they are not subject of interest in present study (Bojilova, Mukhtarov, Miloshev 2020, Evtimov, Ivanov 2008, Ivanov, Evtimov 2014, Chervenkov, Slavov, Ivanov 2019). The goals of reliable air quality studies are the efficient control and protection of population exposure as well as possible emission abatement measures. In recent years the concept of "chemical weather" arises and in many countries respective forecast systems are being developed along with the usual meteorological weather forecasts (Sofiev at al., 2006, Poupkou et al., 2008, Monteiro et al., 2005, San Jose et al., 2006, Mukhtarov, Bojilova 2017, Bojilova, Mukhtarov 2019). Air pollution easily crosses national borders. It would be cost-effective and beneficial for citizens, society and decision-makers that national chemical weather forecast and information systems were networked across Europe.

MODELING TOOLS

The present study is based on air quality simulations with US EPA Models-3 air quality modeling system, consisting of 3 models:

- **CMAQ v.4.6** - Community Multi-scale Air Quality model, http://www.cmaq-model.org /, (Denis et al. 1996, Byun, Ching 1999, Byun, Schere 2006), the Chemical Transport Model (CTM);
- **WRF v.3.2.1** - Weather Research and Forecasting Model, http://www.wrf-model.org/ , (Skamarock et al. 2007), the meteorological pre-processor to CMAQ. The Weather Research and Forecasting (WRF) Model is a next generation meso-scale numerical weather prediction system designed to serve both operational forecasting and atmospheric research needs. It is an evolutionary successor to the MM5 model. The creation and further development of WRF is due to the collaborative efforts of several US institutions like NCAR, NOAA, NCEP and others. The WRF is a fully compressible and non-hydrostatic model with terrain-following hydrostatic pressure coordinate. The grid staggering is the Arakawa-C type. One can find more info on http://www.wrf-model.org/index.php;
- **SMOKE v.2.4** - Sparse Matrix Operator Kernel Emissions Modelling System, http://www.smoke-model.org/ , (Coats, Houyoux 1996, Houyoux, Vukovich 1999, CEP 2003), the emission pre-processor to CMAQ. CMAQ demands its emission input in specific format reflecting the time evolution of all pollutants accounted for by the chemical mechanism used (CB-IV in this

case). Emission inventories are used as row data for anthropogenic emission processing. The inventories are made on annual basis for big territories; many pollutants are estimated as groups (VOC and PM2.5 for instance). Preparation of emission input to a Chemical Transport Model requires emission processing. Such emission processing component in EPA Models-3 system is SMOKE but it is partly used, here, because it's quite strong relation to US emission sources specifics. In this study SMOKE is used only for calculating biogenic (BgS) emissions and for merging Area sources (AS), Large point sources (LPS) and BgS-files into a CMAQ emission input file. The area source emissions and the large point source emissions are prepared by the interface programs AEmis and PEmis.

In the System, WRF model is driven by the NCEP data in GRIB-2 format with space resolution of 1°×1° and 6-hour time resolution. TNO inventory for 2005 (Denier van der Gon et al., 2010) is exploited partly for Bulgaria domain, TNO being the Netherlands's Organization for Applied Scientific Research. For Bulgaria itself and for the other Bulgarian domains, the National inventory for 2010 as provided by Bulgarian Executive Environmental Agency is used. That means TNO inventory is used only for the territories outside Bulgaria in the mother CMAQ's domain.

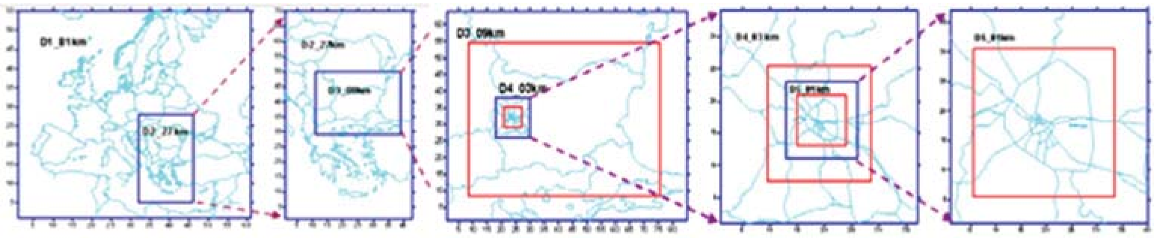

Figure 1. Five computational domains (CMAQ domains are nested in WRF ones)

The nesting capabilities of WRF and CMAQ are used to downscale the simulations from European region to the Sofia city area. The resolution of the mother domain (Europe) is 81 km, big enough as to correspond to met-data space resolution. Four other domains are nested in it and in each other – Balkan Peninsula (27km resolution), Bulgaria (9 km), Sofia municipality (3 km) and Sofia city (1 km) as shown in Fig. 1. The climatic data is used for chemical boundary conditions following the presumption that the errors introduced by this assumption will decrease quickly to the centre of the domain due to the continuous acting of the pollution sources. All other domains receive their boundary conditions from the previous domain in the hierarchy.

The post-processing program XtrCON extracts part of the pollutants for archiving and further handling. Only surface values of the most important pollutants are saved

- 8 gases and 11 aerosols (including PM10 and PM2.5). Part of these pollutants is more or less monitored and they are referred in the European legislation with the respective thresholds. For the moment it presents 4 main pollutants - Ozone, NO_2, SO_2 and PM10 which are used to calculate the Air Quality Indices (AQI). Calculation of the Air Quality (AQ) impact on human health and quality of life in Sofia city is the objective of the present study. The impact is calculated in the terms of the so called AQI – an integral characteristic directly measuring the effects of AQ on human health. The calculations are made on the basis of long term AQ simulations, which make it possible to reveal the climate of AQI spatial/temporal distribution and behaviour.

The AQI is defined as a measure of air pollution seen in the context of its impact on human health. It provides an integrated assessment of the impact of the whole range of pollutants on human health and is calculated based on the concentration of various pollutants obtained from measurements or numerical modeling. The index is defined in several segments (EPA, 2009), each of which is a linear function of the concentration of each considered pollutant:

$$I = ((I_{high} - I_{low}) / (C_{high} - C_{low}))(C - C_{low}) \tag{1}$$

where:
I = the AQI,
C = the pollutant concentration,
C_{low} – the concentration breakpoint that is ≤ C,
C_{high} – the concentration breakpoint that is ≥ C.
I_{low} – the index breakpoint corresponding to C_{low}.
I_{high} – the index breakpoint corresponding to C_{high}.

In that calculation the index falls in one of the ranges of the dimensionless scale. In each range index values are associated with an intuitive colour code, a linguistic description and a health description.

Pretty often in order to evaluate the air quality situation in European cities, all detailed measurements are transformed into a single relative figure: the Common Air Quality Index (CAQI) and this index have 5 levels using a scale from 0 (very low) to > 100 (very high). The index is based on 3 pollutants of major concern in Europe: PM10, NO_2, O_3 and will be able to take into account to 3 additional pollutants (CO, PM2.5 and SO_2).

One of the most commonly used air quality index is the UK Daily Air Quality Index (Leeuw, F. de, Mol, W., 2005), also used in Bulgaria (Etropolska et al. 2010), (Syrakov et al, 2012, 2013, 2014a, 2014b, 2015), (Georgieva, I., 2014), (Georgieva et al. 2015), (Georgieva, I. and Ivanov, V., 2017, 2018), (Ivanov, V. and Georgieva, I., 2017) and (Gadzhev 2018).

RESULTS

Annual recurrence of AQI in “Low”, “Moderate” and “High” bands over territory of Sofia city from 2015 to 2019 and average recurrence for the whole period 2008-2019 (08-19):

Figure 2 demonstrate the spatial and diurnal variation of the annual recurrence of Low band for the chosen hours 04:00, 12:00 and 18:00UTC for the chosen periods. Here we have to mention that in the Low range the air is most clean, so high recurrence values mean more cases with clean air (red colour) and lower recurrence values mean (blue colour), less cases with clean air (worse AQ status). What can be noticed is: the recurrence in Low range is different for all years at 04:00UTC.

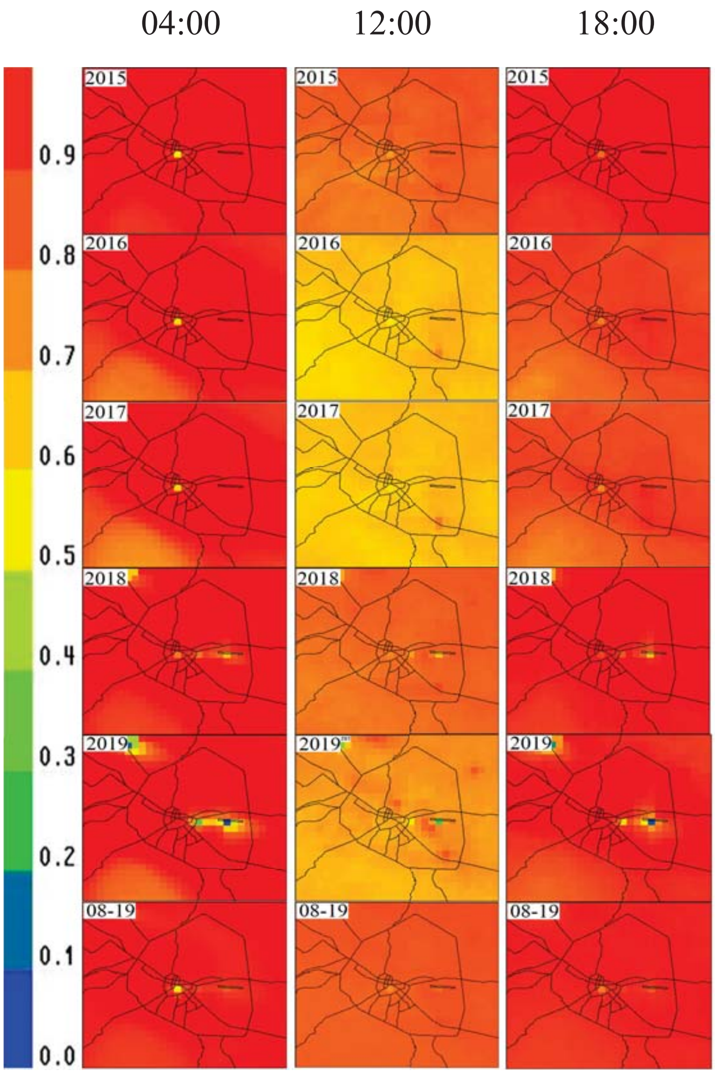

Figure 2. Annual recurrence of AQI in “Low” band over territory of Sofia city from 2015 to 2019 and average recurrence for the whole period 2008-2019 (08-19)

In 2015, 2018 and 08-19 at 12:00 UTC the recurrence in Low band is bigger than this in 2016, 2017 and 2019. While at 18:00 UTC the higher recurrence is in 2015, 2018, 2019 and 08-19. The high polluted areas are the city centre at 04:00 and two spots (Kostinbrod and Sofia airport) in 2019 and they are very well displayed in figure.

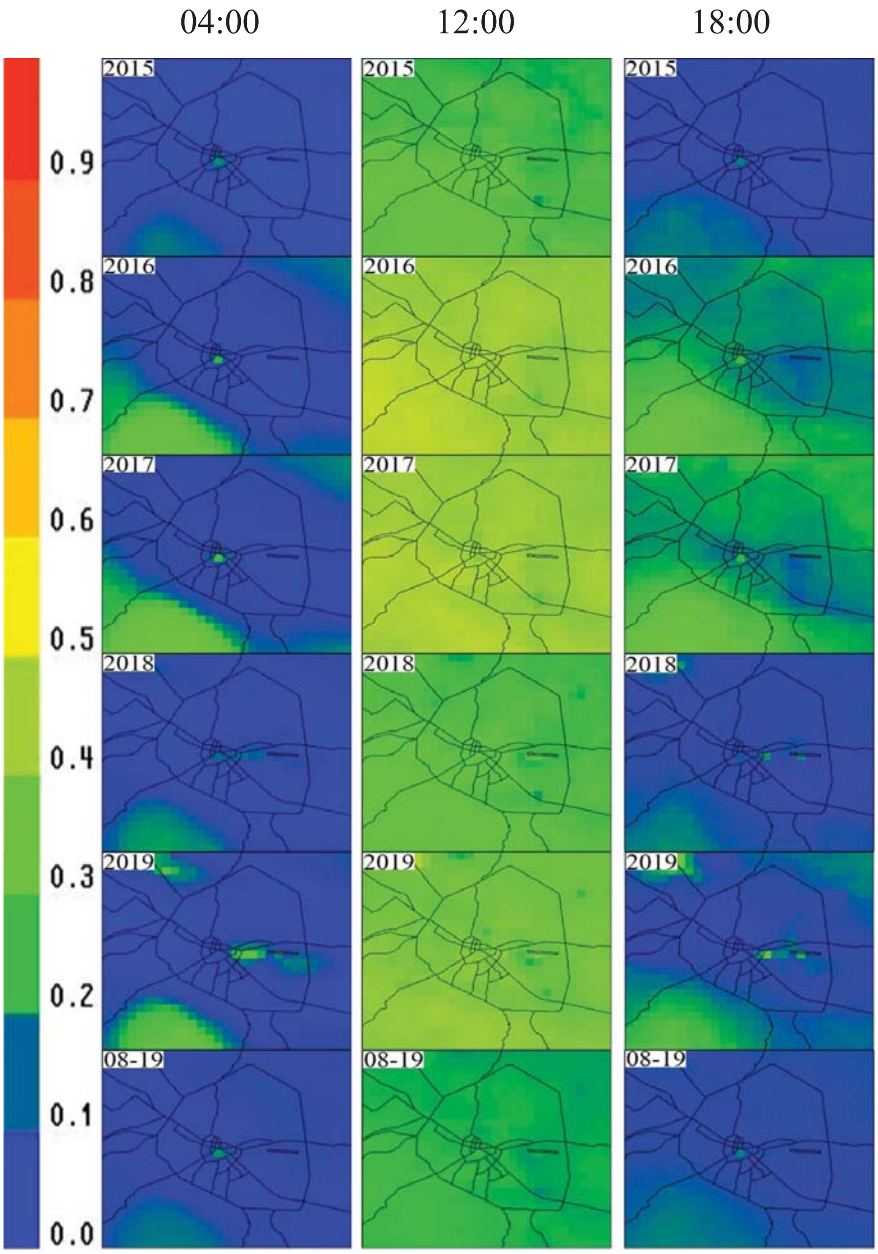

Figure 3. Annual recurrence of AQI in "Moderate" band over territory of Sofia city from 2015 to 2019 and average recurrence for the whole period 2008-2019 (08-19)

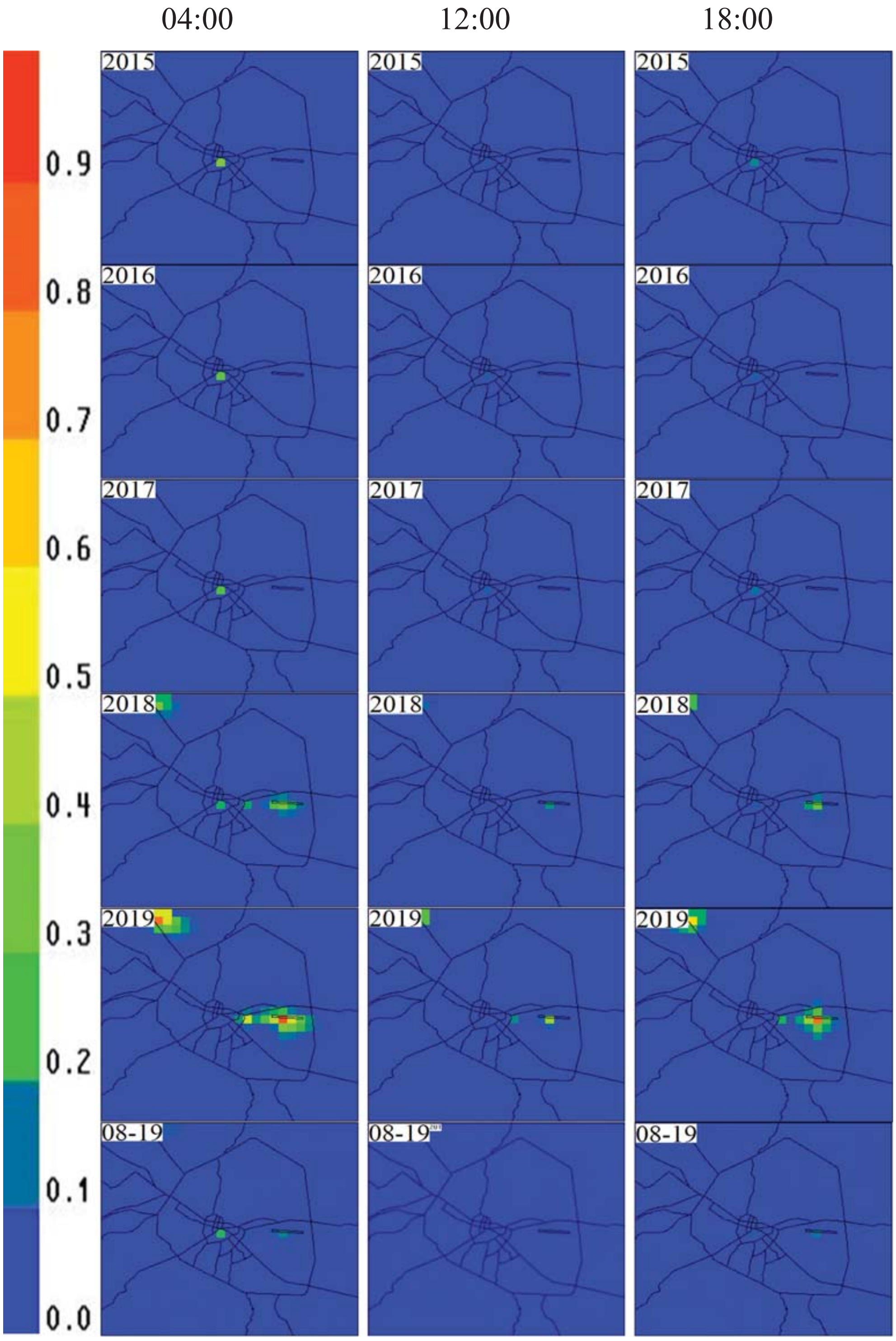

Figure 4. Annual recurrence of AQI in "High" band over territory of Sofia city from 2015 to 2019 and average recurrence for the whole period 2008-2019 (08-19)

In Figure 3 and Figure 4 (Moderate and High ranges) - high recurrence values means less favourable and respectively bad AQ status. It can be seen that most areas with high recurrence of cases with lower AQ status are at noon in the whole domain and mostly over the Vitosha Mountain in other hours. This is due to the intensive O_3 photo-chemistry reactions, the higher NO_2 concentrations lead to production of higher O_3 concentration. The major NO_2 sources in the city are the surface sources (road transport). It can be seen at 18:00 UTC in 2016 and 2017 where over the road network it leads to decreasing of O_3 concentration and with that improving the AQ status. Average for the 2008-2019 in Moderate band at 18:00 UTC it can be also noticed about 10-20% recurrence with not so good AQ status over Vitosha Mountain. Higher values over the Vitosha Mountain in the night and the afternoon are due to the higher concentration of O_3 in mountain areas and intensive ozone transport from higher levels (intensive turbulence during midday). The behavior of the surface ozone is complex. The O_3 in Bulgaria is to a great extent due to transport from abroad and above (Gadzhev et al. 2013 and Kaleyna et al. 2013a, 2013b, 2014). This is the reason why the O_3 concentrations early in the morning are smaller (less intensive transport from higher levels), and higher at noon and afternoon (more turbulent atmosphere (more intensive transport from higher levels) and O3 photochemistry).

The high recurrence of cases in Figure 4 with most polluted air (High band) appears again in the city centre almost at all hours in all years. In the city centre can be observed more than 20% "High" pollution in the night and 10% at the day.

Bad AQ status from the High band almost never disappears. In 2018 and mostly in 2019 it’s make impression that the cases with more worse AQ status are much higher than the other years, as the recurrence around the Kostinbrod, TPP Sofia and Sofia airport can reach about 70% at the different time of the day.

At the plots for average for the 2008-2019 in High band can be seen that at all hours there are places with worst AQ status where the recurrence is almost 20% of all happened cases.

CONCLUSIONS

The simulations for Sofia city show that the air quality status of Sofia is not so good (evaluated with a spatial resolution of 1km).

AQ status falls mostly in Low and Moderate bands, but the recurrence of cases with High pollution is close to 20% mostly at the city center.

The recurrence of cases in Low and Moderate bands has been different for different years.

The pollution in the city is probably due to the surface sources like road transport and also the TPPs in the city and Sofia airport.

Apart from these general features the climatic behavior of the AQI probabilities is rather complex with significant spatial, seasonal and diurnal variability. The areas with slightly worse AQ status are not necessarily linked to the big pollution sources. Wide rural and even mountain regions can also have significant probability for AQI from the Moderate range.

The hot spot in Sofia city, where index with higher impact (High band) is the city center. The recurrence in High band is relatively high - about 20 % in the morning and 10% in the afternoon.

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Air Pollution, Climate and Health

MODELLING OF THE SULPHUR AND NITROGEN DEPOSITIONS OVER THE BALKAN PENINSULA BY CMAQ AND EMEP-MSC-W – PRELIMINARY RESULTS

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Abstract. The air quality US EPA models-3 system consisting of SMOKE - emission model and pre-processor, MM5 – meteorological driver, and CMAQ – chemical-transport model, is used in many studies of the air quality in the Balkan Peninsula, and in particular Bulgaria. It runs in different model resolutions, depending on the domain, from European to city scale. The EMEP-MSC-W model is another chemical transport model, widely used in air quality modelling. Two of the processes involved in the concentration change of some pollutant are the dry and wet depositions. The air quality modelling capability depends on many factors, for example, meteorology and emissions. We study the differences in the simulation of the wet and dry depositions for nitrogen and sulphur compounds, between the CMAQ and the EMEP-MSC-W model for a period of 8 years.

Keywords: modelling**;** CMAQ; EMEP**;** pollution; composition; air quality

INTRODUCTION

The air pollution nowadays forces many countries to take actions for mitigating its adverse effects on human health. Therefore, we need a lot of information, which is increasing in recent years. There are already more direct and indirect data connected to the air quality from different surface-based and satellite-based observing systems. However, we need to understand the different processes involved in the creation, transportation, and transformation of the air pollutant species, which help us to understand their distribution at different spatial and temporal scales. The research community performs these tasks by air quality models systems, with chemical transport models as the main component. We use one of these systems with the chemical transport model CMAQ, for modeling the air quality in the Balkan Peninsula. Previous results from air pollution modelling for the Balkan Peninsula and Bulgaria are published in a lot of research works (Gadzhev et al. 2014, Georgieva 2014, Syrakov et al. 2015, Kaleyna, Mukhtarov, Miloshev 2013a, 2013b, 2014). The air composition is formed by several processes, which involve dry deposition, wet deposition, horizontal and vertical advection, horizontal and vertical diffusion, emission, chemical transformation, aerosol processes, and aqueous chemistry (Gadzhev, Ganev, Mukhtarov 2020, Gadzhev et al. 2011). They interact in between and determine the air composition at different scales. There are some studies with CMAQ of the dry and wet deposition and their influence on the precipitation for Bulgaria (Syrakov et al. 2019a, 2019b, Georgieva et al. 2017, 2019) for different periods up to two years. Another chemical transport model – EMEP-MSC-W is also widely used for air quality studies in Europe (Simpson et al. 2012). Our aim is to make a preliminary study of the model comparison between long-term high-resolution simulations with the CMAQ and the EMEP-MSC-W simulations of the Nitrogen (N) and Sulphur (S) dry and wet deposition processes in the Balkan Peninsula for a long-term period and high spatial resolution.

METHODOLOGY

The study is based on air quality simulations with two chemical transport models over the Balkan Peninsula from 2000 to the 2007 year. One of these simulations is performed with the US EPA Models-3 system, which includes CMAQ (Community Multiscale Air Quality) model (Denis et al. 1996, Byun, Ching 1999, Byun, Schere 2006), SMOKE (Sparse Matrix Operator Kernel Emissions Modelling System) (Coats, Houyoux 1996, Houyoux, Vukovich 1999, CEP 2003) and the regional mesoscale meteorological model MM5. The CMAQ is a numerical chemical transport model for modelling the different processes and their contribution involved in changing the surface and airborne gases and aerosols. That model needs three kinds of input information – initial and boundary conditions, meteorology, and emissions.

We use the regional mesoscale numerical model MM5 for modelling the weather and climate conditions (Dudhia 1993, Grell, Dudhia, Stauffer) over the Balkan Peninsula. It is a non-hydrostatic high-resolution model, providing the needed raw meteorological output for further processing. We use the nesting capabilities of the MM5, where the output from each outer domain excluding the last one, is used as input for the smaller one. The first and the bigger one (D1) is the European domain with background information, provided from the NCEP Global Analysis Data with 1º x 1º (~81 x 81km) horizontal resolution. Our research work is concentrated on the domain D3 geographically limited to the Balkan Peninsula and some adjacent territories. The output from the MM5 model, need to be reprocessed to the right format for ingesting in the CMAQ. For that purpose, we use the Meteorological – Chemistry Interface Processor – MCIP, which prepares all meteorological input information CMAQ needs.

The emissions from the large source sources and area sources for the whole domain excluding Bulgaria and some adjacent territories are ingested from the TNO high-resolution emission inventory with spatial resolution 0.25°x0.125° (Denier van der Gon et al., 2010) in a longitude-latitude grid, reprocessed from the 50-km grid of the EMEP (European Monitoring and Evaluation Programme) database. The emissions for Bulgaria are from the National Emission Inventory. The CMAQ needs also from biogenic emissions. They are provided from the emission pre-processor SMOKE. The input information is provided from the TNO emissions, the MCIP output, and the land-use database.

The CMAQ model accounts for the following processes with a different contribution to the changing of the concentration field for each pollutant: horizontal diffusion (HDIF); horizontal advection (HADV); vertical diffusion (VDIF); vertical advection (VADV); dry deposition (DRYDEP); emissions (EMISS); chemical transformations (CHEM); aerosol processes (AERO); cloud processes (CLOUD). The solution of the transport and transformation equations gives the mean concentration change of $i^{\text{-th}}$ pollutant in the first model layer from time t to time t + Δt.
It is presented as a sum of the contribution of the former processes:

$$\Delta c_i^1 = \left(\Delta c_i^1\right)_{hdif} + \left(\Delta c_i^1\right)_{vdif} + \left(\Delta c_i^1\right)_{hadv} + \left(\Delta c_i^1\right)_{vadv} + \left(\Delta c_i^1\right)_{drydep} + \left(\Delta c_i^1\right)_{emiss} + \left(\Delta c_i^1\right)_{chem} + \left(\Delta c_i^1\right)_{cloud} + \left(\Delta c_i^1\right)_{aero}$$

$$\Delta c_i^1 = \frac{1}{h_1}\int_0^{h_1} \left(c_i(t+\Delta t) - c_i(t)\right)dz$$

We focus on the dry and wet depositions modelled by the CMAQ in this study. The N deposition contains the contribution from NO_2 (Nitrogen dioxide), NO (Nitrogen oxide), NO_3 (Nitrogen trioxide), N_2O_5 (Dinitrogen pentoxide), HNO_3 (Nitric acid), HONO (Nitrous acid), ANH_{4J} (Accumulation-mode ammonium mass), ANH_{4I} (Aitken-mode ammonium mass), ANO_{3J} (Accumulation-mode nitrate mass), ANO_{3I} (Aitken-mode aerosol nitrate mass) and NH3 (Ammonia):

$$N_{deposition} = NO_2 + NO + NO_3 + N_2O_{25} + HNO_3 + HONO + ANH_{4J} + ANH_{4I} + ANO_{3J} + ANO_{3i}$$

The S deposition contains the contribution from SO_2 (Sulphur dioxide), SULF (Sulphate aerosols), ASO_{4J} (Accumulation-mode aerosol sulphate mass), and ASO_{4I} (Aitken-mode aerosol sulphate mass):

$$S_{deposition} = SO_2 + SULF + ASO_{4J} + ASO_{4I}$$

The CMAQ deposition output is in 1-hour frequency. Therefore, we sum up the hourly values of the N and S components for every day of the simulation, finding the daily deposition values.

The second model used for comparison with the previous one is with the Meteorological Synthesizing Centre-West (MSC-W) of the European Monitoring and Evaluation Programme (EMEP). It is a chemical transport model (Simpson et al., 2012), a key tool involving in the European air pollution policy assessments. In the beginning, the model covers the whole of Europe with a resolution of about 50 km x 50 km, with vertical levels up to the tropopause (100 hPa). The model has changed over the years, adding different features, and currently, his horizontal resolution ranging from 5 km to 1 degree with 20 vertical levels. In our study, we use a grid size 0.1° x 0.1°. The EMEP-MSC-W model runs with meteorological fields from the numerical weather prediction system ECMWF-IFS Cycle36r1. The model output is with daily frequency, so we do not need to do further post-processing.

For comparison of the models, we use two kind of error characteristics. The first is Normalised Mean Bias noted as (NMB):

$$NMB = \frac{\sum_i M - \sum_i E}{\sum_i E},$$

and the second is the Mean Bias (MB):

$$MB = \frac{1}{n}\sum_i M - \frac{1}{n}\sum_i E$$

The notions in these equations are i - ith value, M - the output form CMAQ, E - the output from EMEP-MSC-W. The results are revealed with the multiyear averaged values of the NMB for each grid point and the annual spatial-averaged values of the bias of the CMAQ output.

RESULTS

The results are given for the N depositions and for the S depositions, separated in dry component, wet component, and total (dry+wet) component. The multiyear average of the S dry, wet, and total depositions (figure 1) reveals the following features. There is a difference between the CMAQ and the EMEP-MSC-W model due to the difference in the emission inventories. We can clearly note the missing of some of the S sources in one model, but not in the other. We can see from the sum of dry and wet deposition shown on the figure, that the TPP Bobov dol, the TPP Pernik, the Sofia city, the town of Devnia, the Bucharest city and the Istanbul city are noticeable in the CMAQ model output, but not in the EMEP-MSC-W output. On the other hand, Zlatna Panega and Southern Italy sources show up in the EMEP output, but not in the CMAQ one. The influence of the input meteorological data and the meteorological driver for the models have a considerable effect mainly on the wet deposition modelling capability. The wet deposition in the EMEP-MSC-W model has smaller spatial gradients, more intensive and local maximums on larger areas around the corresponding sources. On the other hand, the wet deposition in the CMAQ has smaller values and bigger local spatial gradients.

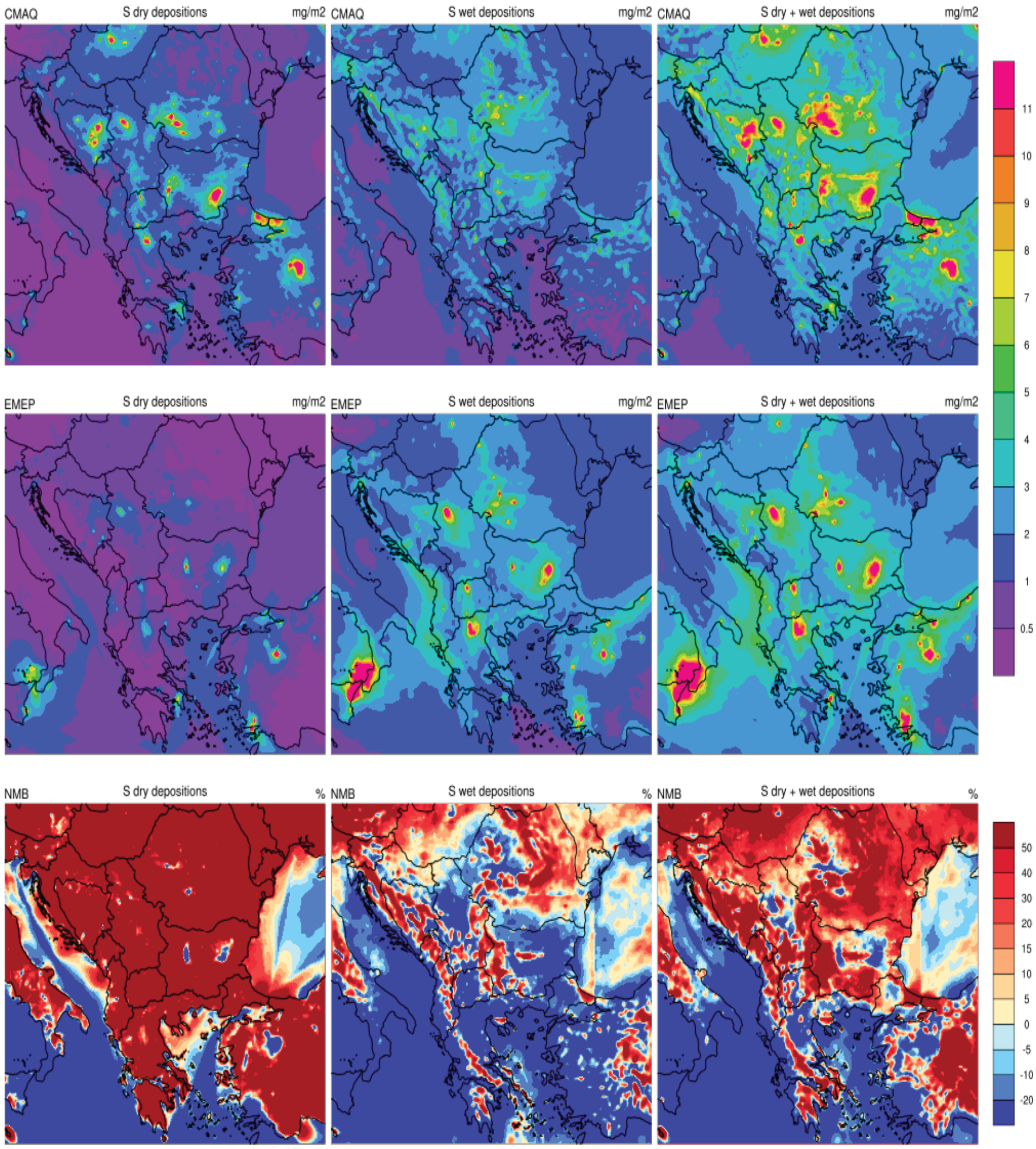

Figure 1. CMAQ (upper row) multiyear average sulphur dry deposition (left plot), wet deposition (middle plot) and dry + wet (right plot). EMEP-MSC-W (middle row) multiyear average Sulphur dry deposition (left plot), wet deposition (middle plot) and dry + wet (right plot). Normalized mean bias [%] of the CMAQ model (lowest row) for sulphur dry deposition (left plot), wet deposition (middle plot) and dry + wet (right plot) in comparison to the EMEP-MSC-W.

The influence of the meteorological conditions and the orography is more notable for figure 1 where the normalized mean biases are shown. The normalized mean bias of the dry deposition over the land areas reaches 50 % and more and only above some of the sources is negative. The normalized mean bias of the sum of the dry and wet depositions has a similar spatial structure with one of the wet depositions for the two models but is more complex. The CMAQ and EMEP-MSC-W simulate the annual area-averaged dry plus wet deposition in a quite similar way from 2000 to 2007, as is shown in table 1. Although more or less different in particular years, they are close. The bias from 2000 to 2003 is negative (figure 2), which is easy to suggest from the area-averaged total depositions and the CMAQ bias for the whole period.

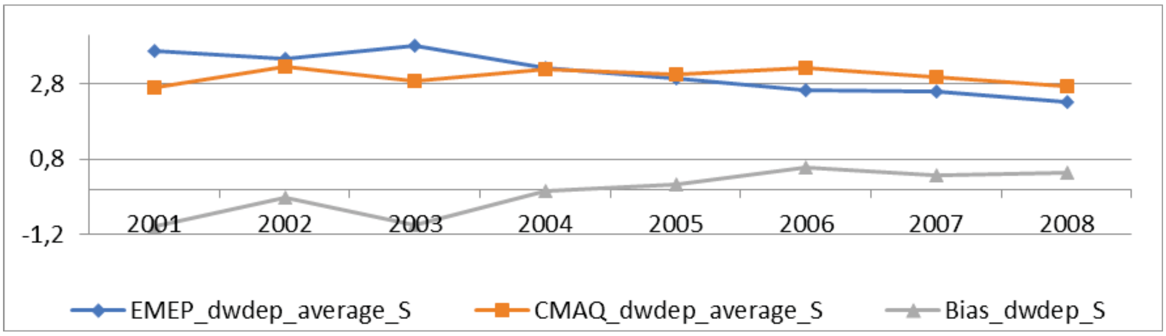

Figure 2. Annual area averaged Sulphur total (dry + wet) depositions and bias of the CMAQ model

Table 1. Annual area averaged and multiyear area averaged (YA) Sulphur total (dry + wet) depositions

Year	EMEP dry + wet average S (mg/m^2)	CMAQ dry + wet average S (mg/m^2)	Bias of dry+ wet S (mg/m^2)
2000	3.6684	2.6886	-0.9798
2001	3.4655	3.2473	-0.2182
2002	3.8176	2.8822	-0.9355
2003	3.2111	3.1706	-0.0405
2004	2.9467	3.0579	0.1112
2005	2.6357	3.2199	0.5842
2006	2.5942	2.965	0.3708
2007	2.3126	2.7426	0.4299
YA	2.9426	3.0188	0.0762

The result for the N depositions is shown in figure 3. They have different spatial and temporal features from the S ones. As is seen in figure 3, the model difference between the dry depositions appears in the almost homogeneous distribution for the CMAQ, in contrast to the clearly outlined sources in the EMEP-MSC-W. The input meteorological data and the meteorological driver for the models exert substantial influence mostly on the wet deposition modelling. The spatial gradient of the mean EMEP-MSC-W wet deposition is smaller than the CMAQ one. However, the CMAQ mean wet deposition is smaller and with bigger local spatial gradients following the orography features. The results for the normalized mean biases of the dry, wet, and sum of the dry and wet depositions (figure 3) suggest a substantial influence of the

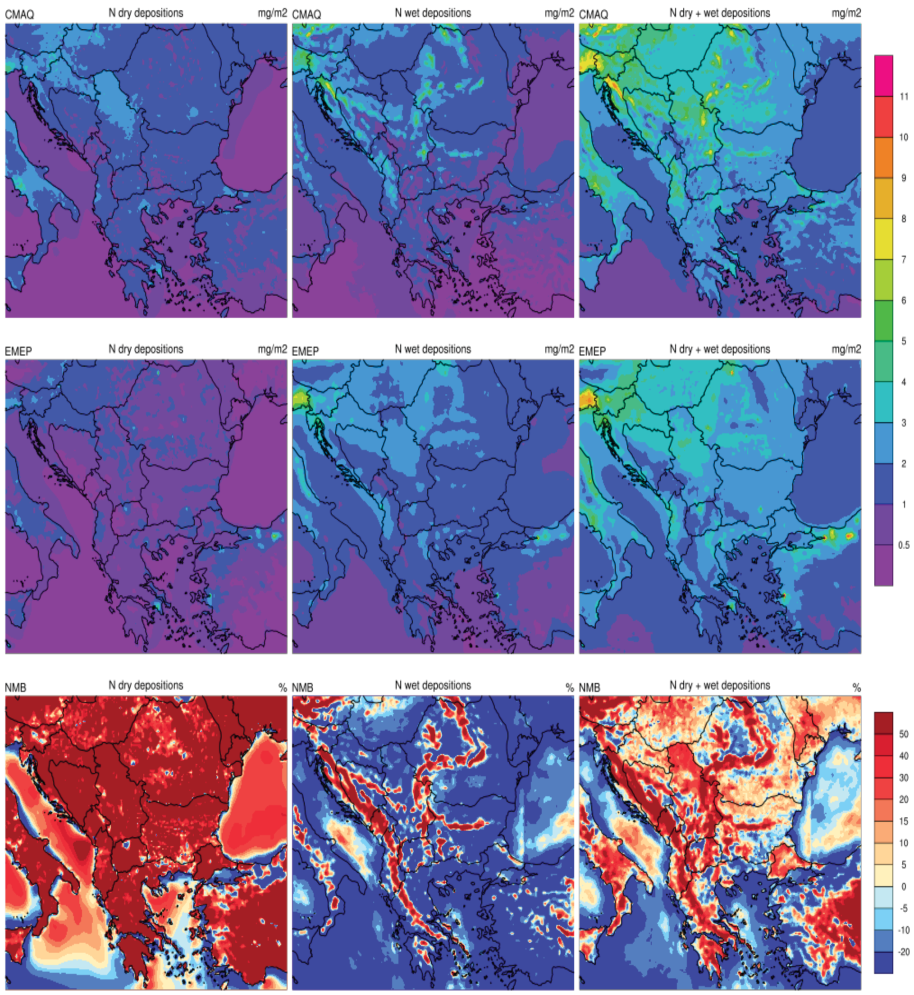

Figure 3. CMAQ (upper row) multiyear average Nitrogen dry deposition (left plot), wet deposition (middle plot) and dry + wet (right plot). EMEP-MSC-W (middle row) multiyear average nitrogen dry deposition (left plot), wet deposition (middle plot) and dry + wet (right plot).). Normalized mean bias [%] of the CMAQ model (lowest row) for nitrogen dry deposition (left plot), wet deposition (middle plot) and dry + wet (right plot) in comparison to the EMEP-MSC-W

meteorological input and the orography on the spatial distribution of the mean wet deposition. The normalized mean bias of the mean dry deposition reaches 50% not only on the land however, is negative in some places. The normalized mean bias of the sum of the dry and wet depositions has a similar, but a more complex structure with the one of the wet deposition, because of the influence of the dry deposition.

The data in table 2 and figure 4 suggest that the simulated annual area-averaged total nitrogen depositions by the CMAQ and EMEP-MSC-W models pretty much the same, although the CMAQ value is smaller in 2002. The results for the multiyear area-averaged total nitrogen depositions are very similar.

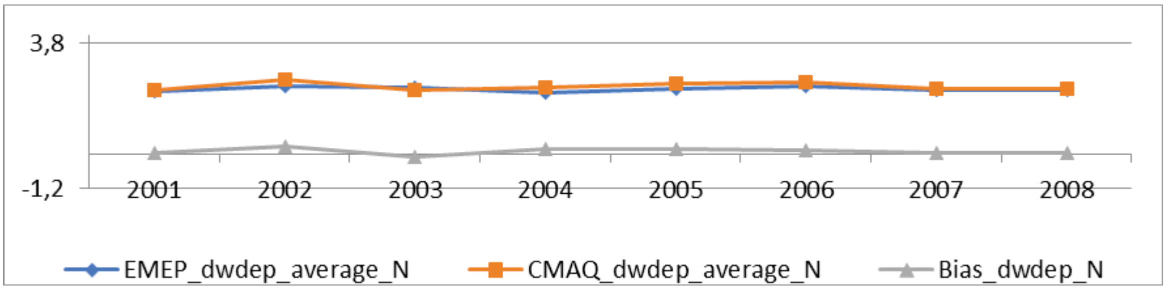

Figure 4. Annual area averaged Nitrogen total (dry + wet) depositions and bias of the CMAQ model.

Table 2. Annual area averaged and multiyear area averaged (YA) Nitrogen total (dry + wet) depositions

Year	EMEP dry + wet average N (mg/m^2)	CMAQ dry + wet average N (mg/m^2)	Bias of dry+ wet N (mg/m^2)
2000	2.1538	2.1827	0.0289
2001	2.3273	2.5671	0.2398
2002	2.2701	2.1798	-0.0903
2003	2.1185	2.285	0.1665
2004	2.2455	2.4198	0.1743
2005	2.3357	2.451	0.1153
2006	2.1773	2.2341	0.0568
2007	2.1989	2.2235	0.0246
YA	2.2331	2.3286	0.0955

CONCLUSION

The results suggest that the Nitrogen annual area-averaged total depositions are represented more similarly by the two models, than the Sulphur ones. There is a large orography influence on the sum of dry and wet deposition for both groups of chemical species. The current research suggests that the orography and meteorology exert substantial influence on the total Nitrogen and Sulphur depositions.

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Proceeding of 1st International Conference on Environmental Protection and Disaster RISKs

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ASSESSMENT OF THE FUTURE CLIMATE OVER SOUTHEAST EUROPE BASED ON ENSEMBLE OF CLIMATE INDICES – PART ONE: CONCEPT AND METHODS

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Abstract: Nowadays there is a strong degree of agreement that the climate change is the defining challenge of our time. The analysis based on climate indices is probably the most widely used non-parametric approach for quantification of extreme climate events. This study which consist of two parts, is dedicated on the assessment of the spatial patterns and the temporal evolution of 6 temperature-based and 3-precipitation based indices in projected future climate over south-east Europe up to the end of the century. The annual means of the daily mean and extreme temperatures are also analysed in consistent manner. The indices are computed from the bias-corrected output of 5 CMIP5 global models, forced with all 4 RCP emission scenarios. The multi model ensemble medians of the temperature-based indices shows considerable warming which is consistent with the increase of the mean temperatures and is statistically significant in most cases. The revealed changes of the precipitation-based indices are more complex when compared with temperature changes.

Keywords: climate indices, CMIP5 ensemble, RCPs, future climate, South-east Europe

INTRODUCTION

There is a strong degree of agreement that the climate change is the defining challenge of our time. It will exert influence on the ecosystems, on all branches of the international economy, and on the quality of life. The globally averaged surface temperature of the Earth increased 0.85°C over the 1880 to 2012 period. It is extremely likely that the observed warming of the climate system was caused by the increased anthropogenic emission of greenhouse gases (IPCC, 2013). However, immediate damages to humans and their properties as well as to ecosystems are not obviously caused by gradual changes in temperature or precipitation but mainly by so-called extreme climate events (Sillmann & Röckner, 2007). The rare occurrence of extremes makes it necessary to investigate long data records to determine significant changes in their frequency and intensity. To this end, global circulation models (GCMs) or, more generally, coupled atmosphere-ocean general circulation models (CAOGCM) are physically consistent way to simulate past, present, and future climate states inclusive extreme events. Regional Climate Models (RCM) applied with higher spatial resolution over a limited area and driven by GCMs can provide more appropriate information on such smaller scales supporting more detailed impact and adaptation assessment and planning (Rummukainen, M., 2010; Belda et al., 2015; Giorgi & Gutowski, 2015). Therefore RCMs have an important role to play by providing projections with much greater detail and more accurate representation of localized extreme events (Gadzhev et al., 2021). The Working Group on Coupled Modelling (WGCM) established the Coupled Model Intercomparison Project (CMIP) as a standard experimental protocol for studying the output of CAOGCMs. CMIP provides a community-based infrastructure in support of climate model diagnosis, validation, intercomparison, documentation and data access (Taylor et al., 2009). The main aim of the fifth phase of CMIP, CMIP5, is to study the climate and climate change in the past, present and future, using a set of simulations with different climate simulators in various spatial and temporal scales (Taylor et al., 2012).

The Mediterranean region lies in a transition zone between the arid climate of North Africa and the temperate and rainy climate of central Europe and it is affected by interactions between mid-latitude and tropical processes. Because of these features, even relatively minor modifications of the general circulation, e.g. shifts in the location of mid-latitude storm tracks or sub-tropical high pressure cells, can lead to substantial changes in the Mediterranean climate (Giorgi & Lionello, 2008). In addition to planetary scale processes and teleconnections, the climate of the Mediterranean is affected by local processes induced by the complex physiography of the region and the presence of a large body of water (the Mediterranean Sea).

Several projects and, consequently, many studies are dedicated in the recent decades on the climate projections over Europe and the Mediterranean basin. The CMIP5 projections generally agree on warming in all seasons in Europe during this century, while precipitation projections are more variable across different parts of Europe and seasons (Belda et al., 2015). Despite of the overall agreement for general reduction of the precipitation amount in the middle and at the end of the 21th century, there are still many differences in the magnitude of the expected changes, annual and seasonal variability and areal distributions (Dai, 2013; Giorgi & Lionello, 2008; Orlowsky & Seneviratne, 2012; Ulbrich et al., 2006). Part of the problems could be attributed to the models deficiencies of the precipitation simulation. The model estimations includes also non-negligible uncertainties which results, in particular, in a less spatially coherent pattern of change, bigger inter-model spread and a lower level of statistical significance when compared with temperature changes (Alexander et al., 2006). In Sillmann et al. (2013a) is demonstrated that GCMs underestimate observed precipitation magnitudes, although CMIP5 models show an improvement compared to CMIP3. The results of Orlowsky & Seneviratne (2012) show that despite the uncertainty in other regions, droughts have increased in the Mediterranean and are projected to increase further, emphasizing the need for proactive adaptation planning. Central and Eastern Europe is a region where precipitation changes remain also still uncertain (Belda et al., 2015). Although regional climate change amplitudes of temperature and precipitation in Europe follow global trends, they can be also affected by changes in the large-scale circulation and regional feedback processes (Kjellstrom et al., 2011). In the comprehensive study of Stagge et al. (2015) is used of the RCMs outcome from CORDEX (the Coordinated Regional Climate Downscaling Experiment – see Kotlarski et al., 2014 for details), forced with CMIP5 climate projections, to quantify the projected change in meteorological drought for Europe during the 21th century, revealing increasing projected drought throughout the Mediterranean, including the eastern Mediterranean. In agreement with previous studies, in Sillmann & Röckner (2007) is evidenced a considerable intensification of heat and water stress in the region.

The free worldwide exchange of methods, software and especially data is from essential importance for the expert community of the geophysical sciences. Such services are provided either from the primary vendors (institutions, organisations or projects) or from single point access portals as the Copernicus Data Store (CDS). They are reliable source for elaboration of objective climatologies, both in regional (Birsan et al., 2014; Chervenkov et al., 2019; Chervenkov & Slavov, 2019; Spinoni et al., 2018) and global (Sillmann et al., 2013a, 2013b; Orlowsky & Seneviratne, 2012) scale for recent and projected future climate as well as for development of various custom-tailored applications. Our working group uses also this possibility in optimal way. The present article, which is the first part of more common work, describes shortly 5 collected and/or implemented by the authors data bases in our general effort to describe the historical, near past and recent as well as the projected future climate over south-east (SE) Europe most concisely and comprehensively.

The work is organized as follows. The CMIP5 scenarios and the used models are described in Section 1. Section 2 is dedicated on the used methods and the considered data bases. Section 3 and Section 4 are the core of the present study. Due to their importance, the first one, ‘Results for the mean temperatures’, is dedicated solely on these variables. In the second one are described the results for the other indices. The concluding remarks are in the last section.

1. CMIP5 SCENARIOS AND USED MODELS

The CMIP5 experiment uses new emission scenarios called representative concentration pathways (RCP) (Moss et al., 2010) to assess the interactions between the human activities on the one hand and the environment on the other hand, and their evolution. Unlike the CMIP3 scenarios, the RCPs are mitigation scenarios that assume policy actions will be taken to achieve certain emission targets. For CMIP5, four RCPs have been formulated: RCP2.6, RCP4.5, RCP6.0 and RCP8.5. They are based on a range of projections of future population growth, technological development, and societal responses. The labels for the RCPs provide a rough estimate of the radiative forcing in the year 2100 (relative to pre-industrial conditions). RCP2.6 represents mitigation scenarios that aim to limit the increase of global mean temperature to <2°C. Different than other RCPs and earlier CMIP3 scenarios, RCP2.6 has a peak in greenhouse gases (GHG) concentration arround 2050 and then declines at a moderate rate. Under RCP4.5, GHG-emissions will peak around the early 2050s and then stabilize, causing a CO_2 equivalent of about 650 parts per million and a temperature increase of approximately 1.8–2.0°C in 2100, compared to the control period of 1986–2005. RCP8.5, on the other hand, predicts a continuous rise of GHG emissions until 2100, causing a CO_2 equivalent larger than 1370 ppm and a global average temperature increase close to 4°C (Spinoni et al., 2018).

The CMIP3 and CMIP5 model output are available from the data archives of the Program for Climate Model Diagnosis and Intercomparison (PCMDI) and the Earth System Grid data distribution portal (ESG). To generate the considered in this study indices for historical and future time periods, bias-corrected climate datasets provided through Inter Sectoral Impact Model Intercomparison Project (ISIMIP 1), Fast Track simulation round have been used. For each simulation round a set of gridded bias-corrected climate variables have been produced to be used as input data for running impact models. These climate datasets contain daily-resolution, bias-corrected climate data from 5 CMIP5 GCMs according Table 1 covering the period 1950-2099 (historical run up to 2005), downscaled to a 0.5°×0.5° lat-lon grid. They cover the global land area.

Table 1. Main Features of the Considered Models

Model Acronym	**Institution**	**Spat. Resolution (Lon×Lat~Lev.)**
GFDL-ESM2M	Geophysical Fluid Dynamics Laboratory, USA	144×90L24
HadGEM2-ES	Met Office Hadley Centre, UK	192×145L40
IPSL-CM5A-LR	Institut Pierre-Simon Laplace, France	96×96L39
MIROC-ESM-CHEM	AORI, NIES, JAMSTEC, Japan	128×64L80(T42)
NorESM1-M	Norwegian Climate Centre, Norway	144×96L26

Note that the models used in this study differ from the models in Chervenkov & Slavov (2020a, 2020b, 2021). ISIMIP offers significantly fewer models, than the applied in Sillmann et al. (2013b) and Orlowsky & Seneviratne (2012) but these studies considers only CMIP5 RCP2.6, RCP4.5 and RCP8.5 (i.e. not RCP6.0) and CMIP3 SRES A2 scenario, correspondingly.

2. METHODS

There are various methods to characterize extreme events, but the computation and analysis of climate indices (CIs) based on daily temperature and precipitation data is probably the most widely used non-parametric approach (Sillmann & Röckner, 2007). The modern sets of such indices, among which the most widely used is the collection of the Expert Team on Climate Change Detection and Indices (ETCCDI, Zhang et al., 2011), are statistically robust, cover a wide range of climate conditions, and have a high signal-to-noise ratio (Alexander & Arblaster, 2009). They are used in several projects on climate change with focus on different spatial scales, from planetary to continental, regional, national or local scale, as prevailing indicators of changes of the extreme events (Birsan et al., 2014). Subsequently, the number of publications on this topic is very large (Alexander et al., 2006; Frich et al., 2002; Kiktev et al., 2003; Klein Tank & Können, 2003; Moberg et al., 2006 and many others). Our group has also previous, partially project-driven, experience in CI-based analysis of historical (Chervenkov & Slavov 2020a, 2020b), near past and present (Chervenkov et al., 2019; Chervenkov & Slavov, 2019; Chervenkov & Slavov, 2021; Malcheva et al., 2016) and projected future regional climate (Gadzhev et al., 2021). The free availability of databases of Cis or other climate indicators, with focus on different spatial and temporal scales, facilitates any assessment which includes these parameters. In Table 2 are listed the main features of some gridded databases recently used in our group. It is worth to emphasize that the information from these sources is rarely suitable for direct implementation in the tasks of the regional climatology. Thus, the data from these sources have to be essentially post-processed in order to fit to the specific needs.

The present study is based entirely on the data from ISIMIP Fast Track. Although this project is intended to be a collection of agroclimatic indicators datasets, most of the indices in scope, inclusive all considered in this study, are based on the ETCCDI definitions which makes them universal. Agricultural indicators in ISIMIP Fast Track have been pre-calculated for this complete matrix of 5 GCMs×4 RCPs combinations. In addition, as a proxy for historical observations, the "Watch Forcing Data methodology applied to ERA-Interim (WFDEI)" (Weedon et al., 2014) were used to generate observational historical Agroclimatic indicators. This dataset is available at the same spatial resolution of ISIMIP climate datasets, covers the time range of 1979 to 2013 and its 30 year long part 1981-2010 is used in the study as reference for the current climate.

Table 2. Mean Features of the Used Data Bases

Acronym	Main Content	Spat. Coverage/ Resolution	Time Span, Scenario(s)	Institution	Basic Reference/ Access
SPI DB	4 data sets of SPI-1, SPI-3, SPI-6, SPI12 based on UDEL/ GEOG/CCR v3.02, GPCC v7.0, NOAA-CIRES 20CR v2c, ECMWF ERA20C	Global, 0.5°×0.5°; 1.5°×1.5°	1900-2010, 1901-2013, 1851-2011, 1900-2010	NIMH, Bulgaria	Chervenkov et al. (2016); ftp://xeo.cfd.meteo.bg/SPI/
CECILIA DB	152 CI based on RCMs	Central&SE Europe, 0.1°×0.1°	1961-1990 2021-2050 2071-2100 SRES A1B	CECILIA project	Belda et al. (2015); http://cecilia.dmi.dk
ClimData	STARDEX&ETCCDI Cis based on E-OBS &CARPATCLIM	E-OBS& CARPATCLIM domains; 0.25°×0.25°, 0.1°×0.1°	1951-2016 1961-2010	NIMH, Bulgaria	Chervenkov et al. (2019); https://repo.vi-seem.eu/handle/21.15102/VISEEM-343.
EIA	ETCCDI Cis based on CMIP5-GCMs	Global, varios res.	1850-2100; CMIP5 RCP2.6, RCP4.5,RCP8.5	Canadian Centre for Climate Modelling& Analysis	Sillmann et al. (2013a); http://www.cccma.ec.gc.ca/data/climdex/climdex.shtml
ISIMIP Fast Track	26 Cis based on CMIP5-GCMs	Global, 0.5°×0.5°	1951-2099; CMIP5 RCP2.6, RCP4.5, RCP6.0, RCP8.5	ISIMIP 1	CDS documentation; https://www.isimip.org/protocol/

After the download from the CDS the ISIMIP-datasets are significantly post-processed. The most essential stages are:

- The datasets for each model and RCP which are downloadable in 30-years time slices are merged in common data streams for 2011-2099
- The indices with equal temporal resolution are joined in common netCDF4 files
- Multi-model (MM) ensemble quantities as multi-model mean (MMM), MM 25-, 50- and 75-percentile which are often refereed as lower quartile, median and upper quartile and traditionally noted as X25, X50 and X75 are computed.
- Due to storage constrains only a spatial subset over Europe is preserved.

All netCDF manipulations are performed with the powerful tool Climate Data Operators (cdo). Additionally, for the current study only, all of the considered indices are aggregated in time on annual basis. The aggregation method depend on the indicator, e.g. min, max, sum, mean. The magnitude of the trend in time as well as its statistical significance are estimated individually for all grid cells and separately for each scenario by means of the Theil-Sen slope estimator (TSE) and the Mann-

Kendall (MK) test correspondingly. Thus far, the study is constrained over SE Europe only as will be shown in the next section and with details in the next part.

3. RESULTS FOR THE MEAN TEMPERATURES

The annual means of the daily minimum, mean and maximum temperature (noted traditionally TN, TG and TX) are important variables, providing information on the current state as well as on the long-term climate variability and change and thus are studied separately from the other considered indices. We analyse the spatial patterns of the multiyear means of the CMIP5 projections of TN, TG and TX as well as the spatial patterns for the reference period. In order to intercompare them, the ensemble median (MMX50) of the listed in Table 1 models for all 4 scenarios is superimposed to the median for the reference period, as shown on Fig. 1.

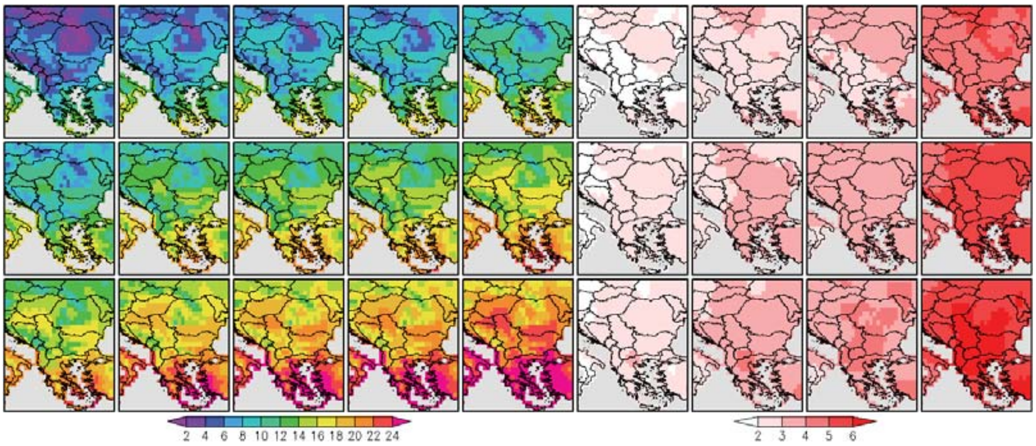

Figure 1. MMX50 of the multiyear means of the TN (first row) TG (second row) and TX (third row) for the reference period (1981-2010) in the first column and multiyear means for 2070-2099 for RCP2.6, RCP4.5, RCP6.0 and RCP8.5 in the second, third, fourth and fifth column correspondingly. The absolute changes of the RCP2.6, RCP4.5, RCP6.0 and RCP8.5 relative to the reference period are shown in the sixth seventh eighth and ninth column correspondingly. The units are ^{o}C.

Figure 1 shows for all variables gradual increase of the projected changes from RCP2.6 to RCP8.5, i.e. proportional to the radiative forcing. The changes are similar in magnitude for all parameters for fixed scenario RCP2.6-RCP6.0 and have not clear spatial structure. For RCP8.5 the changes for TG and TX are exceeding 6^{o}C and are somewhat bigger than the changes for TN. All changes are statistically significant at the 5% level.

The area-weighted regional averages over land of TN, TG and TX are shown on Figure 2.

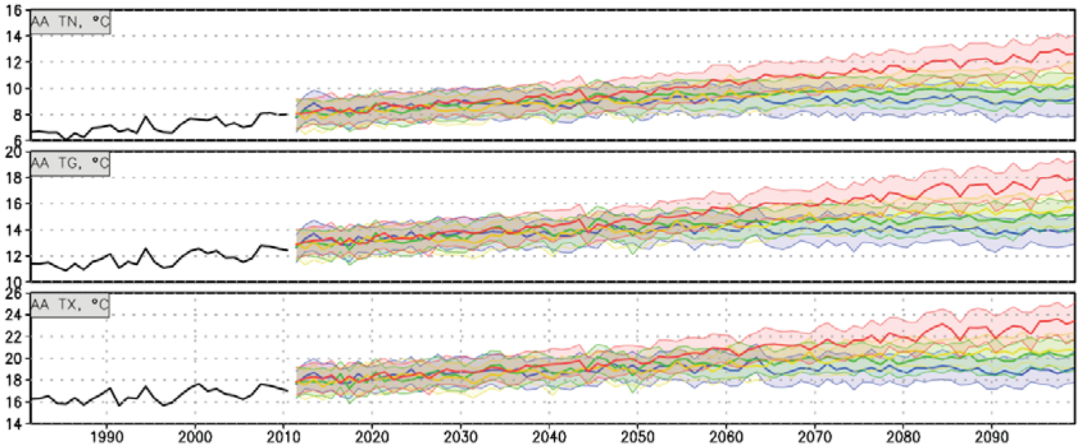

Figure 2. Area-weighted regional averages (index and unit according subplot title) for the reference (solid black line) and simulated by the CMIP5 ensemble for the RCP2.6 (blue), RCP4.5 (green), RCP6.0 (yellow) and RCP8.5 (red). Solid lines indicate the ensemble median (i.e. the 50th quantile) and the shading, respectively the thin lines, indicates the interquartile ensemble spread (25th and 75th quantiles).

Figure 2 shows relatively smooth (in comparison with the other Ci's as will be shown further) but steady increase of the temperatures with apparent difference between scenarios in the second half of the century.

The importance of assessing trends in climate extremes is often emphasized (e.g. Klein Tank & Können, 2003; Meehl et al., 2000; Moberg et al., 2006). The

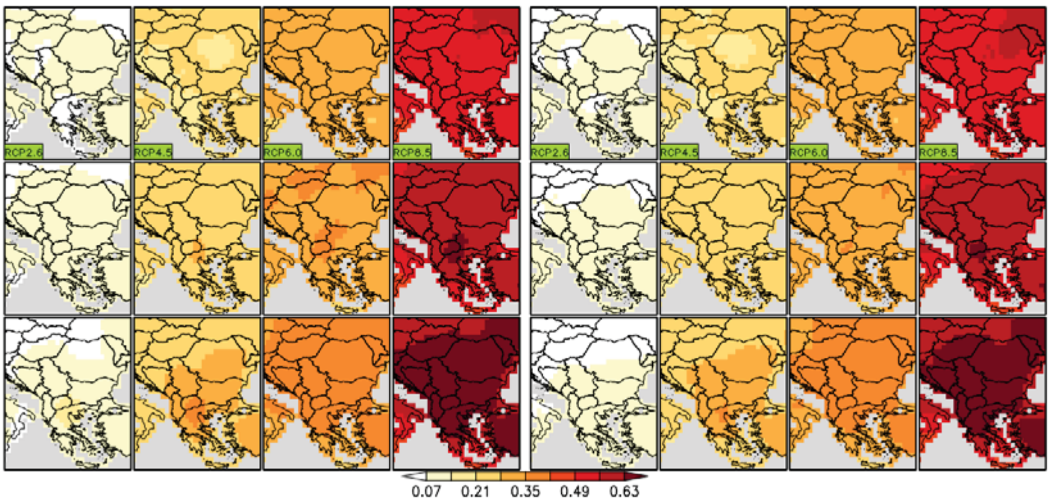

Figure 3. Trend slopes (unit: °C/10 years) of the TN (first row) TG (second row) and TX (third row) of the MMM (left pane) and MMX50 (right pane) for the scenarios according the subtitles in the first row.

main reason is that extreme weather conditions related to temperature, precipitation, storms or other aspects of climate, can cause loss of life, severe damage and large economic and societal losses. Thus, the trend assessment is essential part of the recent climate studies (Alexander et al., 2006; Frich et al., 2002; Sillmann et al., 2013b; and many others). Figure 3 shows the slope of the estimated by means of TSE linear trend of the MMM and MMX50 of the TN, TG and TX for the whole future period 2011-2099.

The most apparent result of analysis of Figure 3 is that the fields of the slopes for MMM and MMX50 are practically identical for each corresponding variable and scenario. As expected, the lowest values are for the scenario with the modest forcing (RCP2.6) and the highest – for the scenario with the strongest forcing (RCP8.5).

CONCLUSION TO PART ONE

The referenced in Table 2 projects and initiatives contributes to the availability of a valuable sets of spatially and temporally representative data to prepare relevant climate change studies in the corresponding domains. These datasets are reliable sources of various climate indicators, which can be presented as continuous, both in space and time, digital maps. The positive consequences to the end user community in exploration of the single point access data portal Copernicus Climate Data Store are manifold, but the free access of data sets standardised file formats via unified transfer protocols seems most significant.

Relevant outcome of the presented part one of the study, is the clearly expressed warming signal in the field of the mean temperatures. It is spatially dominating over the domain and everywhere statistically significant. The amount of warming by scenario generally ranges from high to low as follows: RCP8.5, RCP6.0, RCP4.5 and RCP2.6 which shows principal proportion of the temperature increase to the radiative forcing.

Part two of this study is dedicated on the analysis of the spatial patterns and the time evolution of the other considered indices.

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Proceeding of 1st International Conference on Environmental Protection and Disaster RISKs

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Air Pollution, Climate and Health

ASSESSMENT OF THE FUTURE CLIMATE OVER SOUTHEAST EUROPE BASED ON ENSEMBLE OF CLIMATE INDICES – PART TWO: RESULTS AND DISCUSSION

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Abstract: Nowadays there is a strong degree of agreement that the climate change is the defining challenge of our time. The analysis based on climate indices is probably the most widely used non-parametric approach for quantification of extreme climate events. This study which consist of two parts, is dedicated on the assessment of the spatial patterns and the temporal evolution of 6 temperature-based and 3-precipitation based indices in projected future climate over south-east Europe up to the end of the century. The annual means of the daily mean and extreme temperatures are also analysed in consistent manner. The indices are computed from the bias-corrected output of 5 CMIP5 global models, forced with all 4 RCP emission scenarios. The multi model ensemble medians of the temperature-based indices shows considerable warming which is consistent with the increase of the mean temperatures and is statistically significant in most cases. The revealed changes of the precipitation-based indices are more complex when compared with temperature changes.

Keywords: climate indices, CMIP5 ensemble, RCPs, future climate, South-east Europe

INTRODUCTION TO PART TWO

This part is dedicated on the analysis of the considered indices except the mean temperatures. The study is continuation of our scientific work, documented in suite of publications (Chervenkov et al., 2019; Chervenkov & Slavov, 2019, 2020a, 2020b, 2020c, 2021) which first part is described in Chervenkov et al., (2021). As in Chervenkov & Slavov, (2021), the present study is inspired from the comprehensive study of Sillman et al., (2013b) and fits in the same conceptual framework. Beside the different models, considered indices and significantly finer grid spacing, this study differs, however, from Chervenkov & Slavov (2021) in other two substantial aspects: first and foremost, the input data (i.e. daily temperatures and precipitation sums) are bias-corrected, as described by Hempel et al., (2013), prior the computation of the indices. Although some criticism exists, the general view in the expert community is that the bias-corrected climate change signal is more reliable compared with the uncorrected one and thus is more suitable for impact assessments (Chervenkov & Spiridonov 2020, 2021). Second, the study is focused on the multi-model statistics (mean, MMX25, MMX50, MMX75) rather than the simulation output of the individual models. This is modern common approach, adopted in many recent studies (Orlowsky & Seneviratne, 2012; Sillman et al., 2013a, 2013b).

4. RESULTS

4.1. TEMPERATURE INDICES

4.1.1. ABSOLUTE AND THRESHOLD INDICES

We start our analysis with a comparison of the spatial patterns of the multiyear means of the CMIP5 projections of the extreme temperatures, TNn and TXx with their counterparts for the reference period. In order to intercompare them, the ensemble median (MMX50) for all 4 scenarios is superimposed to the median for the reference period, as shown on Fig. 1. for the annual extreme temperatures

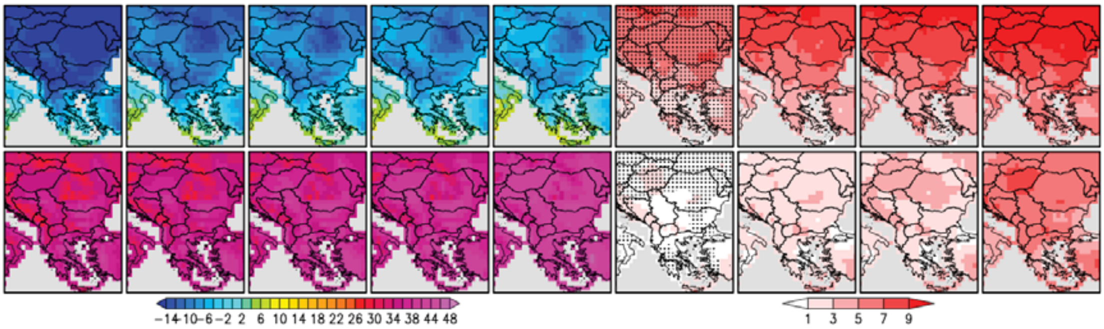

Figure 1. MMX50 of the multiyear means of the TNn (first row) and TXx (second row) for the reference period (1981-2010) in the first column and multiyear means for 2070-2099 for RCP2.6, RCP4.5, RCP6.0 and RCP8.5 in the second, third, fourth and fifth column correspondingly. The absolute changes of the RCP2.6, RCP4.5, RCP6.0 and RCP8.5 relative to the reference period are shown in the sixth seventh eighth and ninth column correspondingly. Stippling indicates grid points with changes that are not significant at the 5% significance level. The units are ^{o}C.

Figure 1 shows gradual increase of the projected changes of the both indices from RCP2.6 to RCP8.5, i.e. proportional to the radiative forcing. The greatest changes in TNn, exceeding 9°C, are simulated in RCP8.5 over the northern half of the domain. The most apparent difference between the spatial patterns of the changes of the TNn and TXx is the stronger temperature increase for TNn. This difference is well expressed for all four scenarios. Alexander et al., (2006) documents analysis of global data base of historical records, revealing such asymmetric warming. According to their global study (for data since 1951), changes in daily maximum temperatures are less marked, implying that our world in many places has become less cold rather than hotter. Other studies, however, based solely on assimilated European data (see Moberg et al., 2006 and references therein) suggest that this conclusion is not representative for Europe if the entire twentieth century is considered. An overall warming is observed also in Moberg et al., (2006), but they find only a small difference, or no difference at all, between average trends in daily minimum and maximum temperatures when they average trends for 75 stations across Europe. According to the future in the CMIP5 projections, Sillmann et al., (2013b) outlines the differences in the changes of the daily extreme temperatures. In particular, TNn increases more strongly in higher latitudes of the Northern Hemisphere. It is worth to emphasize also that our previous study Chervenkov & Slavov (2021), which is conceptually similar to the present one as underlined above, do not detects clear enough and rigour evidences for 'warming asymmetry' between the indices, based on the minimum temperature from the one hand and these, based on maximum temperature, from the other hand.

The widely used threshold indices tropical nights (TR) and frost days (FD), both based on the daily minimum temperature, have limited applicability over the domain. In the climatological study of the Carpathian region Birsan et al., (2014) is stated that the changes in the occurrence of TR are substantial only in low-elevation areas (below 800 m.), located outside the Carpathian Mountains range, which are particularly exposed to persistent and intense warm spells in summer. Generally, TR are not characteristic to the climate of the mountain regions, which are significant

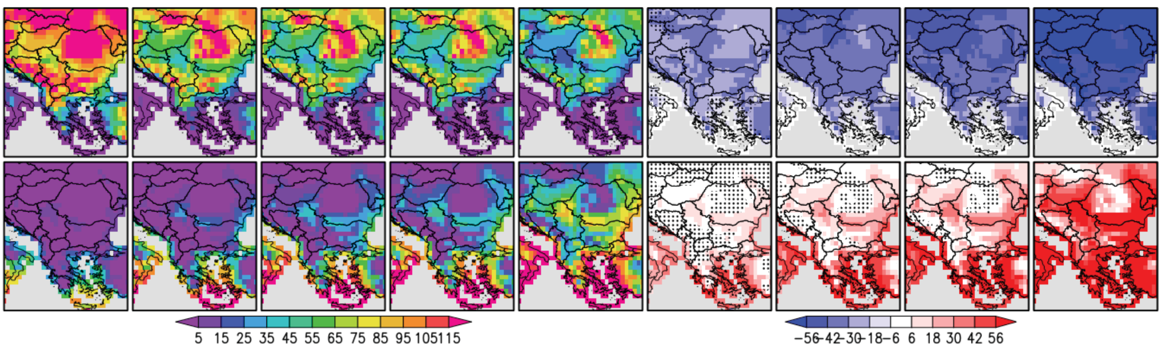

Figure 2. Same as Figure 1 but for the FD (first row) and TR (second row). The units are days.

part of the domain. Similarly, the FD are not very meaningful for maritime climate – this is valid for the southern half of the model region and especially for the areas along the fragmented coastline. Nevertheless, at least for methodological reasons, analysis of these indices have to be performed as shown on Figure 2 in the case for their spatial patterns.

Consistent with the changes of the minimum temperature, the fields of the threshold indices shows progressive (i.e. from RCP2.6 to RCP8.5) decrease of FD and, contrary to FD, increase of the TR. The vertical gradient of the FD is well expressed especially along the main Carpathian ridge. The increase of the TR under RCP2.6, RCP4.5 even RCP6.0 is, over the bigger part of the domain, relatively small and, which is more important, statistically not significant.

The area-weighted regional averages over land of TNn, TXx, FD and TR, which will be called area-averages (AA) for sake of brevity henceforth, are shown on Figure 3.

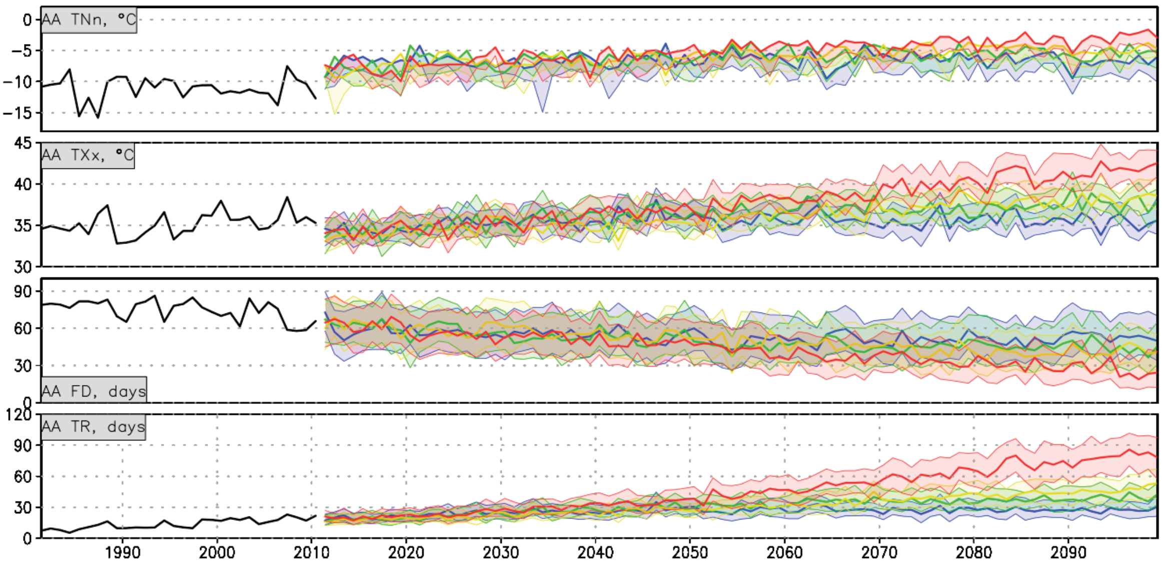

Figure 3. AA of the considered absolute and threshold indices (index and unit according subplot title) for the reference (solid black line) and simulated by the CMIP5 ensemble for the RCP2.6 (blue), RCP4.5 (green), RCP6.0 (yellow) and RCP8.5 (red). Solid lines indicate the ensemble median (i.e. the 50th quantile) and the shading, respectively the thin lines, indicates the interquartile ensemble spread (25th and 75th quantiles).

The overall tendencies, commented above, are markedly expressed for AAs of all indices. In the recent study Chervenkov & Slavov, (2020a), among other problems, are analysed the trends of five temperature-based indices, including TNn and TXx. The trend estimation of the AAs over the domain is based on the gridded data base of the HadEX2 project and is for the period 1900-2010. The study reveals statistically significant increasing trend for the both parameters with bigger lapse for TNn. These conclusions agrees with the present results, suggesting that the projected changes are natural continuation of the already detected changes in the near past and present climate. The analysis of Figure 3 shows also that the CMIP5 interquartile model spreads in the four RCPs practicality remain overlapping for TXx, FD and TR until the middle and for TNn until the end of the 21st century.

4.1.2. DURATION AND PERCENTILE INDICES

The Cold and Warm Spell Duration Indices (CSDI & WSDI) are most frequently used indicators for cold and heat waves respectively (Alexander et al., 2006; Alexander & Arblaster, 2009; Sillmann &, Röckner, 2007 and many others) inclusive in climatological studies of the considered region (Birsan et al., 2014). Hence these indices are calculated using a percentile based, rather than fixed value, threshold, they could be also considered as percentile indices. The spatial patterns of the CSDI and WSDI for the control period as well as for the projected with the CMIP5 future are shown on Figure 4.

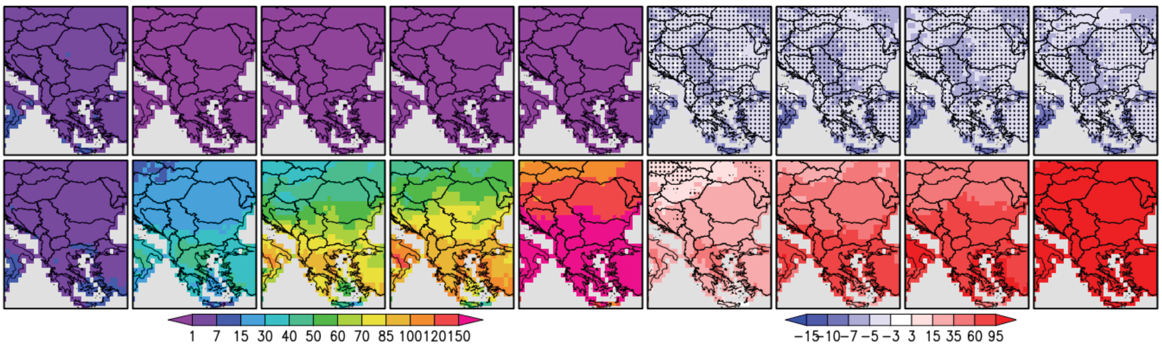

Figure 4. Same as Figure 1 but for the CSDI (first row) and WSDI (second row). The units are days.

Regarding the CSDI, the most obvious result on Figure 4 is that the small on magnitude and uniformly distributed during the reference period index practically disappears in the future even under the scenario with the weakest radiative forcing (RCP2.6). Subsequently, CSDI remains near zero constant under the other three scenarios. The change of the WSDI is very expressive both in magnitude and spatial extent. The differences from RCP to RCP are significant, especially for RCP8.5 compared with others. The absolute increase of WSDI relative to the reference is drastic: more than three months practically over the whole domain. This result, rather embarrassing indeed, is in principal agreement with Sillmann et al., (2013b).

The temporal evolution of the considered duration indices is depicted on Figure 5.

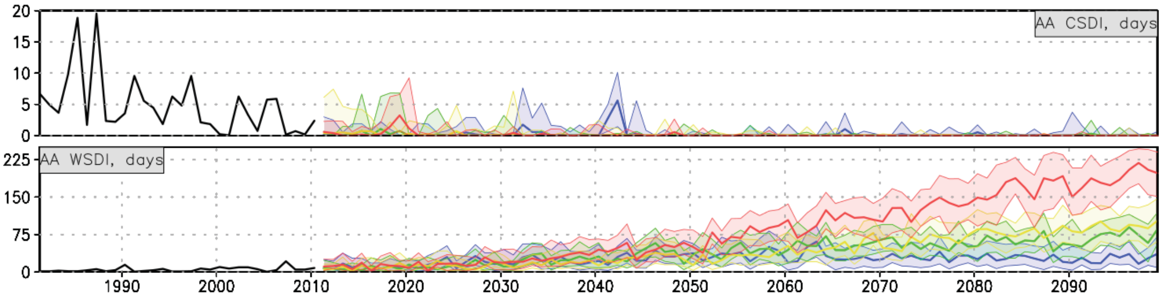

Figure 5. Same as Figure 2 but for the CSDI (first row) and WSDI (second row). The units are days.

Figure 5 confirms the outcomes from the analysis of the spatial patterns of the CSDI and WSDI. Interesting specifics of the dynamics of the AA of the CSDI is considerable changes in both directions for relatively short time during the reference period. This is consequence of single abnormally hot and cold years in this time span documented also in Birsan et al., (2014). The AA of the WSDI during the whole reference period remains with practically negligible values almost constant. In contrast, the dynamics in the projected future demonstrates steady increase, especially for RCP8.5. Consequently, the ensemble median for this scenario is over 150 days around the 2080's.

4.2. PRECIPITATION INDICES

As in many other places of the world, in contrast to the projected changes in the temperature indices, where there is a general agreement on the sign of change independent of the region considered, changes in the precipitation indices over the considered region are less consistent in this regard Sillmann et al., (2013b), Chervenkov et al., (2021).

Our analysis is focused on the indices Annual Precipitation Sum, Heavy Precipitation Days and Consecutive Dry Days, noted RR, RR10mm and CDD correspondingly. These indices are used as key parameters in many studies of present (for example Sillmann and Röckner, 2007) and projected future climate (see Sillmann et al., 2013b and citation therein).

Figure 6 provides a more detailed regional picture of the spatial patterns of the considered precipitation indices for the control period as well as for the future projections. Traditionally, the changes in precipitation sum RR relative to the 1981-2010 reference period are expressed in percentage terms.

First and foremost, Figure 6 demonstrates the complex nature of the expected precipitation changes. Although the total precipitation amount (the first row on Figure 6) shows clear reduction tendency, especially over the southeastern part of the domain, there is no big difference, both in magnitude and spatial distributions, in the relative changes in the scenarios RCP2.6-RCP6.0. Second, which

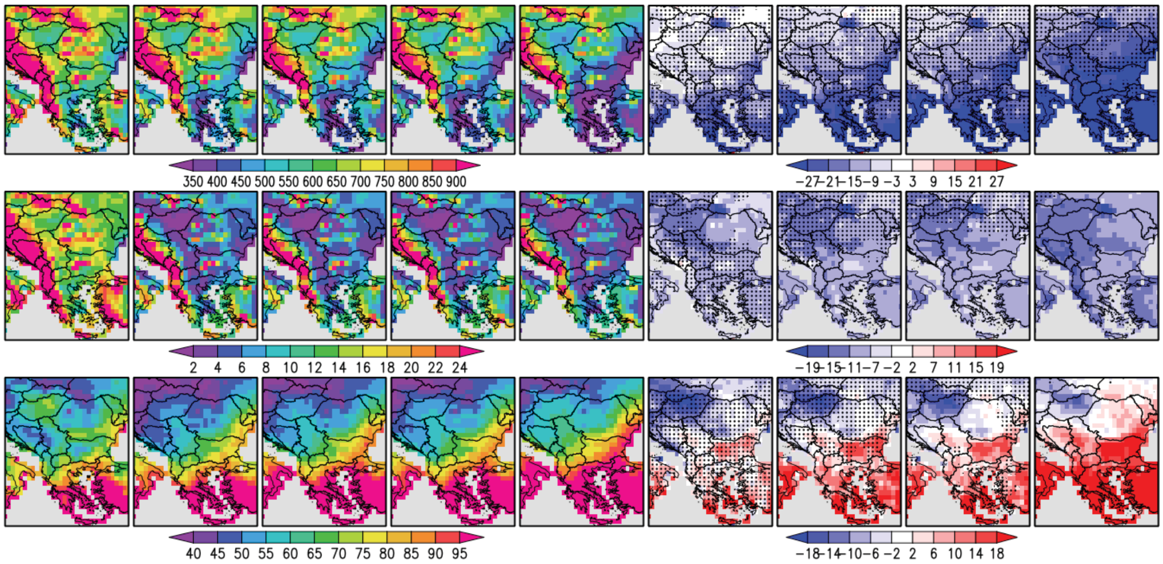

Figure 6. Same as Figure 1 but for the RR (first row), RR10mm (second row) and CDD (third row). Relative instead of absolute changes of the RR are considered. The units of the RR are mm and of the RR10mm and CDD as well as their changes – days. The relative changes of the RR are expressed in %.

is most important, these changes are not statistically significant at the 5% level. This result agrees with Sillmann et al., (2013b). Similar is the overall picture with the days with heavy rain distribution: general reduction, approximately up to a week over the bigger part of the domain, but without substantial difference from scenario to scenario and without statistical significance over wide areas for all RCPs, except RCP8.5. It is notable that this result is somewhat different that the outcomes in Sillmann et al. (2013b): there is shown a small (generally 2-4 days) increase of R10mm over the Balkan Peninsula for all scenarios except RCP8.5 and decrease in the latter of about 2-4 days. It have to be emphasized, however, that in this study is noted that the models disagree even on the sign of change in the total precipitation and R10mm over the Mediterranean. Our recent experiments with the RCM RegCM driven by the GCM HadGEM2-ES (Gadzhev et al., 2021) shows prevailing positive change (i.e. increase) for all seasons except for the summer and on an annual basis. The projected increase is roughly 25–35% for RCP2.6 and 35–45% for RCP8.5. The expected precipitation reduction in the summer reaches values of 35–45% for RCP8.5 over Bulgaria and Romania.

The spatial patterns of the CDD, both in the present and projected future climate is also complex. Most apparent is the well expressed gradient form southeast to northwest. The contrary tendencies in the future, increase of the CDD in southeast and decrease in northwest will leads to strengthening of this contrast. The analysis, performed in Malcheva et al., (2016) which is based on historical records and on the climate reanalysis ERA20C, outlines the drying tendency over SE Bulgaria and the neighboring territories in Greece and Turkey. In Sillmann et al., (2013b) is noted that in the Mediterranean, the increases in CDD are accompanied by increases in the index R95p (very wet days, not considered in the present study) suggesting that dry spells in these regions become longer, but that precipitation may be more extreme when it occurs. Our previous analysis, based on HadEX2 (Chervenkov & Slavov, 2020a), demonstrates also simultaneous increase of the AAs of the CDD and R95p. It have to be kept in mind, however, that the applicability of HadEX2 in regional climate studies, especially for precipitation-related parameters, is disputable. Possible intensification of the extreme precipitation events in generally dryer climate is also discussed in Giorgi & Lionello, (2008).

It is worth to emphasize, that the projected changes under RCP2.6 and RCP4.5, are not significant over the bigger part of the domain which also indicates the complexity of the phenomena.

The temporal evolution of the considered precipitation indices is shown on Figure 7.

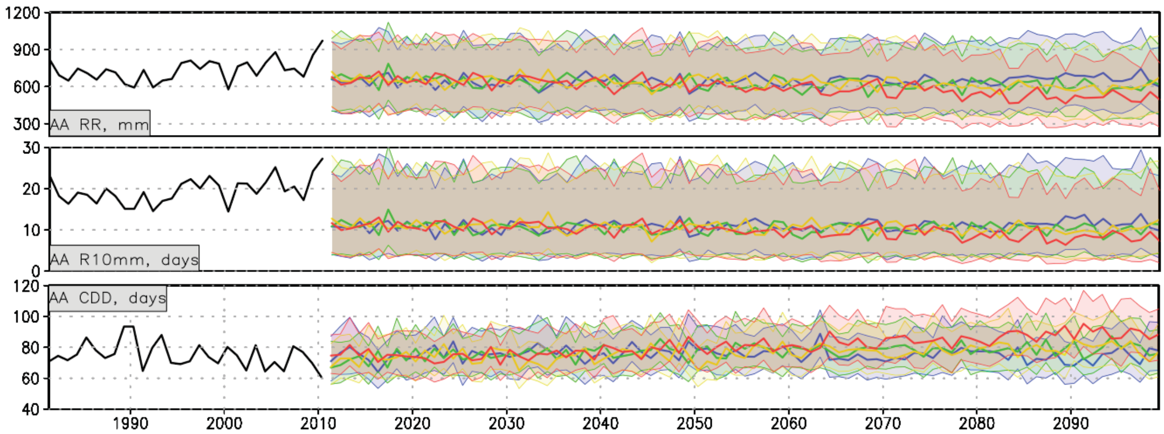

Figure 7. Same as Figure 2 but for the RR (first row) and R10mm (second row) and CDD (third row). The units are according the subplots titles.

As most remarkable on Figure 7 appears the fact that the evolution lines of RR and R10mm and in smaller extent these for CDD, respectively their interquartile ensemble spreads for all scenarios, essentially overlaps for the bigger part of the time span 2011-2099. Such dynamics is expectable, keeping in mind the relatively small changes from RCP to RCP commented above. The absence, at least apparent, of big outliers is also remarkable. The inter-model coherency is demonstrated also in agreement between the models in the simulation of isolated wet years in the 2040s and 2070s in the evolution of the CDD.

SUMMARY AND CONCLUSION

Based on the availability of new sources of information, which represent the state of the art global climate change simulations in the frame of the CMIP5 project and are free accessible from the Copernicus Data Store, we present an updated assessment of future climate change projections over south-east Europe.

In the present study 6 temperature-based and 3 precipitation-based indices, together with the annual means of the daily minimum, mean and maximum temperature are analysed systematically. The indices are calculated in in consistent manner in the frames of the Global Agriculture project and the assessment covers the recent climate (1981-2010) as well as CMIP5 multimodel ensemble projections of the 21st century for all four RCP scenarios. The spatial patterns and temporal evolution of changes presented in this work are in principal agreement with previous studies based on GCM output data (Orlowsky & Seneviratne 2012; Sillmann et al., 2013b; Chervenkov & Slavov, 2021), RCM simulations Belda et al., 2015; Gadzhev et al., 2021) or such based on combined analysis of GCMs and RCMs (Giorgi & Lionello 2008; Ulbrich et al., 2006). The results of this study are also coherent with the consolidated outcomes from all Assessment Reports (AR) of the Intergovernmental Panel on Climate Change (IPCC) (see, for example, IPCC, 2007) concerning the expected long-term regional changes. However, the present results are not directly comparable, at least not quantitatively, to theirs, due to different factors. These factors includes, among others, different time spans and model ensemble members and variations in the applied methodology of estimation. Nevertheless, the most general and important conclusion of the study is the distinct warming, expressed in the spatial patterns and time evolution of all of the considered thermal indices. The climate change of the considered temperature-based indices is consistent with the tendencies of the annual means of the daily mean and extreme temperatures. The warming dominates practically over the whole domain and is statistically significant over its essential part in the most cases. The revealed patterns of climate change intensify gradually with the increasing radiative forcing in the considered scenarios, which also agrees generally with the outcome of the prevailing number of the recent studies. The significantly finer grid spacing of 0.5^{o} than this in Sillmann et al. (2013b), Chervenkov & Slavov, (2021), were it is 1.5^{o}, leads to representation (although still not clear enough) of such structures as the vertical gradients of some indices especially along the main Carpathian ridge and the typical spatial pattern of the CDD. Both of them are poorly resolved in the cited above studies. Beside the revealed spatial details which are well known benefit of the increased resolution, this study differs from Chervenkov & Slavov, (2021) in other substantial aspect regarding the results: the clearly demonstrated 'warming asymmetry' manifested in the fields of the TNn and TXx. Generally, the revealed warming is, evidently, continuation of already detected tendency in the historical records of the twentieth century over the region (Chervenkov & Slavov, 2019; Chervenkov & Slavov, 2020; Malcheva et al., 2016; Moberg et al., 2006).

Concerning the precipitation-based indices, the study confirms the complexity of the expected precipitation-related changes and their inherent ambiguity. The latter is clearly evidenced by the lower level of statistical significance for the scenarios RCP2.6-RCP6.0 when compared with temperature changes. It is worth emphasizing that the projected precipitation reduction over the SE part of the domain and increase of the CDD could amplify the negative impact of the expected hotter climate.

The study could be continued in many directions. Key moments as, for example, seasonal variations and detailed regional specifics, could be focal point of further works. The 10-daily temporal resolution of some indices gives unique possibility even for sub-sesonal analysis. Other way is to utilize more actively the output of RCMs, as demonstrated in Belda et al., (2015) and Gadzhev et al., (2021). Such studies are methodologically reliable scientific basis of various impact studies and the development of adaptation strategies.

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