

## Article

# Computer simulations of air quality and bio-climatic indices for the city of Sofia

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**Abstract:** Air pollution is responsible for any 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 present work is to study the behavior of two bio-climatic indexes 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 WRF-CMAQ model system simulations with a spatial resolution of 1 kilometer. 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. Results: It was found that half of the heat and cold index categories are present in the simulations. Their distribution has some spatial features. All air quality categories are present in the domain, with dominance only of the O<sub>3</sub> and PM10. Conclusions: It was found that Sofia is not so hot and air polluted place, but in some situations, people have to have some concerns when intend to be outdoors for a prolonged time.

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

## 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 affecting the quality of life and human health are as follows:

Chemical composition of atmosphere: 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 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 an only 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, which size varies from 0.01  $\mu\text{m}$  to 50  $\mu\text{m}$ . They have the property to adsorb on their surface various chemical compounds, including some toxic substance (heavy metals, black

carbon and organic hydrocarbons),  $\text{NH}_3$ ,  $\text{NO}_x$  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 which is difficult for quantitative determination. Since 1990 began the separation of particulates in several major fractions:  $\text{PM}_{10}$  (Particulate matter, with diameter  $< 10\mu\text{m}$ ),  $\text{PM}_{2.5}$  (Particulate matter with diameter  $< 2.5\mu\text{m}$ ), and ultrafine particulate matter with diameter  $< 0.1\mu\text{m}$  ( $\text{PM}_{0.1}$ ). 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  $2.5\mu\text{m}$  reach pulmonary alveolus, where along with the adsorbed on their surface compounds, 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, neoplastic diseases, the reduced life expectancy, and air pollution, on the other hand, define the latter as a socially significant 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].

Physical parameters of the atmosphere: 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 dangerous health conditions expressing as unpleasant feelings could occur, such 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 for 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 core temperature decrease. A number of studies [14-17] present different methods for calculating of discomfort index and evaluating the role of thermal comfort on the quality of life and human health.

More complicated methods for calculation of Discomfort Indexes taking into account additional factors, such as wind speed and solar radiation, is also available. Predicted Mean Vote – PMV [18] and Physiologic Equivalent Temperature - PET [19] are based on the human heat balance model [20-24]. These methods account for the total heat effect due to all physical factors that affect the human body's thermal sensation using the human heat balance equation. This equation uses as input the ambient temperature, wind speed, relative humidity, and mean radiant body temperature under different man actions and clothes. Two of the most used indexes are heat index [25-27] and wind chill index [28,29]. They are numerical values in several intervals, called categories, each of which corresponding to a different degree of deviation from the comfort. They are used to study the extreme heat and cold conditions in Bulgaria from observations [30-32] and Southwestern Europe from model simulations [33]. 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 indexes - heat index and wind chill.

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

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 appropriate and up to date **methodology**.

Thus formulated study objectives contain several keywords, which have to be explained:

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

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

**Detailed studies:** This means high enough spatial/temporal resolution of the computer simulations, which to reflect the multi-scale nature of the processes, to make it possible the detecting interactions of different scale phenomena and tracking the basic mechanisms and pathways trough, which low atmosphere characteristics are formed, respectively their 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 [34-43].

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

WRF v.3.2.1 [44] - Weather Research and Forecasting Model, used as meteorological pre-processor; In the System, WRF is driven by the NCEP GFS (Global Forecast System) data that can be accessed freely from [45]

CMAQ v.4.6 - Community Multi-scale Air Quality model [46,47] the Chemical Transport Model (CTM), and

SMOKE - the Sparse Matrix Operator Kernel Emissions Modelling System [48] the emission pre-processor of Models-3 system.

TNO inventory [49] 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.

For calculation of the bio-climatic indexes, we use the air temperature and relative humidity at 2 meters and 10m 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 1 km. The configuration set uses WSM 6-class graupel microphysical parameterization scheme [50], CAM schemes for parameterization of the longwave and shortwave radiation [51]. The land-surface parameterization scheme is Pleim-Xiu [52]. The planetary boundary layer parameterization scheme is ACM2 (Pleim) [53].

One of the most commonly used indices is the UK Daily Air Quality Index [55], also used in Bulgaria [34-36,54]. According to [55] 4 main pollutants – O<sub>3</sub>, NO<sub>2</sub>, SO<sub>2</sub>, and PM10 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. 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 <sub>3</sub> µg/m <sup>3</sup>	NO <sub>2</sub> µg/m <sup>3</sup>	SO <sub>2</sub> µg/m <sup>3</sup>	PM <sub>10</sub> µg/m <sup>3</sup>
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. The reference levels and Health Descriptor used are based on health-protection related limit, target, or guideline values set by the EU, at a national or local level, or by the WHO [1].

**Table 2.** Air Quality Indexes 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

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. In the "Low" band, the air is the cleanest, which means that high values in the fields with the frequency of days with a given air quality index show more cases with clean air, and low values mean fewer cases with clean air, respectively more cases with polluted 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, vapor pressure, and barometric pressure, as well as zero extra radiation [26]. The heat index is composed of a multiple regression formula, valid in air temperatures 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. Because of the possibility that the values for Danger and Extreme Danger conditions are combined in one category – “Danger”. It is calculated according to the [25-27] with regression formula:

$$HI = -42.379 + 2.04901523 * T + 10.14333127 * RH - 0.22475541 * T * RH \\ - 0.00683783 * T^2 - 0.05481717 * RH^2 + 0.00122874 * T^2 * RH \\ + 0.00085282 * T * RH^2 - 0.000000199 * T^2 * RH^2$$

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 [28] is studied for winter, spring and autumn, because these are the times when it is possible for his categories to observe. It is reported in temperature units and is used as a wind chill temperature (WCT) with categories given in Table 4 [29]. 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°C ÷ 32.2°C	Fatigue is possible with prolonged exposure and activity. Continuing activity could result in heat cramps.
Extreme Caution	32.2°C ÷ 40.5°C	Heat cramps and heat exhaustion are possible. Continuing activity could result in heat stroke.
Danger	40.5°C ÷ 54.4°C	Heat cramps and heat exhaustion are likely; heat stroke is probable with continued activity
Extreme Danger	$\geq 54.4^{\circ}\text{C}$	Heat stroke is imminent

The second index is the wind chill index, which categorizes the feeling and health consequences of the wind cooling power in cold weather. It is defined in temperatures lower than or equal to 4.4°C and wind speeds at least 1.34 m/s. The wind chill index is calculated with the formula [28]:

$$WCT = 13.12 + 0.6215 * Ta - 11.37 * V^{0.16} + 0.3965 * Ta * V^{0.16}$$

The  $Ta$  is the air temperatures in degrees Celsius, and the  $V$  is the wind speed in km/h. It is valid for temperatures below 4.4°C and wind speed equal to or above 1.34 m/s. If the values of the air temperature and wind speed are outside the valid intervals, the air temperature, we accept that the WCT is equal to the air temperature.

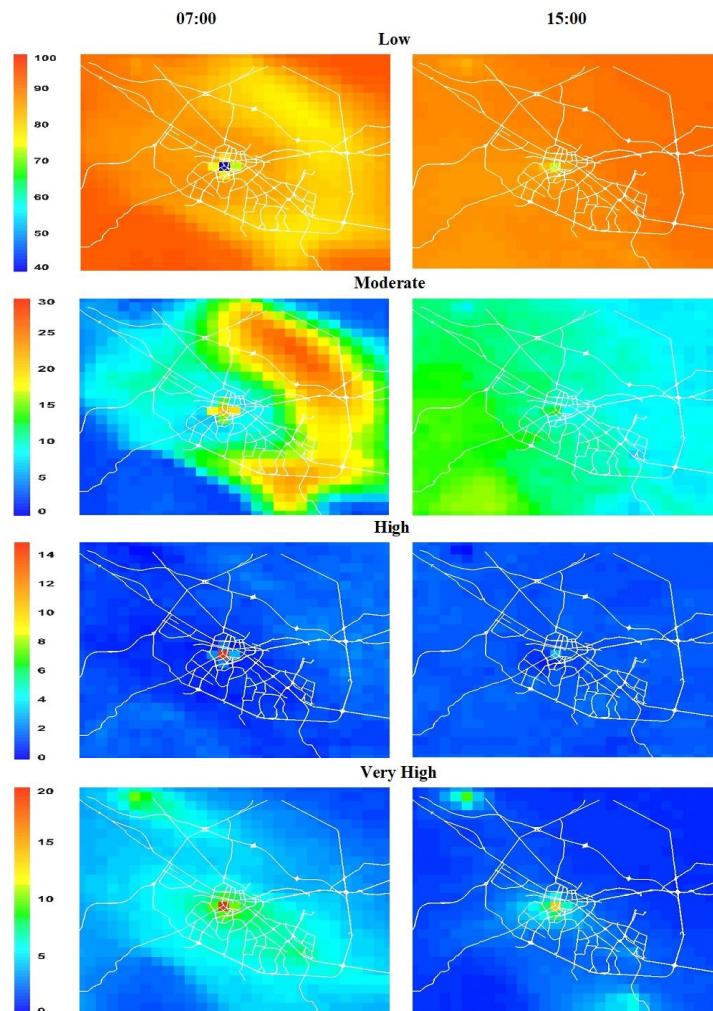
**Table 4.** Wind chill index categories and health effects.

Wind chill Category	Numerical interval	Health Precautions
Light Risk	0 ÷ -9°C	Slight increase in discomfort.
High Risk	-28°C ÷ -39°C	High risk of frostnip or frostbite. Exposed skin can freeze in 10 to 30min; 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 2min; Outdoor conditions are hazardous.

### 3. Results

#### 3.1. Air Quality Indexes

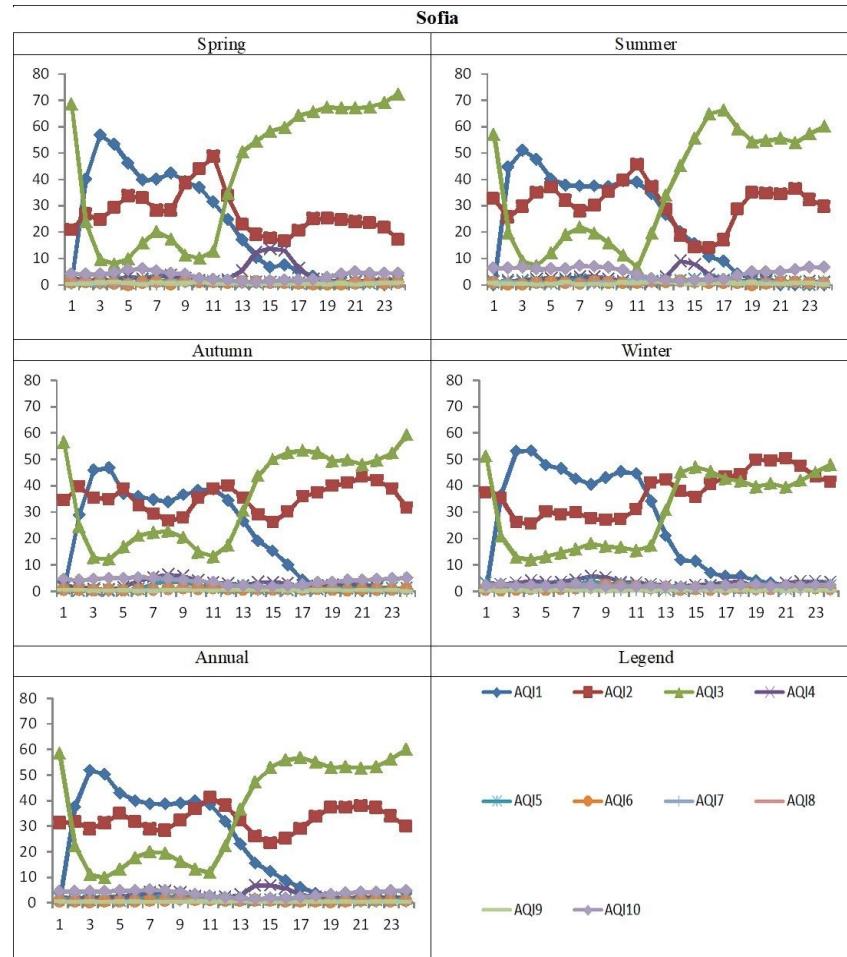
Annually averaged fields of recurrence of days with a certain air quality index are presented in Figure 1. In the category "Low", the areas with a low air quality index are mainly the city's ring road and busier transport routes, as well as the central parts, the most in morning hours. It is also observed in the band "Moderate", early in the morning with about 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. 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) [34-36].



**Figure 1.** Annual recurrences [in %] of the AQI for the band Low, Moderate, High and Very High for the territory of Sofia city.

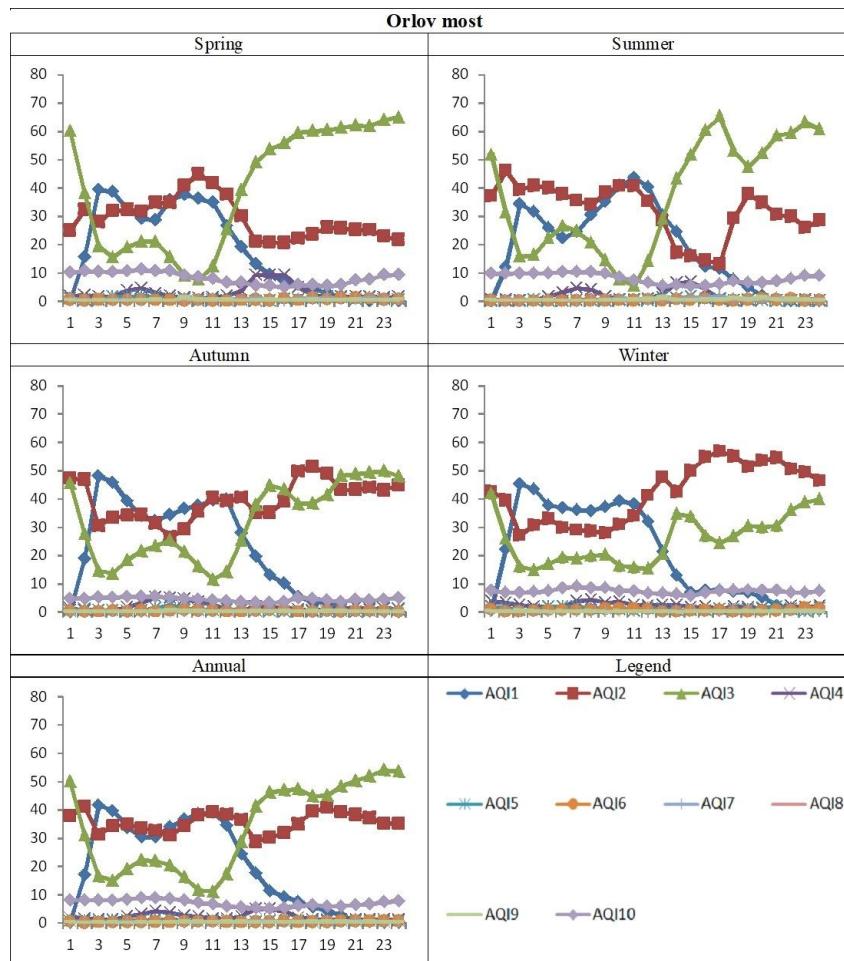
The graphs present the diurnal course and seasonal distribution of the average recurrences in [%] for the different pollution indices (from 1 to 10) for the territory of Sofia (Figure 2), as well as for different selected points of the city – Orlov Most (the city center) and Bistrica (a village in the surroundings of Sofia) (Figure 3, Figure 4).

Figure 2 shows that the indices AQI1, AQI2, AQI3, which fall in the band "Low", have the highest recurrence during the different seasons. The diurnal course of these indices is well defined. In the morning, AQI1, AQI2 have a recurrence of about 40-50%, and at that time, AQI3 has a minimum recurrence. In spring and summer, in the afternoon, AQI4 has a peak with a recurrence of about 10%. In all seasons, AQI10 stands out, which corresponds to the category "Very High" with about 5% repeatability. The other indices have an insignificant recurrence.



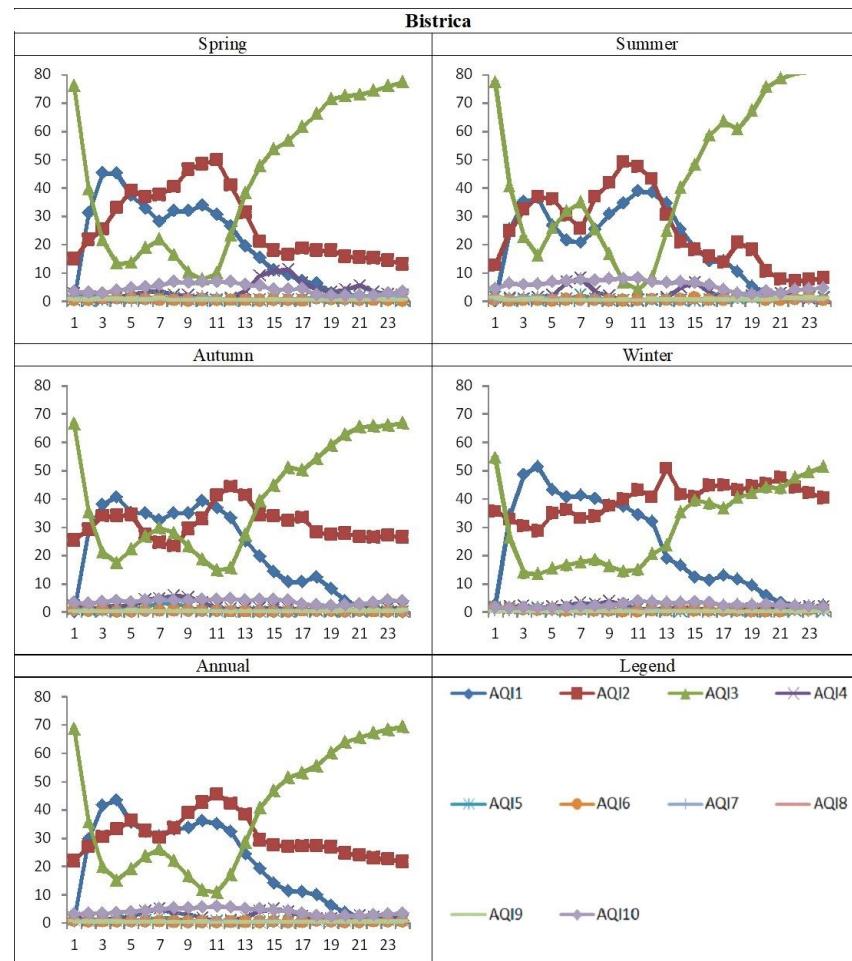
**Figure 2.** Average recurrence [in %] of the different indices (from 1 to 10) for the territory of the city of Sofia.

Figure 3 for the Orlov Most point shows that the indexes AQI1, AQI2, AQI3, which fall in the interval "Low", have the greatest recurrence during the different seasons. The diurnal course of these indices is well defined. In the morning, AQI1, 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 spring and summer. In all seasons, AQI10 stands out, which corresponds to the category "Very High" and, for this point, has a high repeatability of about 10 %.



**Figure 3.** Average recurrence [in %] of the different indices (from 1 to 10) for the Orlov Most (Sofia).

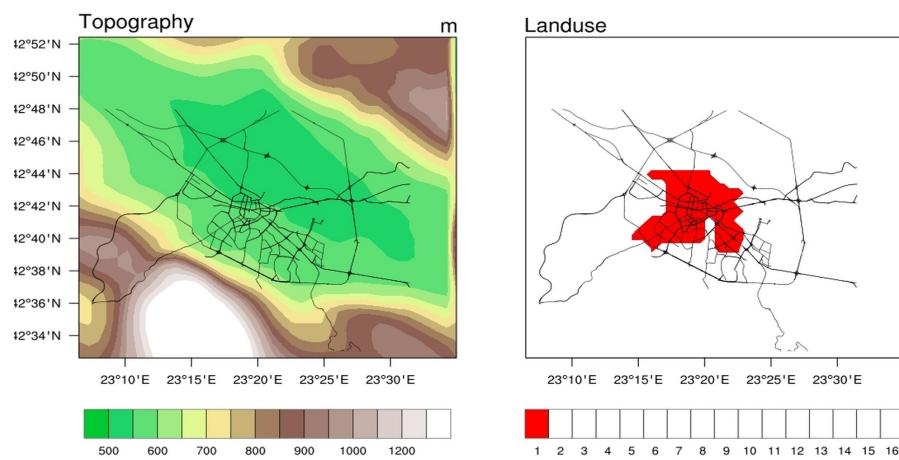
Figure 4 for the Bistritsa point shows that the indexes AQI1, AQI2, AQI3, which fall in the interval "Low", have the greatest recurrence during the different seasons. The diurnal course of these indices is well defined. In the morning, AQI1, AQI2 have a recurrence of about 40%, and in the afternoon, 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 seasons, AQI10 stands out, which corresponds to the category "Very High" and for this point, has a recurrence of about 5% in the morning in all seasons.



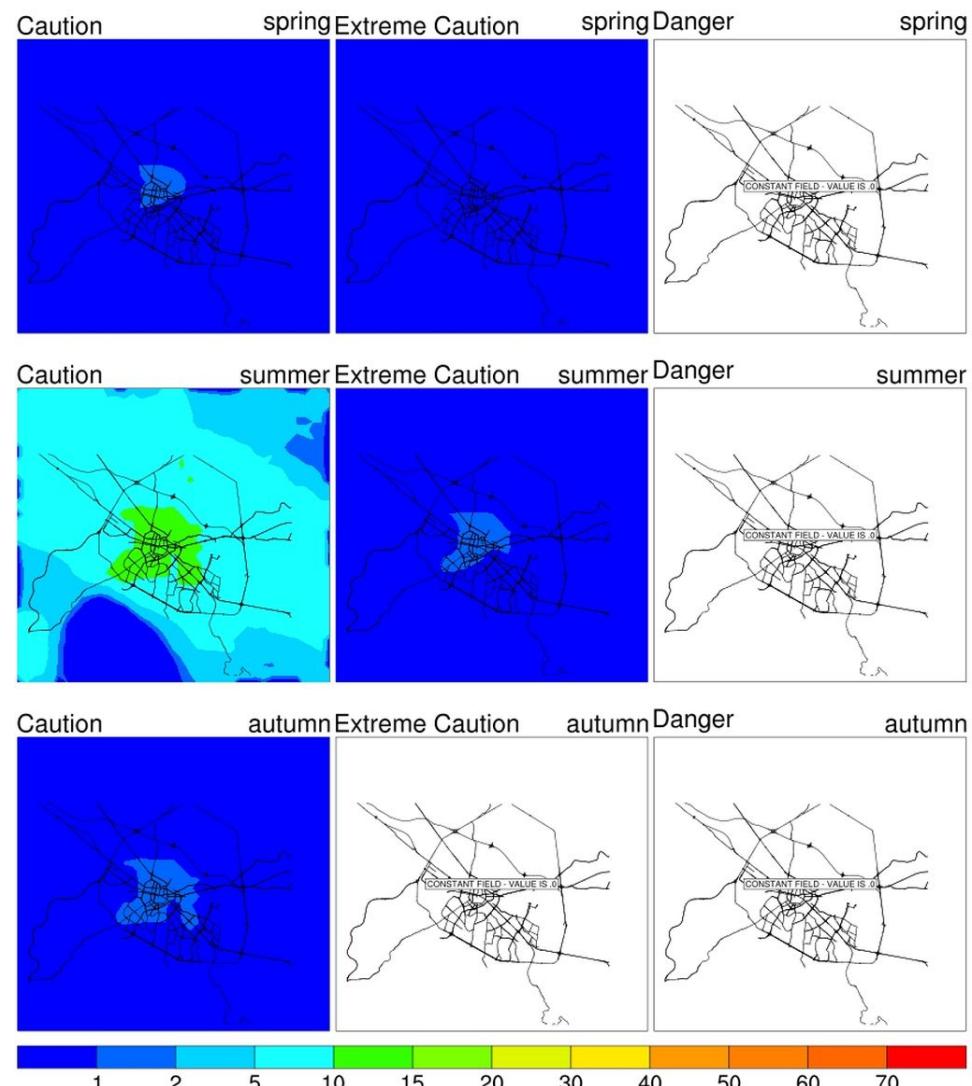
**Figure 4.** Average recurrence [in %] of the different indices (from 1 to 10) for the Bistrica.

### 3.2. Bio-climatic indexes

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 %. The summer cases of Caution conditions are much more and with a more complex 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 increasing the altitude. The spatial distribution of the Extreme Caution conditions on 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 autumn. Therefore, the weather was not as extreme in the autumn as in the spring.

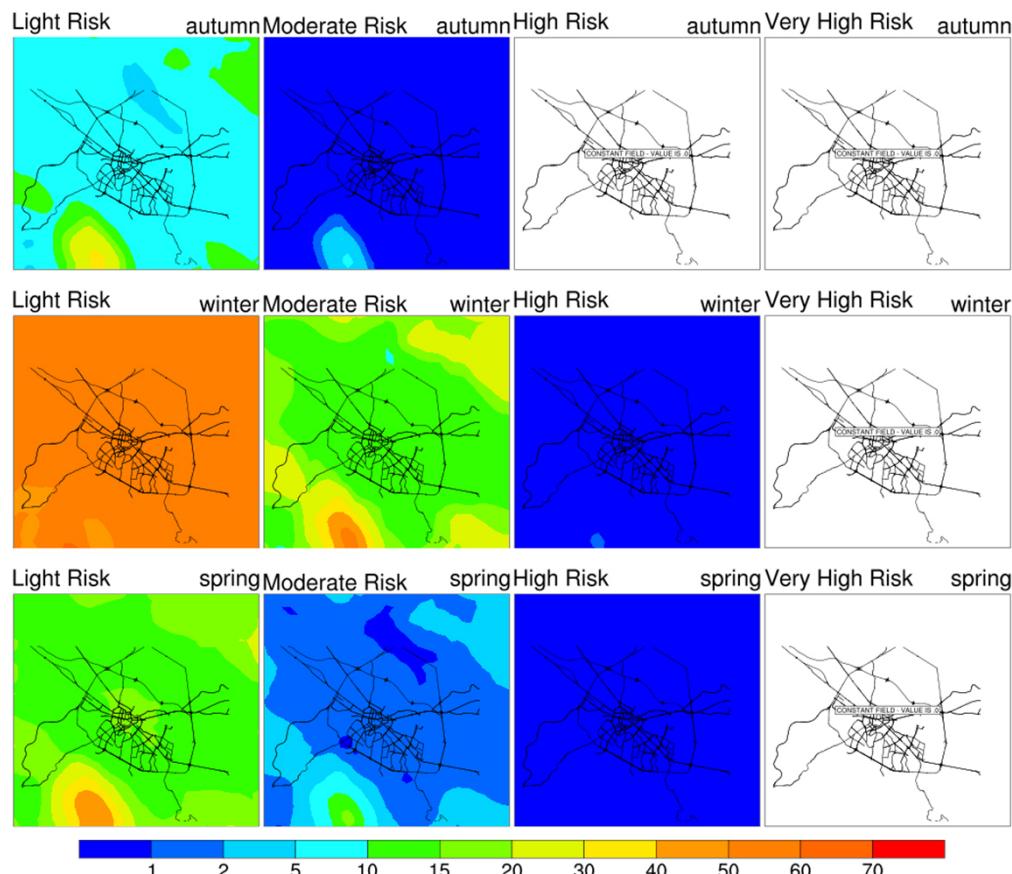


**Figure 5.** Domain elevation (left figure) and Land cover (right figure). The red color in the land cover figure is the urbanized land cover.



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

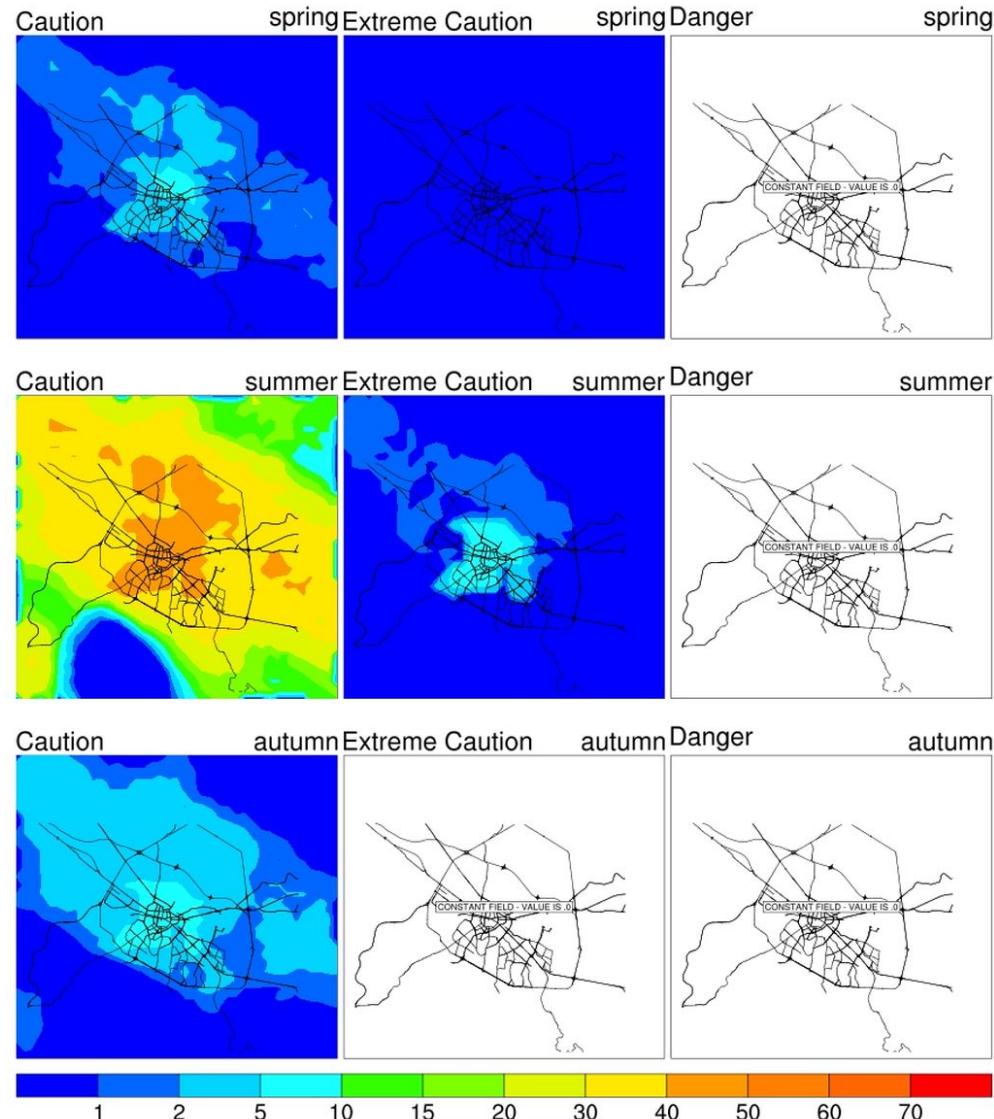
The simulated wind chill categories over the winter and spring are Light Risk, Moderate Risk, and High Risk, and only Light Risk and Moderate Risk in the autumn (Figure 7). There were 5% to 10% of cases with Light Risk in most of the domain, and increasing up to 40 % in higher altitudes. The winter Moderate Risk cases were mostly between 1 and 2%, up to 10% in the 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 mountain 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 spring also follow the terrain height. The percentages are between 1% and 2% in the Sofia Valley, increases to 5% in higher altitudes and 20% in the Vitosha Mountain. The autumn Moderate Risk is up to 1%, except in Vitosha Mountain. There are High Risk cases only in winter and spring.



**Figure 7.** Frequency [in %] 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 in or afternoon, 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 mountain 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 to the 5% to 10% in the more

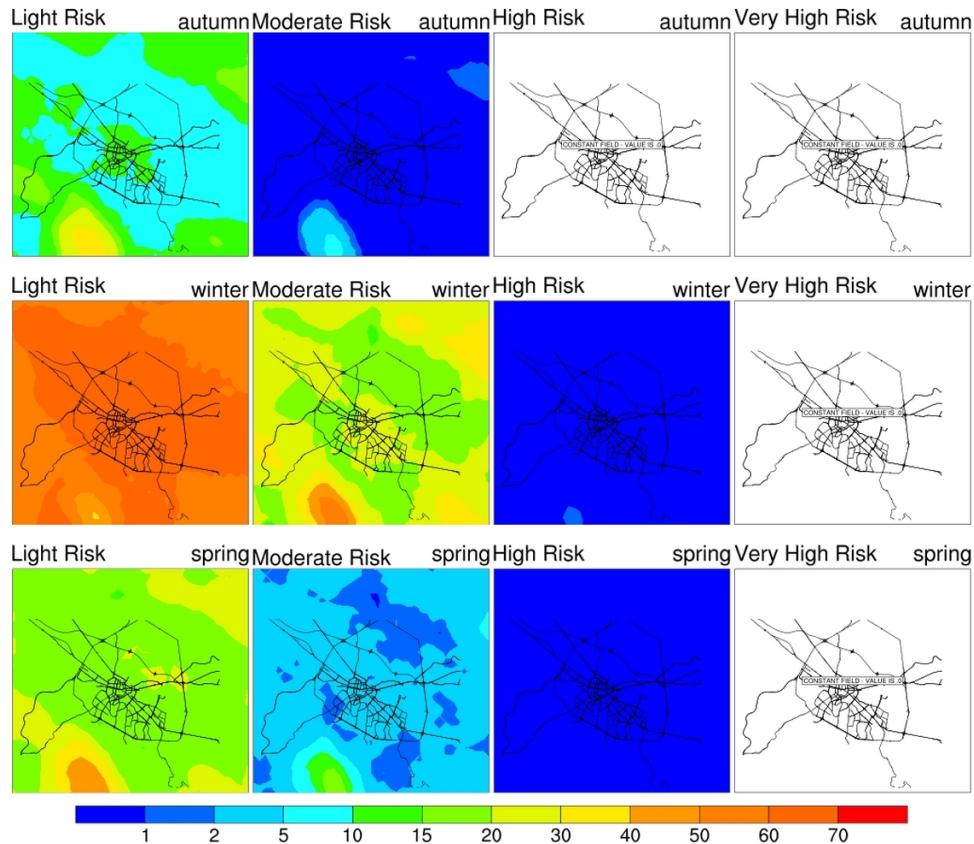
populated area of the city. The autumn percentages are between 5% and 10% in the central city parts, from 2% to 5% in the outer ones and below 2% in the mountainous areas. The spatial distribution during the spring is kind of similar, but the percentages are smaller with 1% to 5%.



**Figure 8.** Frequency [in %] 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).

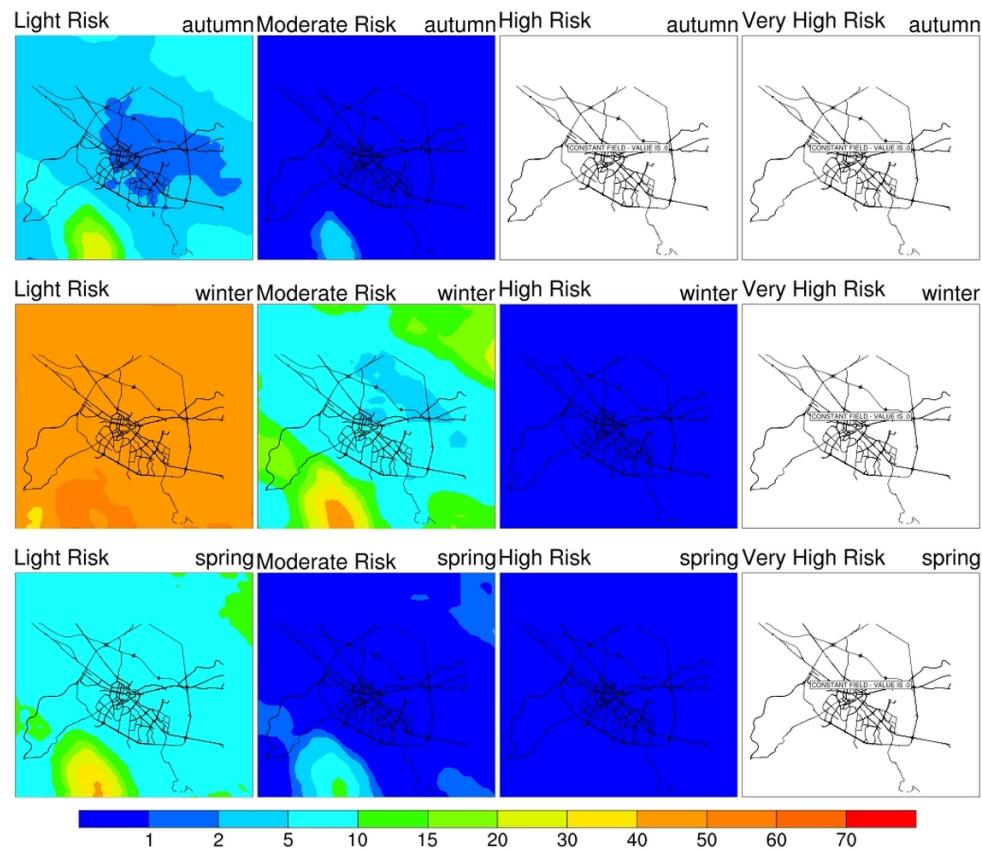
The human's daily life regime implies that it is interesting to study the wind chill index during the early morning and evening hours. The simulated WCT categories at 06 UTC are presented in Figure 9. Only the first two categories are presented in the autumn. The percentages of Light Risk are between 10% and 15% in the central city and mountain 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 on that season are between 20% and 30% in the part of the city limits and mountain areas, 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 per-

centages 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 %] 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 higher in the mountain areas. The winter percentages are mostly between 40 and 50, and the spring ones between 5% and 10%, except in the 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 at the Vitosha mountain, where they reach up to 50%. The High Risk cases are simulated only in winter and spring.



**Figure 10.** Frequency [in %] 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 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 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 afternoon. AQI3 high recurrence can be seen in afternoon hours, 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 recurrence of about 5%-10% during the whole day, all seasons, and for all points.

The pollution in the city is probably due to the surface sources like road transport and 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 a significant probability for AQI from the Moderate range.

The hot spot in Sofia city, where the high-value indices are with higher recurrence, is in the city center. 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 pollution aloft is hampered.

Generally, the adverse heat conditions in the Sofia city region reach up to 15% of the cases. The summer frequency of conditions for fatigue decreases gradually with increasing altitude from the city center to the Sofia Valley and mountain 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 5). 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 5), 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 5) and lower ones in higher altitudes.

The winter slight discomfort is almost the same in the whole domain. It changes with the elevation (Figure 5) in the transition seasons, with 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 5). The spatial distribution of the frequency of the risk of hypothermia, however, shows an opposite behavior – the distribution in 06 UTC is not so complex and similar to the elevation changes (Figure 5) 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 with moderate air quality index are mainly the city's ring road and busier transport routes, as well as the central parts, the most in morning hours. The Moderate pollution in the afternoon over Vitosha Mountain is probably due to 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 maximum in the afternoon hours in spring and summer, and in the morning ones for other seasons and annually. The AQI1 and AQI2 recurrence are higher in the morning hours.

We suggest that at least two factors could play a role in these features of the bio-climatic indexes. 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 5) 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 its frequencies in mountainous areas. Still, it is not always valid for the city limits and the Sofia Valley.

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## References

1. World Health Organization (WHO), Health Aspects of Air Pollution. Results from the WHO Project Systematic Review of Health Aspects of Air Pollution in Europe, 2004.
2. Fact Sheet Number 187, World Health Organization (WHO), 2000
3. European Parliament Directive 2002/3/EC of 12 February 2002 relating to ozone in ambient air, Official Journal of the European Communities (9.3.2002) L 67, 14-30.
4. European Parliament: Directive 2008/50/EC of the European Parliament and of the Council of 21 May 2008 on ambient air quality and cleaner air for Europe, Official Journal of the European Union (11.6.2008), L 152, 1-44.
5. Brunekreef, B; Holgate, S. Air pollution and health., *Lancet*, 2002; 360, 1233-1242.
6. Katsouyanni K., Ambient air pollution and health, *British Medical Bulletin* 2003, 68, 1, 143-156, <https://doi.org/10.1093/bmb/ldg028>
7. WHO Air quality guidelines for particulate matter, ozone, nitrogen dioxide and sulphur dioxide. Global Update 2005. Summary of risk assessment, WHO Regional Office for Europe, Copenhagen
8. Atkinson, R. W.; Yu, D.; Armstrong, B.; Pattenden, S.; Wilkinson, P.; Doherty, R.; Hea, MR.; Anderson, HR. Concentration-Response Function for Ozone and Daily Mortality: Results from Five Urban and Five Rural U.K. Populations, *Environ Health Perspect* 2012, 120, 1411-1417
9. Nikiforov, B.; Antova, T.; Lolova, D. Health issues for the population in the town of Pleven related to ambient air pollution, *Problems of Hygiene* 2002 ,3, 39-44 (Bulgarian)
10. Nikiforov, B.; Antova, T.; Lolova, D. Ambient air quality in the municipality of Rousse and public health risk, *Problems of Hygiene* 2003, 1, 15-22 (Bulgarian)
11. Antova, T.; Nikiforov, B.; Lolova, D. Ambient air quality and health risk to the population of the town of Dobrich, *Problems of Hygiene* 2002, 2, 27-32. (Bulgarian)
12. Pattenden, S. B.; Nikiforov, B.; Armstrong, B.G. Mortality and temperature in Sofia and London, *J. Epidemiol. Community Health* 2003, 57, 628-633
13. Starr, C., McMillan, B. Human Biology. Publisher: Brooks/Cole Cengager Learning, 2010
14. Giles, B. D.; Balafoutis, C. H.; Maher, P. Too hot for comfort: the heatwaves in Greece in 1987 and 1988. *International Journal of Biometeorology*, 1990, 34, 98-104.
15. Stathopoulou, M.I.; Cartalis, C.; Keramitsoglou, I.; Santamouris, M. Thermal remote sensing of Thom's Discomfort Index (DI): comparison with in situ measurements. *Proceedings of SPIE—The International Society for Optical Engineering* 5983, art. no. 59830 K, 2005
16. Sajani Z. S.; Tibaldi, S.; Scotto, F.; Lauriola, P. Bioclimatic characterisation of an urban area: a case study in Bologna (Italy). *International Journal of Biometeorology*, 2008, 52, 779-785.
17. Da Silva, V. D. P. R.; De Azevedo, P. V.; Brito, R. S.; Da Cunha Campos, J. H. B. Evaluating the urban climate of a typically tropical city of northeastern Brazil. *Environmental Monitoring and Assessment* 2010, 161, 45-59.
18. Fanger, P.O. Thermal comfort: analysis and applications in environmental engineering. McGraw-Hill (New York), 1972
19. Höpke, P. Die Thermische Komponente der Stadtklimas. *Wiss Mitt Meteorol Inst Univ München* 1986, 53, 94-108
20. Matzarakis, A.; Mayer, H. The extreme heat wave in Athens in July 1987 from the point of view of human biometeorology. *Atmos Environ* 1991, 25, 203-211.
21. Matzarakis, A.; Mayer, H. Heat stress in Greece. *Int J Bio-meteorology* 1997, 41, 34-39.
22. Höpke, P. The physiological equivalent temperature - a universal index for the biometeorological assessment of the thermal environment. *International Journal of Biometeorology* 1999, 43, 71-75.
23. Matzarakis, A.; Rutz, F.; Mayer, H. Estimation and calculation of the mean radiant temperature within urban structures. In: R. J. de Dear, J. D. Kalma, T. R. Oke and A. Auliciems (Eds.) *Biometeorology and urban climatology at the turn of the millennium. Selected Papers from the Conference ICB-ICUC'99*, Sydney, WCASP-50, WMO/TD No. 1026, 2000, 273-278

24. Matzarakis, A.; Rutz, F.; Mayer, H. Modelling radiation fluxes in simple and complex environments - application of the RayMan model, *Int. J. Biometeorol.*, 2007, 51, 323-334.

25. Rothfusz, L.P. NWS Technical Attachment (SR 90-23), 1990

26. Steadman, R. G. The assessment of sultriness, Part I: A temperature-humidity index based on human physiology and clothing science. *J. Appl. Meteorol.*, 1979, 18, 861-873

27. The NCAR Command Language (Version 6.6.2) [Software]. (2019). Boulder, Colorado: UCAR/NCAR/CISL/TDD.

28. Osczevski, R.; Bluestein, M. The new wind chill equivalent temperature chart *Bulletin of the American Meteorological Society* 2005, 86, 1453-1458.

29. Wind chill index. Accessed 20 May 2019, <https://www.canada.ca/en/environment-climate-change/services/weather-health/wind-chill-cold-weather/wind-chill-index.html>

30. Ivanov, V.; Evtimov, S. Heat Risks in Bulgaria during 2003-2012 period. *Bulgarian Geophysical Journal* 2014, 40, 3-13.

31. Ivanov, V.; Evtimov, S. Wind chill hazard in Bulgaria during 2003-2012 period. *Comptes Rendus De L'Academie Bulgare Des Sciences* 2014, 67, 1521-1530.

32. Ivanov, V.; Chervenkov, H. Modelling human biometeorological conditions using meteorological data from reanalysis and objective Analysis—Preliminary results. *Studies in Computational Intelligence* 2021, 961 SCI, 170 – 181

33. Chervenkov H., Slavov K., Ivanov V. STARDEX and ETCCDI Climate Indices Based on E-OBS and CARPATCLIM. *Numerical Methods and Applications. NMA 2018. Lecture Notes in Computer Science* 2019, 11189.

34. Georgieva, I.; Ivanov, V. Computer simulations of the impact of air pollution on the quality of life and health risks in Bulgaria. *International Journal of Environment and Pollution* 2018, 64, 35-46.

35. Ivanov, V.; Georgieva, I. Air quality index evaluations for sofia city. In 17th IEEE International Conference on Smart Technologies, Proceedings of EUROCON 2017, Ohrid, North Macedonia, 2017

36. Georgieva, I.; Ivanov, V. Impact of the air pollution on the quality of life and health risks in Bulgaria. In HARMO 2017, Proceedings of 18th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes, Proceedings, 2017

37. Georgieva I.; Gadzhev G.; Ganev K.; Prodanova M.; Syrakov D.; Miloshev N., Numerical study of the air quality in the city of Sofia – some preliminary results, *International Journal of Environment and pollution* 2015, 57, 162-174.

38. Georgieva, I.; Gadzhev, G.; Ganev, K.; Prodanova, M.; Syrakov, D.; Miloshev, N., Numerical study of the Air Quality in the city of Sofia, 8th Congress of the Balkan Geophysical Society 2015, BGS 2015

39. Georgieva, I.; Gadzhev, G.; Ganev, K.; Prodanova, M.; Syrakov, D.; Miloshev, N., Numerical study of the air quality in the city of Sofia - Some preliminary results, HARMO 2014 - 16th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes, Proceedings, 2014, 356-360.

40. Georgieva, I.; Gadzhev, G.; Ganev, K.; Melas, D.; Wang, T., HPC simulations of the atmospheric composition in Bulgaria and the city of Sofia. *Cybernetics and Information Technologies (CIT)* 2017, 17, 37-48.

41. Georgieva, I.; Gadzhev, G.; Ganev, K.; Miloshev, N., Computer simulations of atmospheric composition in urban areas some results for the city of Sofia., Proceedings of the Tenth International Conference on "Large Scale Scientific Computations", LSSC2018, Sozopol, Bulgaria, June 5-9 2017, 2018, LNCS10665, 474–482.

42. Georgieva, I.; Gadzhev, G.; Ganev, K.; Miloshev, N., Analysis Of Dynamical And Chemical Processes Which Form Atmospheric Composition Over Bulgaria, *SGEM* 2018, 2018, 18, 4.3

43. Georgieva, I.; Miloshev, N. Computer Simulations of PM Concentrations Climate for Bulgaria, International Conference on "Numerical Methods for Scientific Computations and Advanced Applications", NMSCAA'18, 2018, 46-49.

44. Shamarock, W. C.; Klemp, J. B.; Dudhia, J.; Gill, D. O.; Barker, D. M.; Wang, W.; Powers, J. G., A Description of the Advanced Research WRF Version 2 (No. NCAR/TN-468+STR), 2017, University Corporation for Atmospheric Research. <http://www.dtic.mil/cgi/tr/fulltext/u2/a487419.pdf>

45. <http://www.ftp.ncep.noaa.gov/data/nccf/com/gfs/prod/>

46. Byun, D.; Ching, J. Science Algorithms of the EPA Models-3 Community Multi-scale Air Quality (CMAQ) Modeling System. 1999, EPA Report 600/R-99/030, Washington, D.C., EPA/600/R-99/030 (NTIS PB2000-100561). [https://cfpub.epa.gov/si/si\\_public\\_record\\_report.cfm?Lab=NERL&dirEntryId=63400](https://cfpub.epa.gov/si/si_public_record_report.cfm?Lab=NERL&dirEntryId=63400)

47. Byun, D. Dynamically Consistent Formulations in Meteorological and Air Quality Models for Multiscale Atmospheric Studies part I: Governing equations in a generalized coordinate system. *J. Atmos. Sci.* 1999, 56, 3789-3807.

48. CEP: Sparse Matrix Operator Kernel Emission (SMOKE) Modeling System, 2003, University of Carolina, Carolina Environmental Programs, Research Triangle Park, North Carolina.

49. Denier van der Gon, H.; Visschedijk, A.; van de Brugh, H.; Droge, R. A high resolution European emission data base for the year 2005, 2010, TNO-report TNO-034-UT-2010-01895 RPT-ML, Apeldoorn, The Netherlands.

50. Hong, S.-Y.; Lim J.-O. J. The WRF Single-Moment 6-Class Microphysics Scheme (WSM6), *J. Korean Meteor. Soc.* 2006, 42, 129–151.

51. Collins, W. D. et al. Description of the NCAR Community Atmosphere Model (CAM 3.0), NCAR Technical Note, NCAR/TN-464+STR 2004, 226.

52. Xiu, A.; Pleim J. E. Development of a land surface model part I: Application in a mesoscale meteorology model. *J. Appl. Meteor.* 2001, 40, 192–209

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53. Pleim, J. E. A combined local and non-local closure model for the atmospheric boundary layer. Part 1: Model description and testing, *J. Appl. Meteor. and Clim.* 2007, 46, 1383–1395.
54. Georgieva, I. Air Quality Index Evaluations for Bulgaria, Proc. of the international conference on numerical methods for scientific computations and advanced applications, May 19-22, 2014, Bansko, 2014, 39-42.
55. de Leeuw, F.; Mol, W. Air Quality and Air Quality Indices: a world apart., 2005, ETC/ACC Technical Paper 2005/5 <http://acm.eionet.europa.eu/docs/ETCACC> TechnPaper 2005 5 AQ Indices.pdf