

# The impact of plume rise on modelled SO<sub>2</sub> concentration profiles

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2021

## Introduction

Above the elevated sources, which are usually the industrial stacks with high emissions, the plume rise is occurring due to the escape velocity of the pollutants from the stack and upward acceleration due to buoyancy caused by higher temperature of the emitted pollutants compared to the ambient air. The plume rise is defined as the difference between the effective source height - a height at which the plume becomes passive and follows the motion of the atmospheric flow, and the source height (Seinfeld, 2006).

The plume rise is heavily affected by the meteorological situation - especially wind and stratification of the atmosphere - it grows for unstable conditions and is suppressed during stable conditions. Therefore, it needs to be computed at every time step of the model simulation for all selected sources. To simulate this process in Eulerian models, a sub-grid algorithm is required. Without the plume rise algorithm, the source remains passive - the pollutants are emitted with no exit velocity and no temperature difference from the surroundings, the effluent immediately follows the atmospheric flow. In a model simulation, a passive source remains in a specific grid cell, in which the elevated source is positioned. The plume rise algorithm effectively spreads the emission source throughout multiple model layers.



Fig.1: The plume rise.

CMAQ v5.2 (US EPA, 2017) provides an in-line algorithm for the plume rise calculation, which was not available in the previous versions of the model (it was only available in some emissions preprocessors, e.g. SMOKE). Our intention in this paper is to quantitatively evaluate the effect of the plume rise calculation on the SO<sub>2</sub> concentrations. The effect is evaluated by comparison of simulations without and with the plume rise (case A and B, respectively).

## Simulation specification

CMAQ v5.2 was used for the simulation of SO<sub>2</sub> concentrations for the period of January 2017 in the Nováky region, Slovakia. The model domain consisted of 29x33 cells with 1570x1570 m of horizontal resolution and 31 vertical layers. The meteorological inputs were provided by the WRF model. Two point emission sources were included in the simulation, which correspond to two major stack sources of the Nováky coal-fired power station. The first stack is 150 m high, positioned in the third vertical model layer and emitting 1.12 mol·s<sup>-1</sup> of SO<sub>2</sub>. The second stack is 300 m high, positioned in the fourth layer, emitting 2.28 mol·s<sup>-1</sup> of SO<sub>2</sub>. Both stacks are situated in the same grid cell x = 16, y = 14. The simulation was computed twice - with the plume rise calculation (case B) and without it (passive source) (case A). Simulations were computed on SHMU's high-power computer using 32 cores.

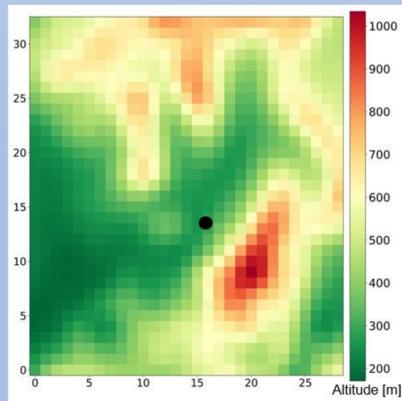


Fig.2: Terrain elevation in Nováky region; position of the simulated sources is indicated by the black dot.

## Results

### Dispersion of the emissions

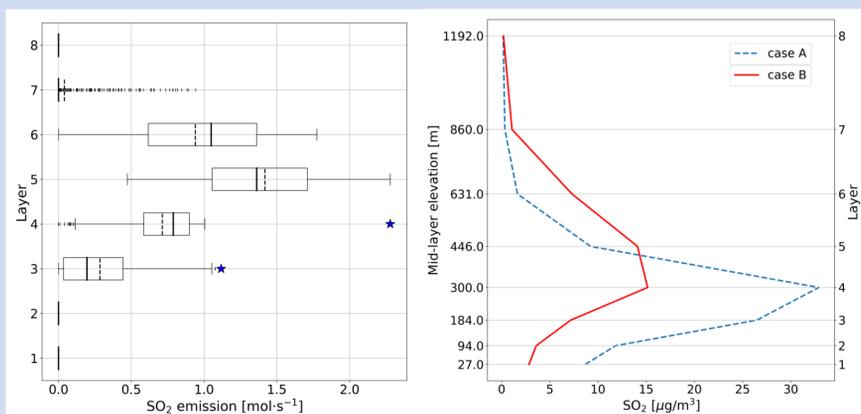


Fig.3: The dispersion of the SO<sub>2</sub> emissions in the individual layers with the plume rise. The stars represent position and magnitude of the emission sources without the plume rise. The bold line within the box is a median and the dashed line is an average.

Fig.4: Mean hourly SO<sub>2</sub> concentration profiles without (case A) and with (case B) the plume rise in the vicinity of the source (5x5 grid cells around the source).

The plume rise calculation effectively spreads the emission sources to higher model layers, which strongly affects the concentration profiles of pollutants. The dispersion of the emission sources varies significantly in time. Figure 3 shows a box plot of the dispersion of the emission sources due to the plume rise calculation. We can see that the emissions are reduced in the 3<sup>rd</sup> and 4<sup>th</sup> vertical layer and increased greatly in the 5<sup>th</sup> and 6<sup>th</sup> layer.

The mean hourly SO<sub>2</sub> concentration vertical profiles for 5x5 grid cell vicinity of the source are presented in Figure 4 for both cases. For case B, the concentrations are reduced substantially in the first 4 vertical layers and are increased for layers 5 to 7. The total amount of SO<sub>2</sub> in the selected volume of the domain has decreased for case B by around 30%, due to stronger mean winds in the upper layers, which enhance the pollutant advection from the selected volume.

## Literature

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- Šedivá, Tereza, 2020: Impact of the physical parametrisations of CMAQ model on the resulting pollutant concentrations, Master Thesis, Comenius University, Bratislava.
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### Comparison of the surface concentration values

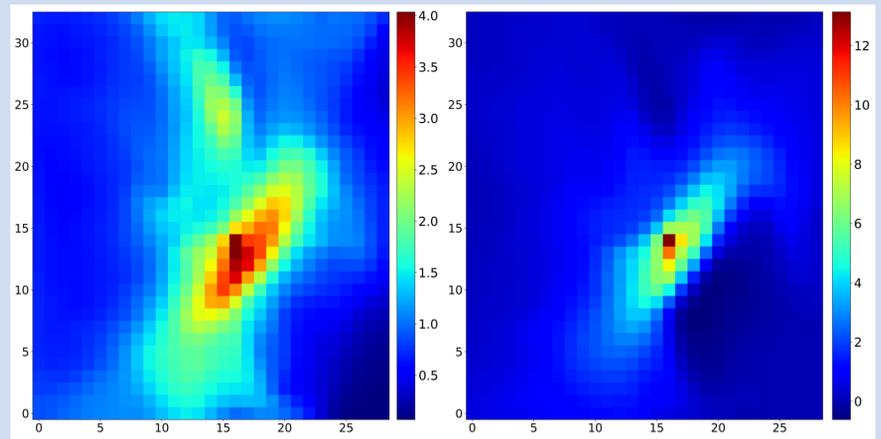


Fig.5: Mean hourly SO<sub>2</sub> concentrations in the surface layer with the plume rise in μg·m<sup>-3</sup> (case B).

Fig.6: Mean hourly SO<sub>2</sub> concentration differences between cases A and B (A-B) in μg·m<sup>-3</sup>.

Figure 5 shows the mean hourly surface concentrations for the simulation with the plume rise computation (case B). In the vicinity of the source, the concentrations are around 4 μg·m<sup>-3</sup>. Figure 6 shows the difference between cases A and B in the surface layer. In the source grid cell the concentrations are more than 12 μg·m<sup>-3</sup> higher for case A, which is 328% of the value for case B. The differences decrease steeply around the source, however, the majority of the valley around the source has an increase in concentrations above 5 μg·m<sup>-3</sup> in case A. A detailed comparison of simulations with and without plume rise can be found in Šedivá (2020).

### Daily profile of concentration differences

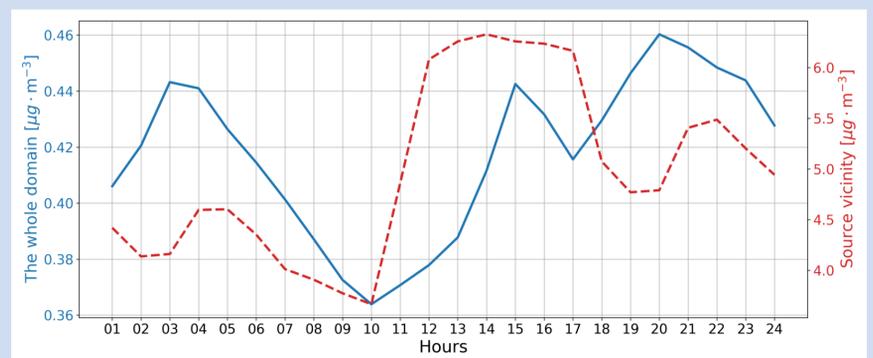


Fig.7: Mean daily profiles of SO<sub>2</sub> concentration difference without and with the plume rise for the whole domain - blue line (33x29 grid cells, first 8 vertical layers) and source vicinity - red dashed line (5x5 grid cells, first 8 vertical layers).

The stability of the atmosphere has a distinct daily regime determined by the sunshine (Stull, 1988), which correspondingly affects the plume rise. Figure 7 shows mean daily profiles of concentration differences between cases A and B for the first 8 layers of the whole domain and source vicinity of 5x5 grid cells. For the whole domain the mean differences are below 0.5 μg·m<sup>-3</sup>, but for the source vicinity the differences are substantial, reaching up to around 6 μg·m<sup>-3</sup>. The response of the concentrations to changes in the plume rise is delayed further from the source and becomes negligible for distant areas. Therefore, we further analyze only the profile in the vicinity of the source in relation to diurnal changes.

After sunset (around 5 PM) the differences in concentrations probably decrease due to formation of the residual layer (Stull, 1988), where turbulence is equal in all directions, which eliminates the differences between cases A and B. The 2 peaks formed during the night are probably a consequence of the stable nocturnal layer (Stull, 1988) growing from the ground above the first and, eventually, the second source. As the stable layer grows above the source, it prevents the emissions from reaching the upper layers (Bednář, 1984) for case A; however the plume rise in case B is able to "shoot" above a narrow stable layer, where the pollutants disperse more rapidly, increasing the differences between cases A and B. As the stable layer grows, it suppresses the plume rise and therefore eventually decreases the differences between cases A and B.

The rapid increase of the differences after 10 AM is difficult to explain properly due to varying daily regimes during the month. However, upon analysis of the regimes of the individual days, we observed some patterns. During the month of January, there were many days with high inversions forming during the nights, reaching several layers above the stacks. These inversions were then dispersed after sunrise by formation of the turbulent mixed layer from the ground, however, the mixed layer often reached only up to layers 3 or 4. This kind of situation produced the largest concentration differences between the two cases, since for case A the pollutants were mostly dispersed into the lower layers, while for case B, the emissions spread to higher layers with limited downward mixing. Needless to say, this effect is heavily affected by the wind profile, making each day's regime different.

## Conclusion

Our simulations showed how the in-line calculation of the plume rise process affects the emissions and concentration profiles of SO<sub>2</sub> in the case study of Nováky region, Slovakia. The elevated sources were located in the 3<sup>rd</sup> and 4<sup>th</sup> vertical layers of the CMAQ v5.2 model.

Our results showed, that the plume rise calculation effectively disperses the emission sources into 5<sup>th</sup> and 6<sup>th</sup> layers (Figure 3), while substantially reducing the emissions in the lower layers. The 7<sup>th</sup> layer was affected only rarely and the 8<sup>th</sup> layer was unaffected. SO<sub>2</sub> concentrations increased in layers 5 to 7, decreased in layers 1 to 4, and have not changed in layer 8 (Figure 4).

The surface concentrations with the plume rise calculation reach values around 4 μg·m<sup>-3</sup> in the source vicinity, while the concentrations without the plume rise in the source grid cell reach values more than 12 μg·m<sup>-3</sup> higher (Figures 5 and 6). With the plume rise calculation, the concentrations of SO<sub>2</sub> decreased by around 0.4 μg·m<sup>-3</sup> for the whole domain and around 5 μg·m<sup>-3</sup> for the 5x5 grid cells source vicinity (Figure 7).

Daily profile of concentration differences between cases without and with the plume rise was analyzed and attempted to be explained by the diurnal cycle of the atmospheric boundary layer (Figure 7). An extended simulation including a longer period and different months of the year would provide more insight into the study of the boundary layer behaviour.