"Modelling air quality in the city"

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Abstract

In this thesis we make a start with a 3D model for prediction of air quality during a heatwave at Nijmegen-West and Weurt. The current air quality models are not so specific for this case. These models are studied, to give an idea what is necessary to make a model that is accepted by the government for official studies. But, it is interesting to see what happens if you do not follow the official rules. It could be, that the result is a better prediction of air quality for this case. For the prediction of air quality, the meteorological characteristics are important. So first, we look at the most important meteorological characteristics. Not everything can be included in the new model, because it is too complicated. Also, the weather data and measurements of air pollutants are studied. This data is valuable for the development of the model. Then there is started with the developing of the new model. The software that is used is Comsol Multiphysics, version 5.2. The model uses an advection-diffusion equation. First, a simple 2D model is made, to give an idea what mathematical method is the best to use for a 3D model. The 2D model is easier to solve and check than a 3D model. Unfortunately, these best options cannot always be used in 3D, because of a very large solution time in 3D. Then, there is started with the development of the 3D model. The relevance of advection and diffusion is tested. The expected effect of advection and diffusion can be seen, but there are also negative concentrations where there must be an almost zero concentration. These negative concentrations are related to a meteorologic characteristic. This was just a start with a model and it will takes much more time to get a realistic model.

1 | Introduction

In this thesis I will propose an alternative way to model air quality. There are several large scale models for air quality that are accepted by government for official studies. Each model has its own (dis)advantages. In general, they are not suitable for specific cases. The new modeling approach will be for specific events such as a heat wave period, 'events' which lead to more traffic, like the "Nijmeegse Vierdaagse" and calamities like a big fire. In this thesis, it is about a heat period.

The intention is to develop a medium scale model for the air quality in urban. As case study we use the area known as Nijmegen-West and Weurt. This is an area where industry, harbor and houses combine. Industry, traffic and harbor leads to a lower quality of air. The town Nijmegen wants to get more insight in the processes that lead to bad air quality. Therefore they placed seven measurement stations for particulates.

The air quality measurements are valuable for the development of the new model. Also, meteorologic characteristics are important for this. There is measurement data from the weather, like temperature, wind-speed and wind-direction. It would be useful if all data is validated, before using it in the new model, as currently not all data appear equally reliable.

The new model is based on differential equations. The software to use is Comsol Multiphysics, version 5.2.

The central question is: is it possible to develop a good air quality model based on the idea written above.

The structure of this thesis is as follows:
Chapter 2 reviews air quality literature in general. It contains information about air pollutants, their measurements and meteorology. Chapter 3 is a description of the current air quality models and methods. In chapter 4 weather data and measurements of air pollutants for the case study Nijmegen-West and Weurt are considered. In chapter 5 a 2D test case model is presented, to analyze whether Comsol is suitable and which method is the best to use for the 3D model. In chapter 6 a 3D model will be developed. Finally, chapter 7 contains a summary, conclusions and some recommendations for further development.

7 | Summary and recommendations

In this thesis a model for air quality in Nijmegen-West and Weurt during a heat wave was initiated and implemented in Comsol Multiphysics, version 5.2. In section 7.1 a summary of the thesis is given. In section 7.2 some recommendations for future developments are presented.

7.1 Summary

In this thesis an alternative way to model air quality is investigated. This model is on medium scale of a few kilometers and specific for a heat wave at Nijmegen-West and Weurt. Current air quality models are not so specific for this case. The new model is based on the advection-diffusion equation. The software that is used is Comsol Multiphysics, version 5.2.

Relevant processes that should be incorporated in the model
To model air quality, there are a few meteorologic characteristics of interest. Also deposition and plume rise is important. This is all described in chapter 2.
First the stability of the atmosphere. In a stable atmosphere the air quality is worse than in an unstable atmosphere at the same amount of air pollution. The spread of emission is hindered in a stable atmosphere. Through this, air pollutants are almost not diffused with the air. In an unstable atmosphere the spread of emission is very good. Therefore, the air pollutants are diffused with the air. With the Monin-Obukhov length, the stability can be determined.
Also important for the spreading of air pollutants is the mixing layer height. Beneath this layer there is turbulence, above there is not. If there is emission of some pollutants above the mixing layer height then these pollutants do not reach the earth's surface, because they cannot break through the mixing layer height. But if the emission is beneath this layer then the pollutants can reach the earth's surface. So, the mixing layer height determines the contribution from a source to a receptor.
Besides this, the wind-speed and wind-direction is of interest. The wind-speed is growing with height and depends on the Monin-Obukhov length. The wind-direction should also changing with height. Since the literature is not very clear about how much this is changing, the wind-direction is keeping constant in height in the model.
There is also deposition: wet and dry. This is too complex for now. Also, indus-

try is producing gas out of stacks. Then there is plume rise, occurred by heat emission or the exit velocity of the gas out of the stack. The height of a plume is different for a stable atmosphere than for unstable or neutral atmosphere. These heights influences the concentration of the plume at a certain place. This is also too complex for now. The focus is on air transport, so deposition and production is not included yet.

Existing models not suitable

There are a few air quality models, which are allowed by governement, to use for Nijmegen-West and Weurt. To compute the air quality, a few rules must be followed. This is described in chapter 3.

First, the background concentrations must be calculated with the OPS model. Then, local contribution can be calculated with a model, based on SRM. There are three methods: SRM-1, SRM-2 and SRM-3. SRM-1 is for roads inside urban areas. SRM-2 is for roads outside urban areas. SRM-3 is for other point and area sources. The new model that is developed in this thesis is for Nijmegen-West and Weurt, so it must be based on SRM-1 and SRM-3. There are two models officially accepted for these two: STACKS (version 2015.1, owned by DNV-GL) and ADMS URBAN (version 2.2, owned by Flow Motion). So, if we want our new model to be officially accepted, then it must follow all these rules. Since for the current air quality models there can be an uncertainty between 20% and 95% and the largest uncertainties are for local situations and deposition, it can be interesting not to follow the rules. Maybe, this gives better, more accurate, results for the specific case: a medium scale model for air quality during a heat wave at Nijmegen-West and Weurt. Also, rules can be changed in the future. So, this thesis does not follow the official rules.

Useful data

There is some weather data, which can be an input of the model and there is some air pollutants measurement data. The last can be used to check the results of the model. The data is presented in chapter 4.

For the weather data, there are stations of KNMI, but there are also two weather amateurs around Nijmegen providing data. This are people who are living in Nijmegen and they have a weather station in their own garden. This can give more accurate result of weather in the city, like urban heating.

In Nijmegen-West and Weurt there are measurements of air pollutants done by RIVM with LML and Nijmegen itself with the particulate monitoring network. The only data that is used at this moment, is the validated data of the wind-speed and wind-direction at Cabauw. Since the current model is just an empty block, the situation can be compared with open air. Therefore, the data of weather amateurs are not useful at this moment. Also, the wind-speed at de Bilt and Volkel are not so many times measured as in Cabauw. Through this, these data looks too much discrete for using it in Comsol. The model get better results with a continue data input. Therefore, the data of Cabauw is used, which looks more continue. There are no new measurements anymore for air pollutants coming from the particulate monitoring network. Therefore, the validated data of LML must be used in the future, to check the results of the model.

Alternative model

Now, all necessary information was complete to make a start with the new model.

First, a 2D model is put forward in chapter 5. With this 2D model, a numerical experiment can be executed. This gives information whether Comsol can be used and, if so, a good method can be found for the 3D model. In Comsol we used the 'Transport of Diluted Species' module, in the conservative form.

The method that is used to solve the equations is BDF with max order 5. The mesh refinement showed that a finer mesh gives better results. Also, refinement of relative tolerance gives better results. Without diffusion there is converge of order 2. With diffusion, there are some really small instabilities, it is more a kind of noise. The best results are for the mesh with adaptive mesh refinement. So, this suggest to use this method for the 3D model. The instabilities are spurious modes: if the max order of BDF was set to 1, then these instabilities changes into undershoots. You cannot use this lower order of BDF because the tops are not correct anymore. The instabilities were also depending on the inflow (sharp transitions). These results are good enough to work further with Comsol for the 3D model.

Then there is started with developing the 3D model in chapter 6. The computation time to find a solution will be very big (about 2 weeks and problems with memory). Therefore, the recommended methods of the 2D model cannot be used at this moment. So, a little bit coarser mesh and bigger relative tolerance is used. In this model the solution is stored every 5 minutes, for 24 hours. The domain is a rectangular block. There is advection, that is the wind, it is changing in time and height and there is diffusion, with mixing layer height, also changing in time and height. There are two inflows, that are Gaussian blobs. The first one is at night, the second at day, because of the difference between day and night for diffusion. There is no production in the block. So, the inflows are coming from outside the domain and via the boundaries blowing into the domain.

The effect of advection and diffusion was visible. For this, Comsol has good results. Unfortunately, there were negative concentrations above the mixing layer height (above the inserted inflow). This is not physically correct. But there are no instabilities anymore. The finest mesh, gives better result than the coarser mesh: the negative values were smaller for the finer mesh. The absolute values of the negative concentrations for the finest mesh for the model with correct diffusion but advection constant in time are compared with the maximum value $1.08681 \cdot 10^{-6}$ maximal 0.8% of this value. Compared with the model without mixing layer height, at the same points, these are approximately 7 times smaller than those without mixing layer height. So at this point, Comsol is not very good. But there are some possibilities to avoid this maybe, which are listed in the conclusion and also later on in the recommendations.

For all models, in general: the numerical accuracy is good for models without mixing layer height. If there is a mixing layer height, the numerical accuracy for these models is less above the inserted inflow, which also shows negative concentrations. But, these negative concentrations are smaller (so better) for a finer mesh. So, maybe with smaller meshes, the results are better and more equal for the different meshes which suggest also a good numerical accuracy for these points. This is not tested at this moment, because each model will takes more than 2 weeks to find a solution with a smaller mesh.

Conclusion
The effect of advection, diffusion and the mixing layer height are visible in the model. So that is good. A disadvantage is the negative concentrations found above the mixing layer (above the inserted inflow). Of course, this is not good because it is not physically. In absolute values the values were approximately 0.8% of the maximum value $1.08681 \cdot 10^{-6}$. A reason for this negative values could be that the mixing layer was too low. If this layer is placed higher, the transition zone for the amount of diffusion is bigger and maybe than the concentrations are positive. But this is not always realistic, it is possible that the mixing layer is placed much lower than used here. It is also possible that you see this, because of the strict upper boundary of the inflow (where the values are around 1% of the maximum value).

Another problem was the computation time to find a solution. The most advanced model takes around 6 days to find a solution, with 8 CPU's. Since this model was just a simplified version of the reality, I expect that when there is a very realistic model, the time to find a solution is very big. If you want the model to use for predicting the air quality for short-term on real time, it will be possible that the solution is found after the time for which the solution is computed.

So, to answer the central question: is it possible to develop a good air quality based on the presented ideas with Comsol? At this moment it is too early to answer this question. The model was not very realistic, because of the empty block. But the first results gives hope and thus it is interesting to develop this model further. However, more research is needed to definite get an answer. For this, there are some recommendations in the next section.

7.2 Recommendations

In this section there are some recommendations for further research and improvement of the model.

Decreasing computation time
Since we already saw that there was a very high computation time, the first step will be to find a way for a shorter computation time. The most advanced model takes now around 6 days with a cluster of 8 CPU's to find a solution. There was also a test with a finer mesh, but this fails because of memory problems and too much computation time (more than 2 weeks). For instance, take a "super computer" for your computations. Then, probably, the recommended solution methods of the 2D model can be used for the 3D model. The model can also be made more complex with a "super computer".

Incorporate emmissions
The inflow was defined as a boundary condition. This is good for background concentrations. But, there are also air pollutants produced inside Nijmegen-West and Weurt. These can come from stacks or traffic. For background concentrations you need to know how much from each air pollutant flows into Nijmegen-West and Weurt for every time-step. Also, for air pollutants produced in Nijmegen-West

and Weurt, you must know how much from each is produced at which time. This is not so easy. So, this can be a problem for developing the model. There are emission-registrations of air pollutants in kg per year from factories in Nijmegen-West and Weurt from the past, so this can gives an idea. This is available at: http://www.emissieregistratie.nl
You also want to know, how relevant the air pollutants are that are produced around Nijmegen-West and Weurt. Therefore, first test the relevance of an air pollutant at different distances from a source. Then you know, how big the area around Nijmegen-West and Weurt is of interest for the air quality in Nijmegen-West and Weurt.
The rate of emission is not the only problem. In section 2.4 we saw that for calculating the plume rise from a stack, you also need to know the stack height, the inside diameter of the stack and the stack exit velocity and the temperature of the gas at the exit of the stack. These data is difficult to get (if it is possible at all). Then, there is also traffic, which produces air pollutants. There is data from the past, with an average of how many cars are passed at a few points of Nijmegen-West and Weurt. This is available at: www.westenweurt.nl. You can add this traffic as a road (a surface at the ground boundary), which produces some air pollutants. This is not constant in time. And also, it can be different for the different road sections. But this must be researched first with the mentioned website.

Despite, it will be useful to test the effect of an inflow from a stack. Possibilities for a stack are: a stack ending under the mixing layer height and a stack ending above the mixing layer height. Maybe, with production from a stack or traffic the negative concentrations disappear, because then the "inflow" is not separated by the mixing layer height.

Disappear negative concentrations

Another option, to let these negative concentrations disappear, is adding a small begin concentration. Now, at the start of the model, the block is clean, so a zero concentration. This new begin concentration must be very small then, because of the small inflow concentration. This new begin concentrations ensures less sharp transitions when there comes an inflow. Also, a finer mesh can be an option (just mentioned earlier).

Add building

Then, at this moment there is just open air and no buildings. With buildings, the air flows are interrupted and the mesh is more complicated. Then adaptive mesh refinement is really needed. This can also gives more instabilities in the solution and it will increase the solution time. It is possible to add each building in Comsol, but it will takes a lot of time to do this. Therefore, add some levels with different sizes and height, which are related to the surface roughness.

Add deposition

There was also no deposition in the model. Since we saw this is also an important part, a first idea for this can be a small percentage of the concentrations will be deposited. First see the effect of this, before making the deposition more complicated and realistic. In section 2.3 there is a part of the process described. So, before adding realistic deposition, this must be researched further. For example, when it is raining, (a part of) the air pollutants will be deposited, so this improves the air quality.

Add different air pollutants
It must also be possible to model more than one type of air pollutant in once. Because traffic can have other emissions than factories. Adding other air pollutants is easy to do in Comsol; just add them.
Also it is possible that different air pollutants influences each other. Therefore, you need to know everything about the effect of each air pollutant on another. This must also be researched first. But then, you can easy add reactions in Comsol.

Model calibration
Later on, when the model is more realistic, the measurements of chapter 4 can be used, to check and improve the solutions. You can just check the solution at points where some concentrations are measured. It is not useful to interpolate these to check the solutions at points where is not measured. Because then, the model will be based on these interpolations (so a data-driven model) and that is not what you want. But for the weather data, you need maybe more data to know the exact circumstances for each small part of Nijmegen-West and Weurt. A possibility is interpolating of available data together with some knowledge about the influences of buildings/traffic on weather conditions at small parts. It is possible to add weather data for small parts of the domain in Comsol, but you take into account sharp transitions (if they are already present).

Predicting air quality
Also, when it is about predicting the air quality, the weather must also be predicted. Therefore, it should be communicate with weather predicting models. If you can get the results of some weather prediciting models, then it is possible to use this in Comsol. But, values like Monin-Obukhov length and mixing layer height must then be computed first, if they are not present in the predicted weather data. This is possible in Comsol. But if for example the mixing layer height is changing a lot, this makes it more difficult to find a correct solution. Also, as mentioned earlier, this layer leads to negative concentrations. The expectation is that this can be worse if the height of this layer is changing rapidly. Because then, the diffusion (in which the mixing layer is processed) is also changing rapidly. But on the other side, a higher mixing layer height gives possibly no negative concentrations anymore, because of a bigger transition zone. This should be easy to test: use the model with a higher mixing layer height but make first the domain higher, to get 'real high' mixing layer height and enough space above it, to see the effect there.

You also want to know something about the uncertainties of your model for predicting the air quality. This is possible with the prediction of the past compared with the measurements of that time. But there are not so much measurement points, so this is not so easy.

Officialy accepted model
Another difficulty, when this model must be used official, it must follow the rules of the law, as described in chapter 3. But, as mentioned earlier: it was interesting to

see, what is happening if you do not follow the rules. If you really want to follow this rules, you have to do more research. Then you need to know exactly all rules. This will be a lot of work and maybe, you have to make big changes in your model.

Other options
A really different option: forget Comsol and make your own numerical method to solve the problem with another software like Matlab. The initial and boundary conditions and advection and diffusion can be used in the same way as here. This is really complex, but maybe you have more insight in what is happening in mathematical view. But, I think, Comsol is easier and better to use.

Conclusion
So, the conclusion is: work further with Comsol. It is not clear if the results will be good, when you have everything in your model, that is mentioned here. But at first sight: most of the things mentioned in this thesis are possible in Comsol. So, the first next step should be adding some building and an inflow from a stack or traffic with a really faster computer.