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## ANALYSIS AND COMPARISON OF TWO MODELS RESPONSE TO AN EMISSIONS ABATEMENT SCENARIO

Yelva Roustan<sup>1</sup>, Isabelle Coll<sup>2</sup>, Nicolas Yan<sup>1</sup>, Aurélie Quemener<sup>2</sup>, Arthur Elessa<sup>2</sup>

 <sup>1</sup> CEREA, Joint laboratory École des Ponts ParisTech -EDF R&D – Université Paris-Est, Champs-sur-Marne (France)
<sup>2</sup> LISA, UMR CNRS 7583, Paris-Est Créteil University - Paris Diderot University - CNRS, Créteil

(France)

Corresponding author(s): Roustan, roustan@cerea.enpc.fr

**Abstract**: One crucial issue about energy scenarios is their ability to sufficiently improve local air quality, in view of the strong orientation of current regulations towards energy efficiency and  $CO_2$  emission reduction issues. In this presentation, we discuss the impact on air quality of the implementation of an ambitious energy scenario that was recently developed by The French Environment and Energy Management Agency (ADEME) for the time horizon of 2030. With this aim, the abatement of air pollutants emissions arising from this scenario was evaluated, and the scenario was simulated. Simulations were conducted at the urban/regional scales, with two "state of the art" chemical transport models (CTM), over three different urban areas. The main species/indicators of interest for the impact of the emission scenario on air quality are nitrogen dioxide (NO<sub>2</sub>), particulate matter (PM<sub>10</sub> and PM<sub>2.5</sub>) and ozone (O<sub>3</sub>). The results show that the three urban areas give specific responses to the emissions changes, that are discussed against air quality indicators in view of their different characteristics. The differences between the results of each model will be analysed to assess the uncertainty in the evaluation of the scenario efficiency.

Key words: prospective evaluation, emissions abatement scenario, air quality, uncertainties

#### **INTRODUCTION**

One of the reasons that motivate the development of atmospheric dispersion models is their expected ability to support prospective studies in the framework of air quality management. Such studies may rely on the constitution of a dedicated emission scenario to evaluate the impact of pollutant release on the observance of regulatory thresholds, and on the exposure of urban populations to potential pollution events. In such studies, the range of model responses to emission abatement has to be considered and exploited in order to give uncertainty attributes to the results.

In this work we aim at addressing the question of the air quality impact of current environmental regulations, that are mostly driven by energy efficiency and by the "Factor 4" objective on the emission of greenhouse gases. With this goal, we propose to use two different chemistry-transport models to evaluate the impact (and the associated uncertainty) on air quality of an assertive energy scenario developed by The French Environment and Energy Management Agency (ADEME) for the time horizon of 2030. The first part of this short paper presents the structure of the two models and their common configuration, as well as the simulated areas and periods. The second part presents the specificities of the ADEME energy scenario. Finally the results are presented through one case study.

### MODEL PRESENTATION

#### **Polyphemus model**

Polyphemus is an air quality modeling platform which aims at covering the scope and the abilities of modern air quality systems (<u>http://cerea.enpc.fr/polyphemus/</u>). It deals with applications from regional scale to continental scale and among other tools provides a modular model based on an Eulerian formulation. For this study the CB05 chemical mechanism (Yarwood et al., 2005) is used to represent the chemical reactions between gaseous species with photolysis rates computed by the preprocessors Fast-JX

(Wild et al., 2000). The ISORROPIA (Nenes et al. 1998) models is used to describe equilibrium between the inorganic aerosol components and the H<sup>2</sup>O model (Couvidat et al., 2012) the equilibrium between the organic aerosol components. A simplified aqueous model (Tombette, 2007) is used to represent the interactions within the aqueous phase between particles and dissolved gaseous species. All these models are used together through the SIREAM Model (Debry et al. 2007) based on a sectional approach to represent the aerosol size distribution. For this study five size sections are considered from 10 nm to 10  $\mu$ m. The dry deposition of gaseous species is described using a resistant analogy approach following Zhang et al. (2003). The dry deposition of particles are computed following the parameterization of Zhang et al. (2001). The wet deposition of gaseous and aerosol species represent deposition flux from incloud and below cloud scavenging. For in-cloud scavenging a common parameterization based on a constant collection efficiency of 0.9 (Seinfeld and Pandis, 1998) is used both for gaseous and aerosol species in cloud water. For below cloud scavenging the parameterization of Sportisse and du Bois (2002) is used for gaseous species, the parameterization proposed in Seinfeld and Pandis (1998) is used for aerosol species.

### **Chimere model**

The CHIMERE model (http://www.lmd.polytechnique.fr/chimere/) can be run from the regional to the continental scale, with horizontal resolutions ranging from 1 to 100km. To account for atmospheric chemistry, CHIMERE uses by default the MELCHIOR2 gas-phase chemical scheme (120 reactions for 44 gaseous species) which is adapted from the original EMEP mechanism and is a reduced version of the MELCHIOR1 mechanism, obtained by Carter's method. Aerosol particles are described using 8 size bins ranging from 10 nm to 40 µm, through the concentrations of 7 particulate species: primary particle material, nitrate, sulfate, ammonium, biogenic SOA, anthropogenic SOA and water (Bessagnet et al., 2008; Schmidt et al., 2001; Bessagnet et al., 2004). Physical processes taken into account are coagulation (Gelbard and Seinfeld, 1980), absorption (Nenes et al., 1998) and nucleation for sulfuric acid (Kulmala et al., 1998). The equilibrium concentrations of inorganic species are computed by the thermodynamic module ISORROPIA (version 1.7) presented in Nenes et al. (1998). The gas-phase chemical mechanism for secondary organic aerosol has been described in detail by (Pun et al, 2006). In the model, horizontal advection is calculated using the Van Leer second order scheme and boundary layer turbulence is represented as a diffusion phenomenon, following Troen and Mahrt (1986). Vertical winds are diagnosed through a bottom-up mass balance scheme. Dry deposition is coded as in Wesely (1989) and photolytic rates may be attenuated using liquid water or relative humidity. Finally, the numerical time solver uses the TWOSTEP method.

#### Simulation configuration

The simulation of three different French urban areas is considered in this study: 52 Nantes, Paris and Strasbourg. These urban areas were chosen due to their different 50 profiles, in terms of both meteorological conditions and anthropogenic emissions. For <sup>48</sup> example, Nantes and Paris have a Western 46 European oceanic climate while Strasbourg is under continental influence. Also, despite 44 the fact that NOx emissions of the three cities are dominated by road traffic, the 42 main contributors to PM emissions in Nantes and Paris are residential heating, road traffic and manufacturing industries



Figure 1: Simulation domains considered for the study.

while in Strasbourg the emissions of PM are dominated by wood burning in the residential sector. The models were run over two large nested domains in order to provide robust boundary conditions to the urban areas (Figure 1): a continental domain with an horizontal resolution of 60x60km<sup>2</sup>, a national domain (15x15km<sup>2</sup>). The three urban domains are then simulated with 2 increasing resolutions : 3x3km<sup>2</sup> and 1x1km<sup>2</sup>.

Meteorology for both models is provided by WRF simulations forced by NCEP meteorological fields at the scale of each domain. Boundary conditions for the continental domain come from MOZART simulations (Polyphemus) or LMDzT-INCA (Chimere). Finally, for the two largest domains, the EMEP emission dataset was used and submitted to each model's processing chain, while local Air Quality Network emission inventories at 1km resolution are provided for the 3 urban areas. The simulations were launched for the whole



Figure 2: Simulated annual mean concentrations of  $PM_{2.5}$  (in µg m<sup>-3</sup>) for the year 2009.

year 2009. Annual mean averages for  $PM_{2.5}$  in the reference emission scenario are presented in Figure 2 for the four nested domains that include the city of Paris.

## **EMISSION SCENARIOS**

The ADEME energy scenario is originally designed to implement the political will to reduce international energy dependence of France. It is focused on 1) the rational use of energy, especially in the buildings sector and the urban planning, 2) an increased use of sustainable energy sources. The main assumption for the building sector is a 25% decrease of the energy consumption between 2010 and 2030 based on construction of new buildings construction with low energy consumption, thermal rehabilitation of existing buildings and an increase of urban density. The transportation sector is also particularly considered. The main assumptions concerning this sector rely on an increased use of vehicle sharing, public transportation and bicycle, an evolution of the vehicle fleet (with more hybrid and electric vehicles) and the decrease of vehicle consumption.

### **RESULTS AND DISCUSSION**

In a preliminary phase two set of measures concerning the road traffic and the biomass combustion have been evaluated independently of the other measures considered in the energy scenario. The figure 3 shows distributions of hourly concentrations of  $NO_2$  in regional domain for Pays de Loire and Île-de-France regions. It compares the reference situation with the implementation of measures for road traffic.





These set of measures is efficient to decrease the annual mean concentrations for both regions (from 7.5 to 4.6  $\mu$ g m<sup>-3</sup> for Pays de Loire and from 29 to 21  $\mu$ g m<sup>-3</sup> for Île-de-France). It is however notable that the peak concentrations are more dramatically reduced for Pays de Loire than for Île-de-France (from 75 to 34  $\mu$ g m<sup>-3</sup> and from 106 to 90  $\mu$ g m<sup>-3</sup> respectively).

If we consider map of concentrations (figure 4), it is clear that the set of measure is also efficient for Alsace. The decrease of  $NO_2$  mean concentrations mainly occurs in the vicinity of the altered sources (main roadway and densely populated area). The impact of this set of measures on the concentrations of  $PM_{2.5}$  is also sensible even if relatively less important than for  $NO_2$ . This is especially true for the Alsace region where the fine particle emissions are dominated by the contribution of wood burning in the residential sector.

Another preliminary work based on a theoretical 30% decrease of particulate matter emissions in France was performed. The figure 5 shows the impact on the  $PM_{2.5}$  annual mean concentrations for the Île-de-France region. These results clearly show that even a strong abatement of primary particles does not ensure compliance with air quality standards. It is essential to simultaneously of



**Figure 4**: Evolution of NO<sub>2</sub> annual mean concentrations (in µg m<sup>-3</sup>) due to the implementation of road traffic measures in Alsace.

quality standards. It is essential to simultaneously consider abatement of gaseous precursors as ammoniac (NH<sub>3</sub>), NO<sub>2</sub> or volatile organic compounds.



Figure 5: Evolution of PM<sub>2.5</sub> annual mean concentration (in  $\mu$ g m<sup>-3</sup>) after a 30% decrease of the particle emissions.

This study will be achieved by the evaluation of the ADEME energy scenario as a whole. This evaluation performed with two models for the three different regions will allow a comparison of the impact on air quality for different environmental background. The comparison of the two models response will provide an assessment of the modelling uncertainties in this evaluation.

#### REFERENCES

- Couvidat, F., É. Debry, K. Sartelet, and C. Seigneur, 2012: A hydrophilic/hydrophobic organic (H2O) aerosol model: Development, evaluation and sensitivity analysis, *Journal of Geophysical Research*, **117**, D10304.
- Debry, E., K. Fahey, K. Sartelet, B. Sportisse and M. Tombette, 2007: Technical Note: A new SIze REsolved Aerosol Model (SIREAM), *Atmospheric Chemistry and Physics*, 7, 1537-1547.

- Bessagnet, B., A. Hodzic, R. Vautard, M. Beekmann, S. Cheinet, C. Honore, C. Liousse and L. Rouil, 2004: Aerosol modeling with CHIMERE: preliminary evaluation at the continental scale, *Atmospheric Environment*, 38, 2803-2817.
- Bessagnet, B., L. Menut, G. Curci, A. Hodzic, B. Guillaume, C. Liousse, S. Moukhtar, B. Pun, C. Seigneur and M. Schulz, 2008: Regional modeling of carbonaceous aerosols over Europe—focus on secondary organic aerosols, *Journal of Atmospheric Chemistry*, 61, 175-202.
- Schmidt, H., C. Derognat, R. Vautard, M. Beekmann, 2001: A comparison of simulated and observed ozone mixing ratios for the summer of 1998 in Western Europe, *Atmospheric Environment*, 36, 6277-6297.
- Gelbard, F. and J. H. Seinfeld, 1980: Simulation of multicomponent aerosol dynamics, *Journal of Colloid* and Interface Science, **78**, 485-501.
- Kulmala, M., A. Laaksonen, and L. Pirjola, 1998: Parameterizations for sulfuric acid/water nucleation rates, *Journal of Geophysical Research*, 103, 8301-8307.
- Nenes, A., C. Pilinis, S. N. Pandis, 1998. ISORROPIA: A new thermodynamic model for inorganic multicomponent atmospheric aerosols, *Aquatic Geochemistry*, 4, 123-152.
- Pun, B. K., C. Seigneur and K. Lohman, 2006: Modeling secondary organic aerosol formation via multiphase partitioning with molecular data, *Environmental Science and Technology*, 40, 4722-4731.
- Seinfeld and Pandis, 1998 Seinfeld, J. and S. Pandis, 1998: Atmospheric chemistry and Physics, Wileyinterscience, New York.
- Sportisse, B. and L. Dubois, 2002: Numerical and theoretical investigation of a simplified model for the parameterization of below-cloud scavenging by falling raindrops, *Atmospheric Environment*, **36**, 5719-5727.
- Tombette, M., 2007: Modélisation des aérosols et de leurs propriétés optiques sur l'Europe et l'Île de France: validation, sensibilité et assimilation de données, PhD Thesis, ENPC, France.
- Troen, I. B. and L. Mahrt, 1986: A simple model of the atmospheric boundary layer; sensitivity to surface evaporation, *Boundary-Layer Meteorology*, **37**, 129-148.
- Wesely, M. L., 1989: Parameterization of surface resistance to gaseous-dry deposition in regional scale numerical models, *Atmospheric Environment*, **23**, 1293-1304.
- Wild, O., X. Zhu, and M. J. Prather, 2000: Fast-J: Accurate Simulation of In- and Below-Cloud Photolysis in Tropopsheric Chemical Models, *Journal of Atmospheric Chemistry*, **37**, 245-282.
- Yarwood, G., S. Rao, M. Yocke, and G. Whitten, 2005: Updates to the Carbon Bond Chemical Mechanism: CB05, report, Rpt. RT-0400675. US EPA, Research Triangle Park.
- Zhang, L., S. Gong, J. Padro and L. Barrie, 2001: A size-segregated particle dry deposition scheme for an atmospheric aerosol module, *Atmospheric Environment*, **35**, 549–560.
- Zhang, L., J. Brook and R. Vet, 2003: A revised parameterization for gaseous dry deposition in air-quality models, *Atmospheric Chemistry and Physics*, **3**, 2067-2082.