Aerosol modeling at regional and continental scales

CEREA - Joint Research Laboratory ENPC/EdF R & D
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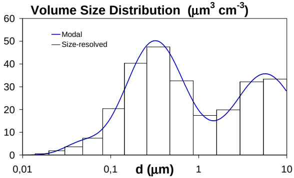
Outline

1. Aerosol modeling in Polyphemus
   - Description of the models
   - Aerosol processes
2. Validation and sensitivity studies
   - Overview
   - over Greater Paris
   - over Greater Tokyo
   - Over East Asia
   - Over Europe

Description of the models



The air quality modeling platform Polyphemus

- http://cerea.enpc.fr/polyphemus/
- Chemistry transport Model Polair3D

Two aerosol models

- SIze REsolved Aerosol Model (SIREAM)*
- Modal Aerosol Model (MAM)**

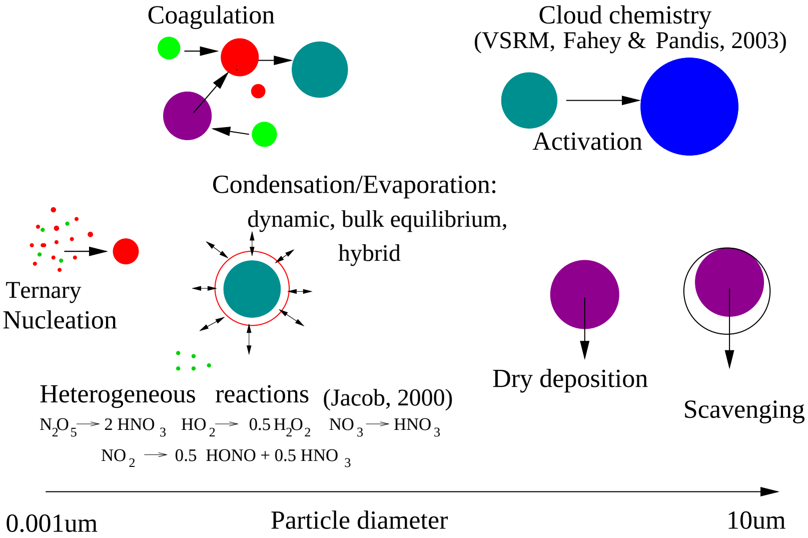
Aerosol composition

- inert: MD, BC; inorganic: Na, SO_4, NH_4, NO_3, Cl; organic

(*)E. Debry, K. Fahey, K. Sartelet, B. Sportisse, and M. Tombette. Technical note: A new SIze REsolved Aerosol Model: SIREAM. *Atmos. Chem. Phys.*, 7:1537–1547, 2007

(**)K.N. Sartelet, H. Hayami, B. Albriet, and B. Sportisse. Development and preliminary validation of a modal aerosol model for tropospheric chemistry: Mam. *Aer. Sci. Tech.*, 40(2):118–127, 2006

Aerosol processes



Overview

Validation

- Measured and simulated mean, correlation
- $$NME = \frac{\sum_{k=1}^{N} |C_k - O_k|}{\sum_{k=1}^{N} O_k}, \quad NMB = \frac{\sum_{k=1}^{N} (C_k - O_k)}{\sum_{k=1}^{N} O_k}$$

Sensitivity studies

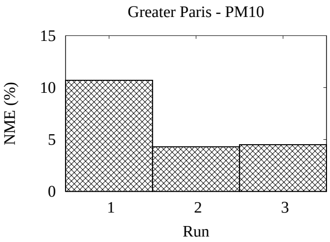
- Impact of aerosol processes and parameterizations
- "Brute Force" method: reference simulation (used to compute scores) compared to simulations where only one process differs from the reference simulation

Over Greater Paris

Validation (May to September 2001)

- 10 sections ([0.01-10μm])
- PM_{10} averaged over 8 stations

Meas. mean	Sim. mean	Corr	NMB	NME
23.0	23.9	59.5	4.0	32.4



Sensitivity study (1 to 15 July 2001)

- Heterogeneous reactions, hybrid: bulk equilibrium for 7 sections (< 1.25μm).
- 1: without heterogeneous reactions
- 2: bulk equilibrium
- 3: dynamic mass transfer

M. Tombette and B. Sportisse. Aerosol modeling at regional scale: Model-to-data comparison and sensitivity analysis over Greater Paris. *Atmos. Env.*, 2007. in press

Over Greater Tokyo

High pollution episodes (9-10 Dec. 1999, 31 July-1 Aug. 2001)

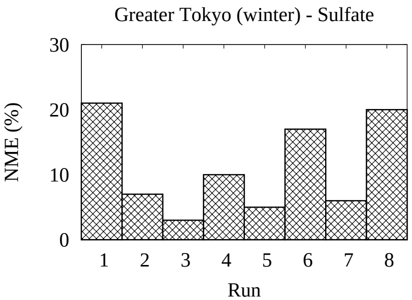
	Meas.	Sim.	NMB	NME
sulfate (winter)	2.6	3.3	-26	41
nitrate (winter)	4.5	4.1	8	111
sulfate (summer)	13.3	14.1	-7	34
nitrate (summer)	5.7	2.1	62	67

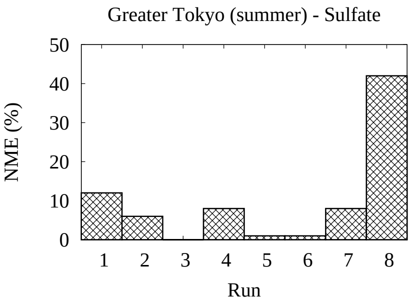
Reference simulation

- With dry deposition, nucleation and coagulation
- Condensation/evaporation: bulk equilibrium
- No Heterogeneous reactions
- 4 modes [0.001-10μm]

K. Sartelet, H. Hayami, and B. Sportisse. Dominant aerosol processes during high-pollution episodes over Greater Tokyo. *J. of Geophys. Res.*, 112(D14214), 2007

Over Greater Tokyo: sulfate

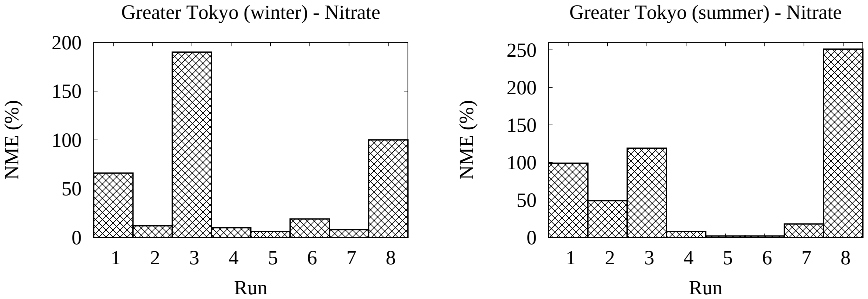




without condensation (1), using the hybrid scheme (2), with heterogeneous reaction (3), without dry deposition (4), without nucleation (5), without coagulation (6), SIREAM (7), CMAQ (8)

- Winter: Sensitivity to condensation, CMAQ, coagulation
- Summer: high sensitivity to CMAQ
- Impact of dry deposition is limited
- Impact of nucleation and coagulation higher in winter

Over Greater Tokyo: nitrate



without condensation (1), using the hybrid scheme (2), with heterogeneous reaction (3), without dry deposition (4), without nucleation (5), without coagulation (6), SIREAM (7), CMAQ (8)

- Impacts of condensation, heterogeneous reactions and CMAQ dominate
- Impact of thermodynamic equilibrium assumption is limited

Over East Asia

Framework

- Model Inter-Comparison Study –Asia Phase II (MICS 2): 8 models are compared over 4 months in 2001 and 2002

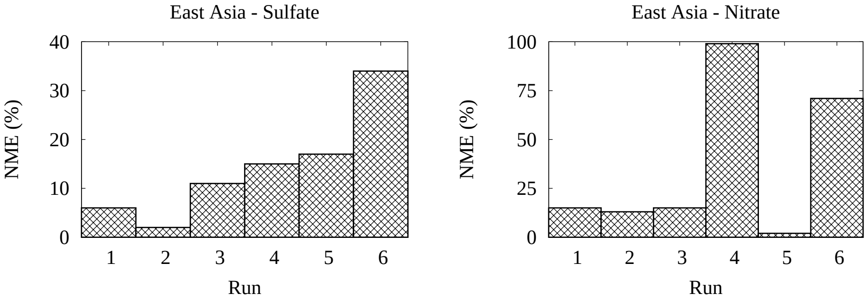
Sensitivity study: March 2001

- Condensation/evaporation: bulk equilibrium
- Heterogeneous reactions and cloud chemistry are ignored
- 10 sections [0.01-10μm]
- 24 stations

	Meas.	Sim.	NMB	NME
sulfate	4.9	5.2	13	13
nitrate	0.9	1.8	24	27

K. Sartelet, H. Hayami, and B. Sportisse. MICS-Asia Phase II: sensitivity to the aerosol module. *Atmos. Env.*, 2007. doi:10.1016/j.atmosenv.2007.03.005, In press

Over East Asia (2)



3 sections instead of 10 (1), with the hybrid scheme (2), without coagulation (3), with heterogeneous reaction (4), with cloud chemistry (5), CMAQ (6)

- Sulfate: CMAQ, cloud chemistry, heterogeneous reaction, coagulation
- Nitrate: heterogeneous reaction, CMAQ

Over Europe

Validation: 1 year (2001)

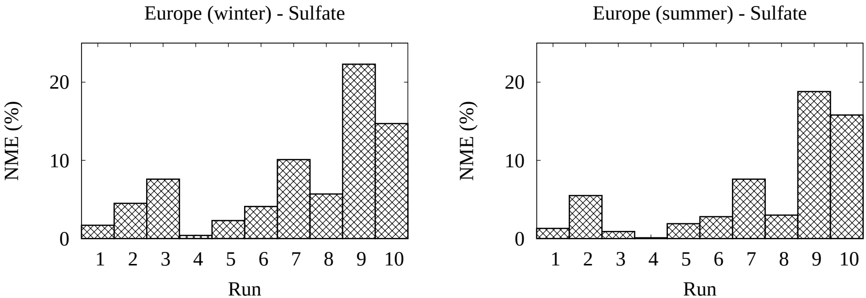
	Meas.	Sim.	Corr	NMB	NME
PM_{10} (EMEP)	16.9	15.6	55	-1	51
PM_{10} (Airbase)	24.9	15.4	44	-33	49
sulfate (EMEP)	2.5	2.1	56	-5	51
sulfate (Airbase)	1.9	2.4	51	73	105
nitrate (EMEP)	2.6	4.1	41	91	122
nitrate (Airbase)	3.5	4.4	72	27	56

Sensitivity study

- 7 July - 8 Aug. and 15 Nov.- 14 Dec.
- Cond/evap: bulk equilibrium
- No nucleation
- 5 sections [0.01-10μm]

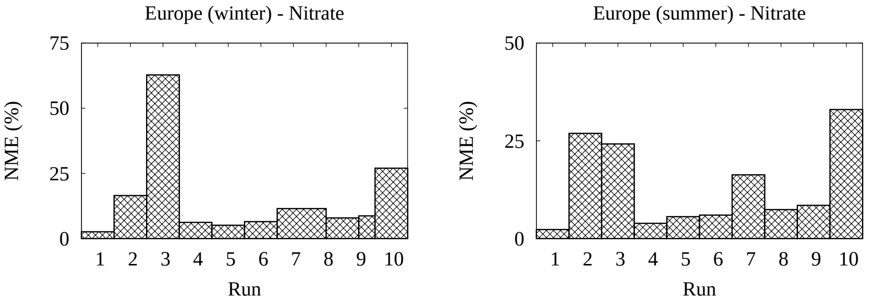
K. Sartelet et al. Simulation of aerosols and gas-phase species over Europe with the POLYPHEMUS system. part I: model-to-data comparison for 2001. *Atmos. Env.*, 2007.

Over Europe: sulfate



10 sections (1), dynamic mass transfer (2), without the het. react. N_2O_5 (3), varying reaction probability for the het. react. N_2O_5 (4), with nucleation (5), criterion LWC < 0.07g m^{-3} to call VSRM (6), cloud fraction to diagnose when to call VSRM (7), parameterization for scavenging (8), boundary conditions (9), parameterization for vertical diffusion (10)

Over Europe: nitrate



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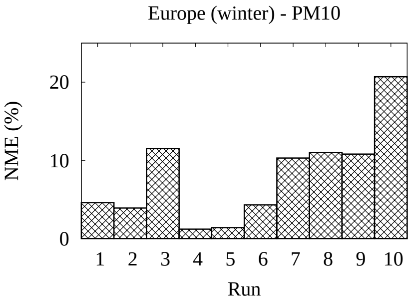
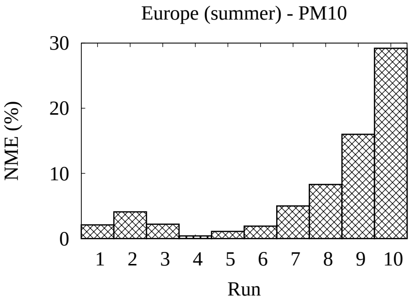
Over Europe: PM_{10}





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Conclusion

- Aerosols are sensitive to configuration choices outside the aerosol module: e.g. vertical diffusion and boundary conditions
- and inside the aerosol module: heterogeneous reaction, cloud chemistry and scavenging
- Size distribution, coagulation and nucleation have lower sensitivities
- The sensitivity to dynamic mass transfer vary depending on conditions
- Low sensitivity to variation of the reaction probability of the het. react. N_2O_5 with temperature, RH and aerosol composition (Evans and Jacob, 2005; Riemer et al., 2003)
- This presentation focused on sulfate, nitrate and PM_{10} integrated over several days/months. Conclusion would be different if focus on small particles, number distribution...