LAGRANGIAN MODELLING OF PLUME CHEMISTRY FOR SECONDARY POLLUTANTS IN LARGE INDUSTRIAL PLUMES

D R Middleton¹, A R Jones¹, A L Redington¹, D J Thomson¹, R S Sokhi², L Luhana² and B E A Fisher³

¹UK Met Office, ²University of Hertfordshire ³Environment Agency.

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Aim of Talk

- Environment Agency funded work to explore tools for Regulating secondary pollutants from large stacks.
- We used NAME III to model the chemistry of an ideal plume mixing with background pollutants in surrounding air.
- Talk summarises this work.
Introduction

- Regulation of NO₂
- Model Set-up: NAME III dispersion model
  - Point Source: NO & NO₂
  - Meteorology
  - Background concentrations: O₃ & VOC
  - Idealised plume of NO & NO₂

- Plume Chemistry Sensitivity Study
- Discussion
- Conclusions

Acknowledgements: This work by University of Hertfordshire and Met Office was funded by the Environment Agency. NAME III is funded by Met Office Research Programmes.

UK Regulation: Local Air Quality Management

- Local Government role
- Monitoring; Inventories; Met Data
- Run dispersion models: maps
- Public consultation: Traffic management & Town planning
UK Regulation: Large Industrial Sources

- Environment Agency role.
- Developer makes permit application.
- Estimate NO\textsubscript{x} downwind in plume at ground level - NO\textsubscript{2}:NO\textsubscript{x} as fixed ratio.
- Agency evaluates modelling.
- Decides on permit.

Questions: Regulating Plumes

- Quantify NO\textsubscript{2} when a plume mixes with polluted air?
- Quantify O\textsubscript{3} increase due to a large point source?
- Sensitivity: Factors affecting the amount of secondary pollutants formed?
- A tool for Regulators, e.g. complex modelling of dispersion & chemistry?
Set-up for NAME III Model

- Point source: Lagrangian particles NO, NO\textsubscript{2}, SO\textsubscript{2}
- Background air: Lagrangian particles O\textsubscript{3}, VOC

- Background concentrations mix & react with plume.
- Inhomogeneous concentrations affect the chemical kinetics.

- Model set-up for 3-hour and 24-hour average concentrations.
- Evaluate concentrations - particles in grid cells 1km×1km×100m deep.
Point Source

- Ideal stack, 200m tall
- Located over the U.K. at 0°E, 54°N.
- No Plume Rise - algorithm switched off.
- Effective plume height 200m.
- Continuous point source – Steady Stream of Lagrangian particles

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<table>
<thead>
<tr>
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<tbody>
<tr>
<td>NO2</td>
<td>50 g s⁻¹</td>
<td>5%</td>
</tr>
<tr>
<td>NO</td>
<td>950 g s⁻¹</td>
<td>95%</td>
</tr>
<tr>
<td>SO2</td>
<td>8000 g s⁻¹</td>
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Meteorological Input

- NAME III – met options:
  1. NWP data from Met Office UM global/mesoscale.
  2. Single site data e.g. synoptic observations.

- Input Uniform meteorology:
  - artificial single site data
  - wind speed: 4 m s⁻¹ at stack height (200m)
  - wind direction: 270°, steady uniform Westerly
  - neutral boundary layer with depth 800 m.
  - temperature: 10° C
  - clear skies & dry atmosphere.
  - solar radiation: 21-22 June; for chemistry.
Background chemical species for NAME III

- Initialize model domain at start of model run.
- We vary input concentrations of chemical species: O₃ & VOC.
- Lagrangian particles in domain are advected about.
- Lagrangian particles emitted by point source in domain are dispersed.
- Species are advected in through the upwind face, using an artificial area source, replacing those swept out downwind.
- Species are diffused across the ceiling and walls of the domain using artificial sources.

Chemistry Domain: 100 km × 40 km × ~2.5 km

- Downwind species loss by advection
- Wall sources are to maintain uniform background

User defined ambient [O₃, VOC]
Background Volatile Organic Compounds

- Total [VOC] in model domain varied for each run: 5, 10, 20, 50, or 75 ppb.

<table>
<thead>
<tr>
<th>Reactive type</th>
<th>Mole ratio</th>
<th>Propene C\textsubscript{3}H\textsubscript{6}</th>
<th>13.48%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Toluene C\textsubscript{6}H\textsubscript{5}CH\textsubscript{3}</td>
<td>32.6%</td>
<td>o-xylene C\textsubscript{6}H\textsubscript{2}(CH\textsubscript{3})\textsubscript{2}</td>
<td>8.511%</td>
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<tr>
<td>Ethane C\textsubscript{2}H\textsubscript{4}</td>
<td>23.4%</td>
<td>Acetaldehyde CH\textsubscript{3}CHO</td>
<td>3.546%</td>
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<tr>
<td>Formaldehyde HCHO</td>
<td>15.6%</td>
<td>Butadiene C\textsubscript{4}H\textsubscript{6}</td>
<td>2.873%</td>
</tr>
</tbody>
</table>

Plume Chemistry...Backgrounds

A large number of particles is used to reduce noise.
- Background: 20 ppb $O_3$ & 20 ppb VOC
- Elevated NO$_2$ seen at plume edges in the night (no photolysis)
Discussion

- Elevated NO$_2$ seen at plume edges in the night, near source, $<$~40 km.
- NO+O$_3$ reaction generates raised NO$_2$.

- Depletion of ozone by night.
- Depletion of ozone by day with low VOC.
- To form significant O$_3$ downwind needs VOC.

- O$_3$ maximum 106 ppb at 15:00 hours – high VOC reacts with downwind plume creates O$_3$ – vanishes as darkness falls.
- Elevated O$_3$ was far from source, $>$~50 km

Discussion

- Model results do not support the use of a fixed NO$_2$:NO$_x$ ratio.

- With NAME III we can vary source, background concentrations, and meteorology.
Conclusions (1)

- NAME III with pre-set scenarios may be a potentially useful Regulatory tool for large NO$_x$ plumes.

- Each run took about 3-6 hours, suggesting a two-step screening protocol is advisable to estimate worst case NO$_2$:
  1. Simple empirical formulae to identify worst cases.
  2. Complex modelling of scenarios, as in this work, and with full NWP data for selected episodes.

Conclusions (2)

- Validation of NAME III simulations using plume measurements is needed.

- Work with Regulators is needed to develop a documented protocol for the use of screening methods, standard models, and complex modelling for secondary pollutants O$_3$, NO$_2$ and aerosols.