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

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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 NO_2
- Model Set-up: NAME III dispersion model
  - Point Source: NO & NO_2
  - Meteorology
  - Background concentrations: O_3 & VOC
  - Idealised plume of NO & NO_2
- Plume Chemistry Sensitivity Study
- Discussion
- Conclusions

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UK Regulation: Local Air Quality Management

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

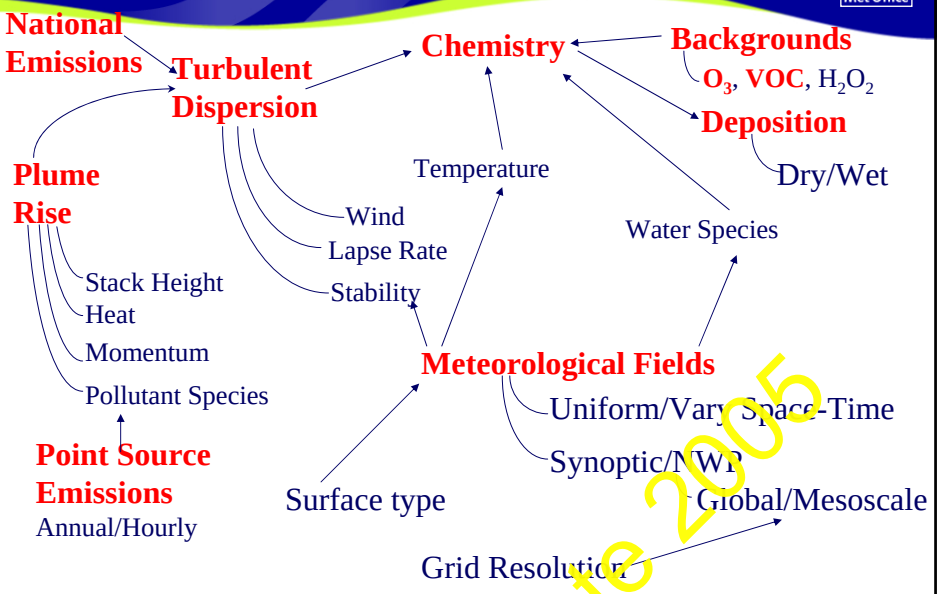
UK Regulation: Large Industrial Sources

- Environment Agency role.
- Developer makes permit application.
- Estimate NO_x downwind in plume at ground. level - NO_2:NO_x as fixed ratio.
- Agency evaluates modelling.
- Decides on permit.

Questions: Regulating Plumes

- Quantify NO_2 when a plume mixes with polluted air?
- Quantify O_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?

Sensitivities



Set-up for NAME III Model

- Point source: Lagrangian particles NO,NO_2,SO_2
- Background air: Lagrangian particles O_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

NO2	50 g s^{-1}	5%
NO	950 g s^{-1}	95%
SO2	8000 g s^{-1}	

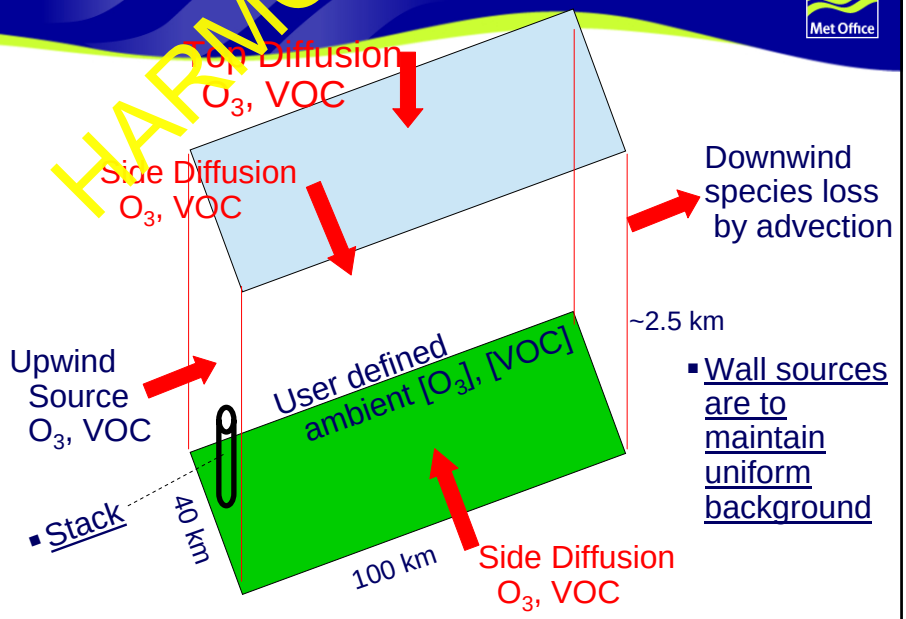
Meteorological Input

- 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 : O_3 & 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



- Wall sources are to maintain uniform background

Background Volatile Organic Compounds

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

Reactive type	Mole ratio
Toluene $C_6H_5CH_3$	32.6%
Ethane C_2H_4	23.4%
Formaldehyde HCHO	15.6%

Propene C_3H_6	13.48%
o-xylene $C_6H_2(CH_3)_2$	8.511%
Acetaldehyde CH_3CHO	3.546%
Butadiene C_4H_6	2.873%

Plume Chemistry... Backgrounds

O3 / VOC	10 ppb	20 ppb	50 ppb	100 ppb	150 ppb
5 ppb	Run 11	Run 12	Run 13	Run 14	Run 15
10 ppb	Run 16	Run 17	Run 18	Run 19	Run 20
20 ppb	Run 21	Run 22	Run 23	Run 24	Run 25
50 ppb	Run 26	Run 27	Run 28	Run 29	Run 30
75 ppb	Run 31	Run 32	Run 33	Run 34	Run 35

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.