

Modelling Ozone

OZONE MODELS AND THEIR MAIN SOURCES OF UNCERTAINTY

Dick Derwent
rdscientific, Newbury, United Kingdom

AAMG Conference
Prague
Czech Republic
25th – 26th September 2007

WHY MODEL OZONE ?

To provide a framework to link together information connecting a disparate range of issues:

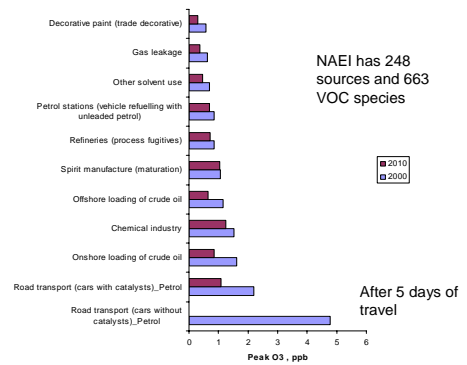
- emissions,
- meteorological data,
- atmospheric chemistry,
- air quality data

WHY MODEL OZONE ?

To provide a vehicle for exploring ignorance and answering questions.

- Where have the elevated ozone levels come from ?
- How important is long-range transport of ozone?
- Which VOCs are the most important to control ?

IMPACT OF VOC REDUCTIONS IN DEFRA PROJECTIONS BETWEEN 2000 AND 2010 USING UK PTM AND MCMv3.1

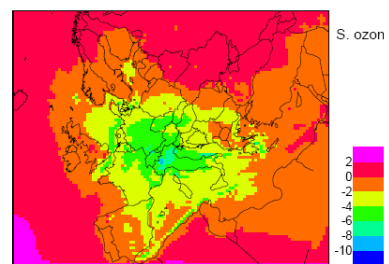


WHY MODEL OZONE ?

To develop a means of prediction for policy-makers.

- What would happen of this source of precursor emissions is controlled ?
- Which sources are best to control ?
- What will happen if nothing is done to control emissions ?

IMPACT OF THE CAFÉ THEMATIC STRATEGY ON SUMMERTIME OZONE

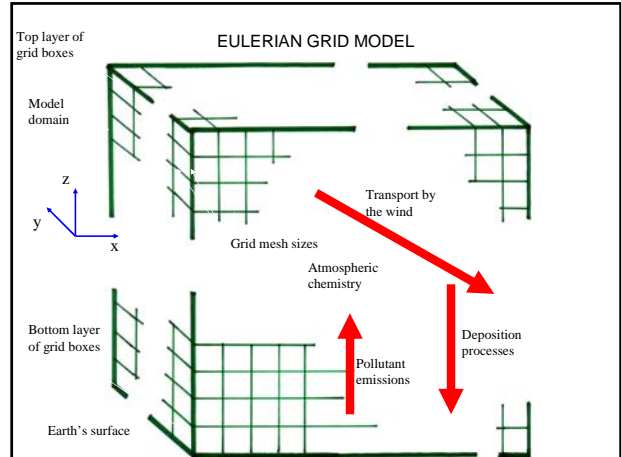


Diff. BL CLE 2010 - 2000. 1997 meteorology
Results from the Unified EMEP Eulerian Model (Tarrason et al., 2005)

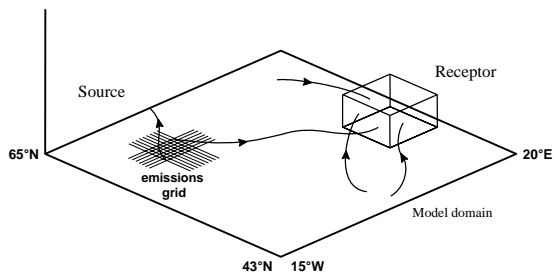
Modelling Ozone

CLASSIFICATION OF OZONE MODELS

- Empirically-based models
- Mathematically-based models
 - Eulerian grid models
 - Lagrangian trajectory models

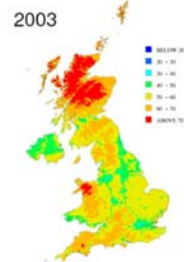


LAGRANGIAN TRAJECTORY MODELS



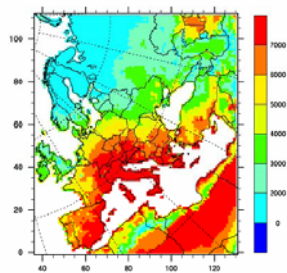
Describe the atmosphere as thousands of individual air parcels or boxes that are moved along with the winds

OUTPUT FROM AN EMPIRICAL OZONE MODEL



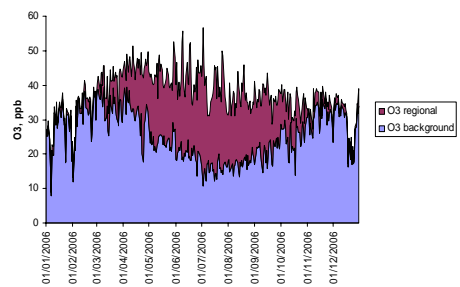
Annual mean ozone concentrations in $\mu\text{g m}^{-3}$ (Stedman et al. 2006)

OUTPUT FROM THE UNIFIED EMEP EULERIAN MODEL



Sum of ozone concentrations above 35 ppb calculated for 1995 – 2002 (Tarrason et al., 2005)

OUTPUT FROM A LAGRANGIAN TRAJECTORY MODEL



Output from the UK Photochemical Trajectory Model for Harwell, Oxfordshire for 2006 showing ozone source attribution

Modelling Ozone

MODELS ARE INHERENTLY SIMPLIFICATIONS OF THE REAL-WORLD

When models are built, they are always simpler than the worlds they represent. This simplification is achieved by:

- Generalisation
- Distortion
- Deletion
- Neglect

EVALUATION OF MODEL PERFORMANCE: IS THIS MODEL VALIDATION OR VERIFICATION ?

- Generally, model performance is evaluated against observations
- Policy-makers expect modellers to establish the trust-worthiness of their models
- Agreement with observations is inherently partial, models agree with some observations but not all
- Validation and verification are not feasible because assumptions and inferences may fail under some circumstances and poorly known fine details may become crucial
- comparison against observations is a good first step in the evaluation of model performance

THE PURSUIT OF COMPLEXITY

Models are always incomplete and efforts to make them more complete can be problematic:

- adding new features and processes may introduce more uncertain parameters
- complex models may contain more parameters than can be calibrated with the available observations
- scientific advances will never make it possible to build the perfect model

MAIN AREAS OF UNCERTAINTY

The simplifications inherent in models introduce uncertainties. There are four main areas of uncertainty:

- theoretical aspects – not fully understood
- empirical aspects – difficult to measure
- parametrical aspects – simplified concepts
- temporal aspects – not stable in time

HOW TO HANDLE UNCERTAINTIES ?

A wide range of possibilities exist for handling uncertainties:

Probabilistic uncertainty analysis

- represent all model uncertainties probabilistically
- compute distribution of output of interest

Scenario assessment or sensitivity analysis

- consider 'pessimistic', 'neutral' or 'optimistic' scenarios for parameters

WHAT ARE THE MAJOR UNCERTAINTIES ?

- missing processes
- weather conditions
- chemical mechanism
- emissions from human activities
- emissions from natural processes

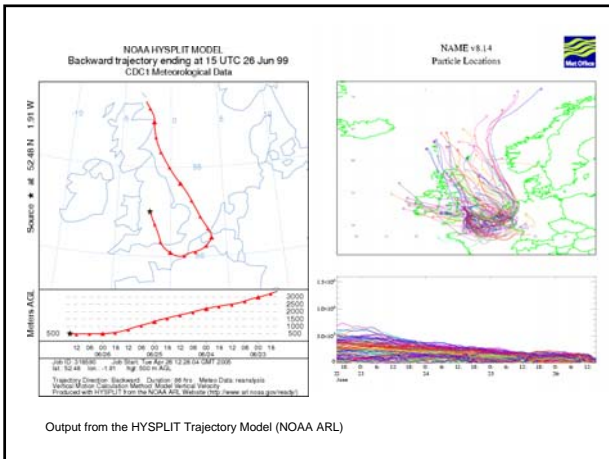
Modelling Ozone

UNCERTAINTY ANALYSIS IN A PHOTOCHEMICAL TRAJECTORY MODEL

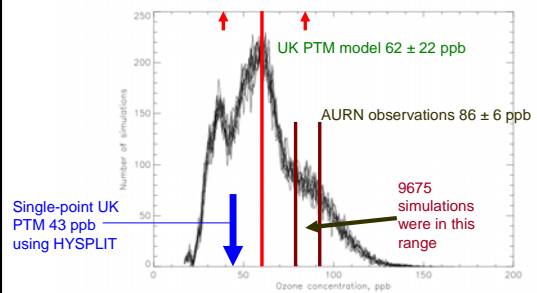
- VOC emissions
- NO_x emissions
- SO₂ emissions
- CO emissions
- methane emissions
- isoprene emissions
- deposition velocities
- initial concentrations
- boundary conditions
- x,y,z trajectory position
- air parcel temperature
- air parcel pressure
- air parcel humidity
- boundary layer depth

MONTE CARLO UNCERTAINTY ANALYSIS IN THE UK PTM

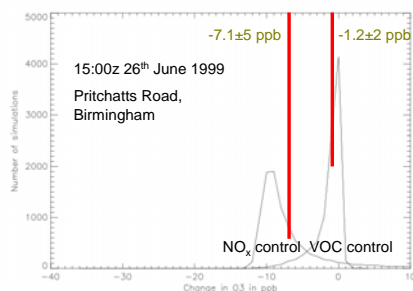
- assign subjective uncertainty ranges for each input parameter
- sample 1000 independent multiple air mass trajectories for that hour from a sophisticated Lagrangian trajectory model
- perform 100,000 UK PTM runs to sample all the uncertain parameters randomly and simultaneously
- 96-hour back trajectories arriving at Birmingham during PUMA campaign on 26th June 1999



100,000 UK PTM OZONE RESULTS FOR PRITCHATTS ROAD, BIRMINGHAM FOR 15.00z 26th JUNE 1999



OZONE RESPONSES TO 30% NO_x and VOC CONTROLS USING 9675 VALID SIMULATIONS



CONCLUSIONS

- ozone models have played an important role in policy development within Europe
- ozone network observations have played a vital role in the evaluation of policy model performance
- uncertainties still remain in policy models and we have barely begun the process of understanding their importance
- if the aim of policy is to reduce ozone exposure levels below air quality guidelines then policy models will need to handle uncertainties

Modelling Ozone

ACKNOWLEDGEMENTS

- To the AEQ Division UK DEFRA for supporting the Photochemical Trajectory Modelling studies under contract no. AQ 03508
- To Claire Witham, Met Office for providing the back-track air parcel trajectory data
- To Leonor Tarrason for providing the results from the Unified EMEP Model