The use of sensitivity analysis in the evaluation of dispersion models

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• Atmospheric dispersion models are commonly used within environmental management and strategic planning:
  - assessment of exceedances of air quality standards
  - atmospheric response to suggested pollution control measures.
• Models incorporate parametrisations of chemical and physical processes which cannot be efficiently computed at a fundamental level:
  - turbulence, surface roughness, kinetic rate constants, etc.
• May also include input data which relate to measurable physical quantities but are not known with certainty:
  - wind speed and direction, emission rates, temperature, pressure etc.
• Model predictions are inherently uncertain and yet we need to use them in a design/decision making environment.
Evaluation of complex models

- Need to evaluate if models are fit for purpose.
- Comparison of model with experimental or field data for simple to complex scenarios.
  - Then what?
- How much confidence can we place in simulations?
- If lack of agreement then how do we find contributing causes?
- **Sensitivity** and **uncertainty analysis** help to answer these questions:
  - models often nonlinear, computationally expensive, many parameter
  - tempting to optimise model by fitting parameters to specific sets of experiments – can we really isolate parameters well enough?
  - need **strong feedback loop** between model evaluation and methods for model improvement.
Sensitivity and uncertainty analysis

• **Uncertainty analysis (UA)** estimates the overall predictive uncertainty of a model given the state/or lack of knowledge about its input parameters.

• UA puts error bars on predictions.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$S_i$, $x=2.2$ m</th>
</tr>
</thead>
<tbody>
<tr>
<td>Structure function coeff. $C_0$</td>
<td><strong>0.7976</strong></td>
</tr>
<tr>
<td>Mixing time-scale coeff. $\alpha$</td>
<td>0.1853</td>
</tr>
<tr>
<td>$\Sigma S_i$</td>
<td>0.9843</td>
</tr>
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**Sensitivity analysis (SA)** determines how much each input parameter contributes to the output uncertainty (usually variance).
• High ranked parameters could then be re-estimated using *ab initio* modelling studies or *simple experiments* which help to isolate their effects.

• If the parameter can be re-estimated with better certainty then the error bars of the prediction are reduced.

• In some cases, even within the error bars, there is no overlap between experimental and modelled outputs. This suggests structural problems with the model e.g. poor parametrisation, missing physical processes or chemical kinetic steps.
• Local methods for sensitivity analysis are most commonly used and are available in many commercial codes.

• They essentially probe sensitivity around best estimate for input parameter using partial derivatives (local, linear).

• But what if the best estimate is way off and the model nonlinear?

• Better to search a wide input space using global sensitivity methods.

  wide ranges of inputs can be tested within multi-dimensional space
  downside is computational cost.
Global methods:
Monte Carlo (MC) simulations

• Conceptually straightforward.
• Based on random or quasi random (Sobol) sample of input parameter space.
• Perform many simulations until output mean/variances converge.
• Interpretation of results difficult for large input space:
  ➢ Scatter plots for each parameter show overall effect.
  ➢ Large scatter often obscures mean effect of individual parameter.
  ➢ Linear effects easily shown using Pearson correlations.
  ➢ How can we rank parameters if non-linear or interactive effects?
  ➢ Its expensive!
The examples show possible nonlinearities and large scatter – obscuring overall sensitivity to parameter.
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Scatter plots for urban dispersion model

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Local sensitivity tends to 0 at edge of parameter range

Local sensitivity close to 0 at short distance from nominal parameter
• Developed to provide detailed mapping of the input variable space to selected outputs – a metamodel.

• Output is expressed as a finite hierarchical function expansion:

\[ f(\mathbf{x}) \equiv f_0 + \sum_{i=1}^{n} f_i(x_i) + \sum_{1 \leq i \leq j \leq n} f_{ij}(x_i, x_j) + \cdots + f_{12\ldots n}(x_1, x_2, \ldots, x_n) \]

• Usually second-order expression provides satisfactory results.
• Metamodle built using quasi random sample and approximation of component functions by orthonormal polynomials.
• Metamodle can be used to generate full Monte Carlo statistics.
Sensitivity coefficients

\[ f_0 \approx \frac{1}{N} \sum_{s=1}^{N} f(x^{(s)}) \]
\[ f_i(x_i) \approx \sum_{r=1}^{k} \alpha_r \varphi_r(x_i) \]
\[ f_{ij}(x_i, x_j) \approx \sum_{p=1}^{l} \sum_{q=1}^{l'} \beta_{pq}^{ij} \varphi_p(x_i) \varphi_q(x_j) \]

- \( k, l, l' \) - order of polynomial expansion, \( \alpha_r^{i} \), \( \beta_{pq}^{ij} \) - coefficients to be determined, \( \varphi '\)s - orthonormal basis functions.
- Optimisation technique implemented to calculate optimal polynomial order and to exclude unimportant component functions.
- Partial variances \( D_i \), \( D_{ij} \) and 1\(^{st}\) & 2\(^{nd}\) order sensitivity indices \( S_i \), \( S_{ij} \) easily calculated from component functions and ranked in order of importance.

\[ D_i \approx \sum_{r=1}^{k_i} (\alpha_r^{i})^2 \]
\[ D_{ij} \approx \sum_{p=1}^{l_i} \sum_{q=1}^{l'_j} (\beta_{pq}^{ij})^2 \]
\[ S_i = \frac{D_i}{D}, \quad S_{ij} = \frac{D_{ij}}{D} \]
Component functions for previous example

(a) Vertical velocity in street

(b) Roof level turbulence

(c) Surface roughness length
Examples

• Need to be able to model formation of secondary pollutants such as $\text{NO}_2$ in order to test the impact of emission reduction strategies.

• Computational fluid dynamics (CFD) models becoming more common in pollution and emergency response management.

• Different turbulence closure schemes in use:
  
  Reynolds Averaged Navier Stokes (RANS), Large Eddy Simulation (LES).

• Also different dispersion schemes:
  
  Lagrangian particle, stochastic fields, eddy diffusivity.

• Urgent need to evaluate where different approaches are “fit for purpose” and the impacts of parametrisations of turbulence, mixing and kinetics.
Ex 1: Brown and Bilger wind tunnel experiments (1996).

**Aim:** to evaluate a combined Lagrangian stochastic model with micro-mixing and chemical sub-models for predicting impact of nitrogen oxide (NO) released into a turbulent grid flow doped with ozone (O$_3$) on NOx/NO$_2$. 

![Diagram of turbulence grid and instantaneous plume](image-url)
Lagrangian particle equations:

velocity increment: \( du_i = a_i(x,u,t)dt + b_{ij}(x,u,t)d\omega_j \)

position increment: \( dx_i = u_i dt \quad b_{ij} = \sqrt{c_0 \varepsilon \delta_{ij}} \)

c_0 - structure function coefficient, \( \varepsilon \) - dissipation rate of tke \( k \)

Using simple Interaction by Exchange with Mean (IEM) mixing model:

\[
\frac{dC}{dt} = -\frac{1}{t_m}(C - \langle C \rangle) \quad t_m = \alpha \frac{k}{\varepsilon}
\]
**Stage 1: Non-reactive tracer plume**

**Model parameters:** Velocity structure function coefficient $c_o$ (5.3-6), mixing time-scale coefficient $\alpha$ (0.75,0.6-3), source size (0.008-0.016m).

Quite large error bars, but overlap with experiment except at plume edges.
First order sensitivities using HDMR for peak \([\text{NOx}]\)

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<tr>
<th>Parameter</th>
<th>(S_i \times=2.2) m</th>
<th>(S_i \times=4.8) m</th>
<th>(S_i \times=5.8) m</th>
</tr>
</thead>
<tbody>
<tr>
<td>Structure function coefficient (c_0)</td>
<td>0.7976</td>
<td>0.7941</td>
<td>0.7903</td>
</tr>
<tr>
<td>Mixing time-scale coefficient (\alpha)</td>
<td>0.1853</td>
<td>0.1918</td>
<td>0.1937</td>
</tr>
<tr>
<td>(\Sigma S_i)</td>
<td>0.9843</td>
<td>0.9874</td>
<td>0.9844</td>
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**Diagram a)**: \(f_i(x_i) + f_0\) vs. \(c_0\)

**Diagram b)**: \(f_i(x_i) + f_0\) vs. \(\alpha\)
**NO₂ mean concentrations and fluctuations**

Mean peak overestimated using nominal values

Slight underestimation of rms values
High sensitivity of mean and rms NO\(_2\) values to \(\alpha\) but not of mean NOx. Adjustment of \(\alpha\) from 0.75 to 1.5 gives better agreement with experiment.
Ex 2: York street canyon simulation

TKE, wind vectors for $\theta_{\text{ref}}=90^\circ$ to canyon axis

Signal controlled intersection

Bootham

Gillygate
Complex model couplings

Traffic Network Information

Traffic micro-simulation model

Vehicle Characteristic

Vehicle speeds

Vehicle acceleration

Instantaneous emissions model

Meteorology

CFD flow model (MISKAM k-ε)

Flow and turbulence

Dispersion model

Emissions

Pollution concentrations

Building layouts
Parameter set varied in global sensitivity study

Model parameters (26 in total):

- velocity structure function coefficient $c_o$
- mixing time-scale coefficient $\alpha$
- surface roughness $z_0$ for inlet, surface and wall
- temperature dependant rate parameters for NO/NO$_2$/O$_3$ reactions, photolysis rate parameters for JO$_3$ and JNO$_2$
- wind direction $\theta_{\text{ref}}$
- temperature
- background [O$_3$]
- NO:NOx ratio
- traffic demand

Model parametrisation

Physical/meteorological

Traffic emissions
Example Fit and Component Functions
Sample sensitivity results ($\theta_{\text{ref}} = 110-130$): average over 6 in-canyon road-side locations: mean [NO$_2$]
Conclusions

• In complex models with large numbers of input parameters, often only a small number of parameters drive output uncertainty.
• Global sensitivity methods provide essential step in model evaluation by identifying this parameter set.
• Further studies can then be focussed on key parameters improving model performance.
• Simple experiments can help to narrow down feasible range for parameters.
• **More careful experiments in controlled conditions very useful!**
• An extended HDMR based method has proven effective in application to a large complex model – providing up to second order sensitivities with relatively low computational cost.
HDMR software with graphical user interface freely available

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