Experiences from the Application of a Parameter Estimation and Identifiability Analysis Methodology to the Operational Street Pollution Model (OSPM)

Thor-Bjørn Ottosen[1,2] Matthias Ketzel[3] Ole Hertel[3] Henrik Skov[2,3] Jørgen Brandt[3] Konstantinos Kakosimos[1]

[1]Department of Chemical Engineering, Texas A&M University at Qatar

[2]Department of Chemical Engineering, Biotechnology and Environmental Technology, University of Southern Denmark

[3]Department of Environmental Science, Aarhus University

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Overview

1 Motivation

Why uncertainty and sensitivity analysis?

- Role of models has changed – need for uncertainty and sensitivity analysis

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- Guide research directions
- Improve scientific communication – transparency
- Has not been performed for air quality models before

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- Originated in other branches of science (ecological modelling, econometrics, engineering etc.)
- Lack of demonstration of feasibility and advantage of approach

2 Objectives

Methodology of choice: The iterative parameter estimation and identifiability analysis of Brun et al. (2001). It has been widely applied in other branches of science.

Aim: To analyse the applicability of applying the parameter estimation and identifiability analysis methodology to a model within atmospheric science, in this case the Operational Street Pollution Model (OSPM^{TM}).

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10. Explore potential bias problems

Iterate until convergence (steps 4–9)

3 Methods

Identifiability analysis: Search for parameters identifiable from data

For a parameter to be identifiable:

- The model have to be sensitive to small changes in the parameter $\left(\left|\frac{\partial f(u,\theta)}{\partial \theta}\right| \gg 0\right)$
- Only small compensation effects in the model output. Analysed via linear dependency of the sensitivity matrix.

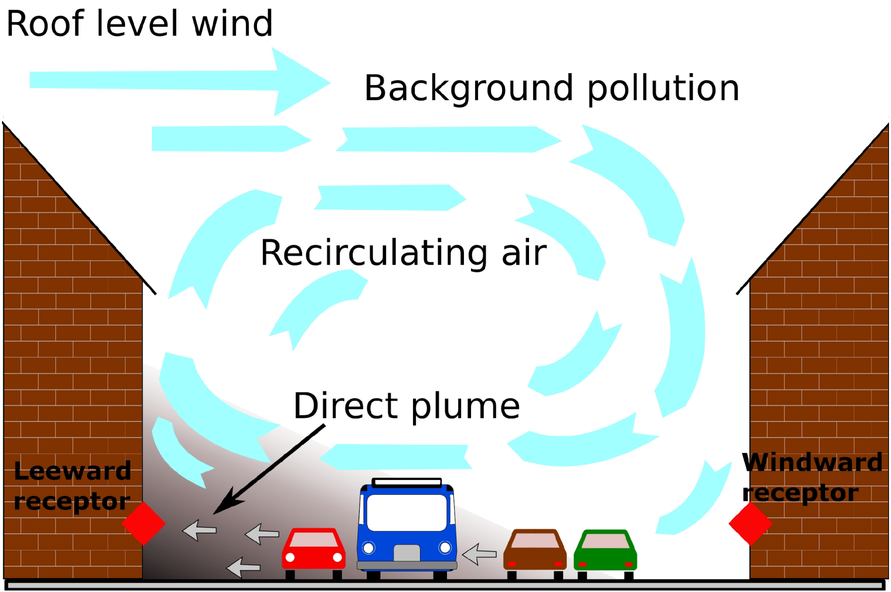
Parameter estimation: Estimation of parameters from data

- Used least-squares minimization criterium
- Weighted to balance species

Model input:

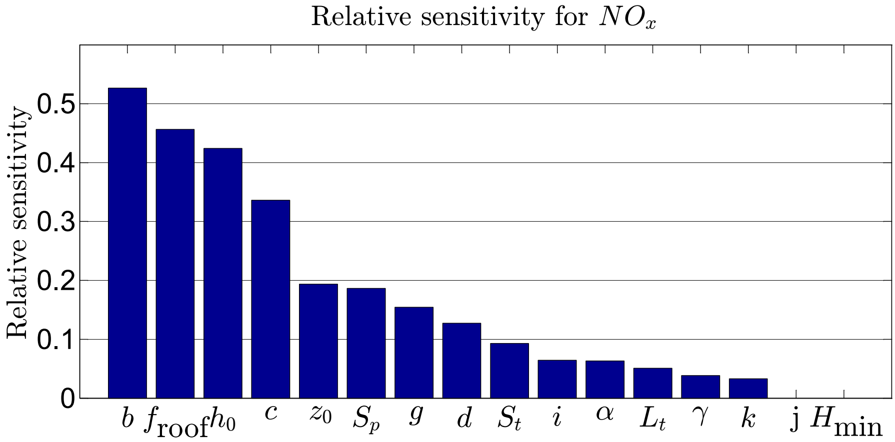
- Species: NO_x and NO_2
- Years: 1994–2010
- Five streets in major cities in Denmark
- Meteorology and urban background concentration from rooftop stations
- Measurements from Ellermann et al. (2013)
- Two data splitting approaches: DUPLEX and Seasonal

4 The Operational Street Pollution Model (OSPM^{TM})

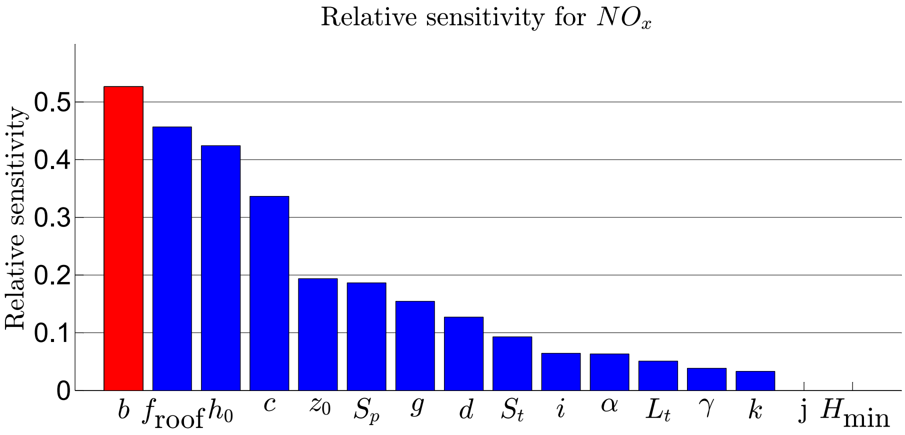


5 Results

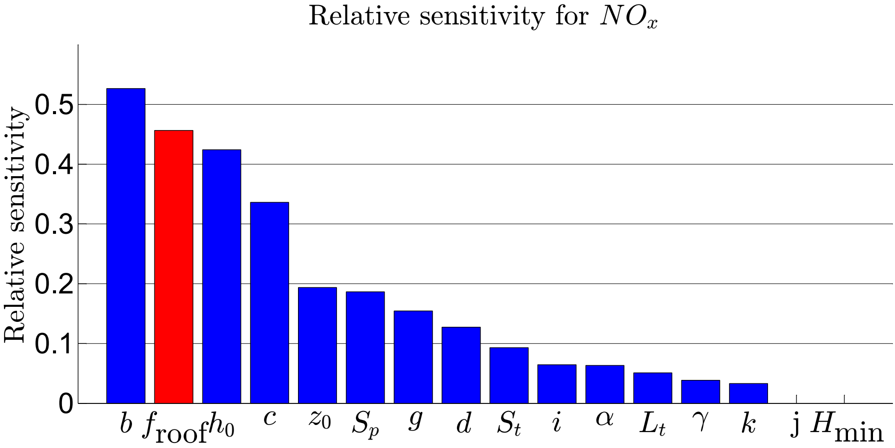
Local sensitivity analysis



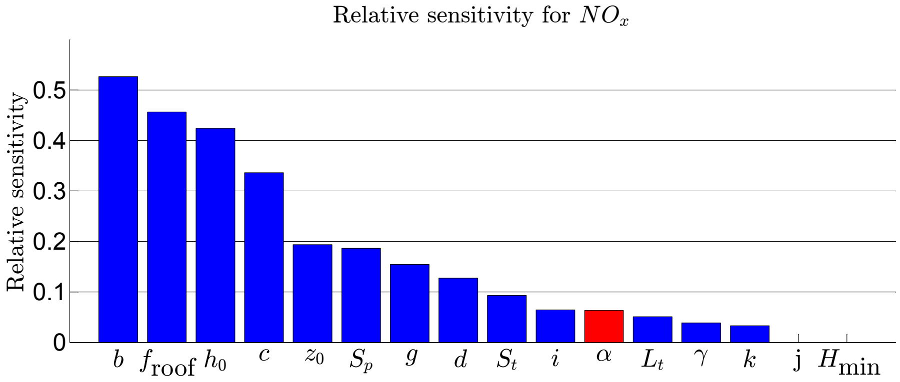
Distinct trend in sensitive and non-sensitive parameters – dependent on parameter values



Scale-factor for traffic-produced turbulence



$$f_{\mathrm{roof}} = \frac{u_{\mathrm{mast}}}{u_{\mathrm{roof}}}$$



Slope of emission plume

Size	Combinations	γ_K range	$\gamma_K < 10$ (%)	Parameters subset for $\gamma_{\min}$

5 Results

Collinearity analysis

Size	Combi-nations	γ_K range	$\gamma_K < 10$ (%)	Parameters subset for $\gamma_{\min}$
2	91	0.71–9.29	100.0	c, L_t
3	364	0.78–42.28	97.8	c, L_t, i
4	1001	0.84–42.30	93.3	c, L_t, i, k
5	2002	1.00–42.30	86.8	d, g, i, k, γ
6	3003	1.07–42.33	78.4	α, L_t, g, i, k, γ
7	3432	1.13–42.43	68.4	α, L_t, d, g, i, k, γ
8	3003	1.53–42.48	56.6	α, L_t, d, g, i, S_t, k, γ
9	2002	2.08–42.50	43.7	α, L_t, d, g, i, S_p, S_t, k, γ
10	1001	2.66–42.52	30.2	α, c, L_t, d, g, i, S_p, S_t, k, γ
11	364	4.92–42.52	17.3	α, c, L_t, d, z_0, g, i, S_p, S_t, k, γ
12	91	8.41–42.53	6.6	α, c, L_t, d, f_{roof}, z_0, g, i, S_p, S_t, k, γ
13	14	20.47–42.54	0.0	α, c, L_t, d, f_{roof}, h_0, z_0, g, i, S_t, b, k, γ
14	1	42.54–42.54	0.0	α, c, L_t, d, f_{roof}, h_0, z_0, g, i, S_p, S_t, b, k, γ

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Parameter estimation

θ	Original value	Limits	Estimate Seasonal	Estimate DUPLEX	% Difference	95 % CL % of mean θ

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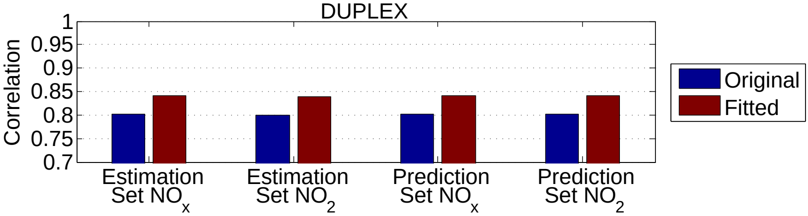
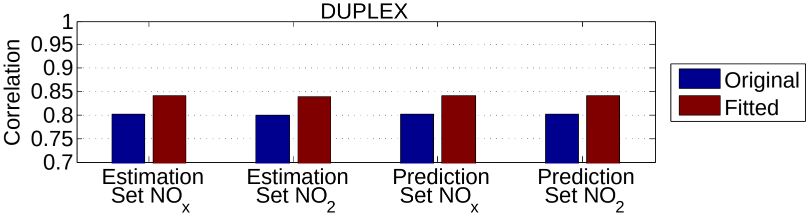
θ	Original value		Limits	Estimate Seasonal	Estimate DUPLEX	% Difference	95 % CL % of mean θ
b	0.3		$[10^{-5} : 0.999]$	0.212	0.288	30.5	± 0.6
f_{roof}	0.4		$[10^{-5} : 0.999]$	0.427	0.422	1.2	± 1.2
h_0	2.0	m	$[0.6 : 10]$	2.177	1.422	42.0	± 0.9
c	2.0		$[0.25 : 10.00]$	6.607	5.685	15.0	± 1.5
S_P	2.0	m^2	$[10^{-5} : 10]$	1.198	0.360	107.5	± 2.5
g	2.0	$\frac{\mathrm{m}}{\mathrm{s}}$	$[10^{-5} : 10]$	0.116	0.085	31.5	± 18.5
d	0.5		$[10^{-5} : 2\pi]$	1.873	1.105	51.6	± 0.3
i	1.0	$\frac{\mathrm{m}}{\mathrm{s}}$	$[10^{-5} : 10]$	0.455	0.713	44.3	± 1.4
α	0.1		$[0.05 : 2.00]$	0.277	0.292	5.5	± 1.0
L_t	0.5		$[10^{-5} : 0.999]$	0.008	$1.335 \cdot 10^{-5}$	199.3	$\pm 1.3 \cdot 10^5$
γ	0.2		$[10^{-5} : 0.999]$	0.789	0.017	191.5	± 52.1
k	0.4		$[0.04 : 0.999]$	0.999	0.999	0.0	± 8.7

In general: More sensitivity $\rightarrow$ less uncertainty



Approximately homogeneous correlation before and after

Validation of estimated parameters – Statistics



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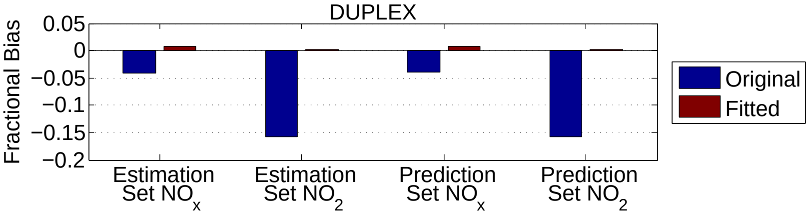
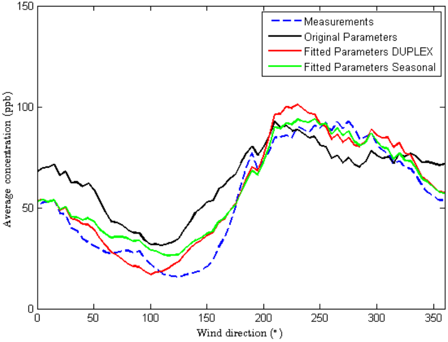
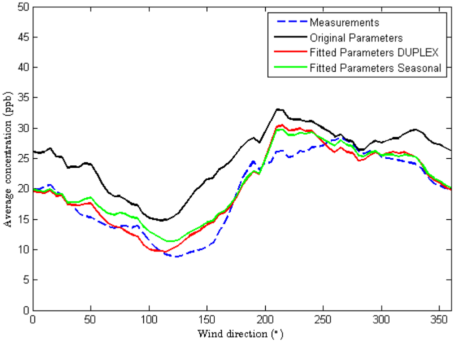


More homogeneous and reduced fractional bias after fit

Wind direction plot: Albanigade, Odense

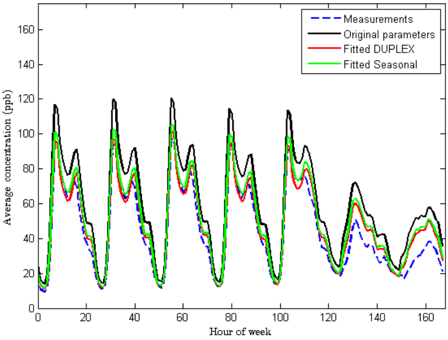


(a) NO_x

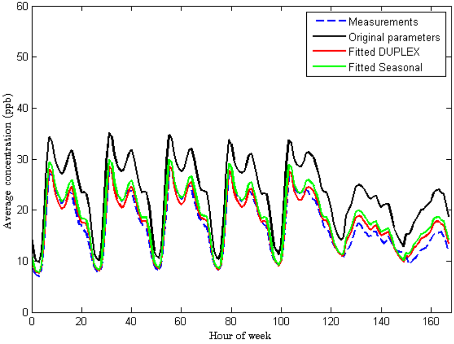


(b) NO_2

Diurnal average plot: Albanigade, Odense



(c) NO_x



(d) NO_2

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Other experiences:

- The 95% confidence intervals underestimates uncertainties

Further reading:

Thor-Bjørn Ottosen, Matthias Ketzel, Henrik Skov, Ole Hertel, Jørgen Brandt, and Konstantinos Kakosimos (2014). "A Parameter Estimation and Identifiability Analysis Methodology Applied to a Street Canyon Air Pollution Model". In: *Environmental Modelling & Software* (in preparation)

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