Source Parameter Estimation Of Atmospheric pollution from accidental releases of gas

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Abstract

This thesis presents the development of an inverse model that may be used to estimate the source term parameters for a polluting gas released into the atmosphere from a point above the ground. The model uses measured pollution concentrations at observation sites on the ground as well as meteorological data such as wind speed and cloud cover. The inverse model is formulated as a least- squares minimisation problem coupled with the solution of an advection-diffusion equation. The least-squares technique allows quantification of the uncertainty of the calculated estimates, which in turn allows estimation of the uncertainty of the simulation model predictions.

The minimisation problem where the pollutants are released instantaneously is well-posed and the source term is calculated with reasonable accuracy. However, the problem with a non-steady extended release source is ill-posed; consequently, its solution is extremely sensitive to errors in the measurement data. Tikhonov's regularisation, which stabilises the solution process, is used to overcome the ill-posedness of this problem. The optimal value of the regularisation parameter in the problem is estimated using both the linear and non-linear L-curve criterion, and a generalised cross-validation approach. The accuracy of the model is examined by using simulated concentration data (generated by the forward model) to which normally-distributed relative noise has been added, as well as some real experimental data.

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Contents

List of Symbols

q	release rate of pollutant gas $[kg\ s^{-1}]$
q_0	release amount of pollutant gas $[kg]$
C	concentration of pollutant gas $[kg\ m^{-3}]$
t	measurement time with respect to release started time $[s]$
T	measurement clock time $[s]$
t_0	measurement started time with respect to release start time $[s]$
S	location of the source
H	height of the source from the ground level $[m]$
X_0	distance in the X-direction between the source and the receptor $[m]$
Y_0	distance in the Y-direction between the source and the receptor $[m]$
λ	regularization parameter
L	regularization operator
n	number of measurements
N	order of regularization
σ	singular values
Σ	singular matrix
W	left singular vector
V	right singular vector
$\mathbf{q}$	mass flux per unit area
$\mathbf{K}$	dispersion tensor
K_x	dispersion coefficient in the X- direction $[m^2\ s^{-1}]$
K_y	dispersion coefficient in the Y- direction $[m^2\ s^{-1}]$
K_z	dispersion coefficient in the Z- direction $[m^2\ s^{-1}]$
U	wind speed in the X-direction $[m\ s^{-1}]$
σ_x	the standard deviation of the concentration in the X-direction
σ_y	the standard deviation of the concentration in the Y-direction
σ_z	the standard deviation of the concentration in the Z-direction
GCV	generalised cross validation
SVD	singular value decomposition
a, b, c, d, e, f, p, r	atmospheric stability parameters
$\mathbf{c}$	measured concentration vector
$\hat{\mathbf{c}}$	estimated concentration vector