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SOURCE PARAMETER ESTIMATION  
OF  
ATMOSPHERIC POLLUTION FROM  
ACCIDENTAL RELEASES OF GAS

A THESIS PRESENTED IN PARTIAL FULFILMENT OF THE  
REQUIREMENTS FOR THE DEGREE OF

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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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## 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	$[m]$
$\lambda$	regularization parameter	
$L$	regularization operator	
$n$	number of measurements	
$N$	order of regularization	
$\sigma$	singular values	
$\Sigma$	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	$[m\ s^{-1}]$
$\sigma_x$	the standard deviation of the concentration in the X-direction	
$\sigma_y$	the standard deviation of the concentration in the Y-direction	
$\sigma_z$	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	

