Solving inverse problems of unknown contaminant source in groundwater-river integrated systems using a surrogate transport model based optimization

Azade Jamshidi 1,1, Jamal Mohammad Vali Samani1,*, Hossein Mohammad Vali Samani2, Andrea Zanini3,*, Maria Giovanna Tanda3, Mehdi Mazaheri1

1 Tarbiat Modares University, Department of Hydro Structures, Tehran, Iran; azade_jamshidi@modares.ac.ir, samani_j@modares.ac.ir, m.mazaheri@modares.ac.ir
2 Islamic Azad University, Department of Civil Engineering, Shahr-e-Qods Branch, Tehran (Iran); hossein.samani@gmail.com
3 University of Parma, Department of Engineering and Architecture, Parco Area delle Scienze 181/A, 43124 Parma (Italy); andrea.zanini@unipr.it, mariagiovanna.tanda@unipr.it
* Correspondence: samani_j@modares.ac.ir; andrea.zanini@unipr.it

**List of Symbols**

| Symbol | Description |
|--------|-------------|
| $T_x$  | Transmissivity tensor at location $x$ |
| $h_p$  | Piezometric head |
| $w$    | Volumetric flux per unit area |
| $S_{stv}$ | Storativity of the porous material |
| $t$    | Time |
| $x$    | Position in the domain |
| $x_0$  | Source location |
| $\phi$ | Effective porosity |
| $u(x,t)$ | Effective velocity at location $x$ and time $t$ |
| $D(x)$ | Dispersion tensor |
| $C(x,t)$ | Concentration at location $x$ and time $t$ |
| $\nabla$ | Nabla operator |
| $s(t)$ | Unknown release function |
| $\delta(t)$ | Dirac delta temporal distribution function |
| $\delta(x)$ | Dirac delta spatial distribution function |
| $g(x,t)$ | Transfer function at location $x$ and time $t$ |
| Symbol | Description                                      |
|--------|-------------------------------------------------|
| $\tau$ | Time                                            |
| $H(t)$ | Heaviside step function                         |
| $F_0$  | Constant and known mass rate input function     |
| $z$    | Observations                                    |
| $T$    | Sampling time                                   |
| $h(s)$ | Vector that describes the transport process     |
| $H$    | Sensitivity matrix                              |
| $x_M$  | Monitoring location                             |
| $\Delta t$ | Numerical model time step                     |
| $N$    | Number of sources                               |
| $n$    | Number of the discretized time values           |
| $m$    | Number of monitoring point                      |
| $Q$    | Discharge                                       |
| $A$    | Cross-sectional area                            |
| $q$    | Lateral inflow                                  |
| $h_w$  | Water level                                     |
| $S_f$  | Flow resistance term                            |
| $\alpha$ | Momentum distribution coefficient               |
| $x_l$  | Curvilinear coordinate                          |
| $M_{tot}$ | Discharged contaminant total masses            |
| $f_r(t)$ | Release histories                              |
| $g_r(x_l)$ | Source spatial distribution in the $r$th source |
| $k(x_{IM},t)$ | Transfer function                      |
| $C(x_{IM},t)$ | Concentration at location $x_{IM}$ and time $t$ |
| $R$    | Number of sources                               |
| $p$    | Number of measurement point                     |
| $t_j$  | Time                                            |
| $h$    | Model function                                  |
| $v$    | Random vector                                   |
| $f_s$  | Vector of discretized release history           |
| Symbol | Description |
|--------|-------------|
| $w_0$  | Unknown input vector value of injected source flux |
| $w_{\text{max}}$ | Upper value of injected source flux |
| $C_i$  | Measured concentration |
| $\hat{C}_i$ | Estimated concentration |
| $\text{objF}$ | Optimization objective function |
| $x_n$  | Position in the domain |
| $C_{\text{sampled}}(x_n, t)$ | Sampled true concentration data at location $x_n$ and time $t$ |
| $C_{\text{new, sampled}}(x_n, t)$ | Corrupted concentration data at location $x_n$ and time $t$ |
| $\delta_n$ | Random number |
| $\alpha$ | Error amplitude |
| $\alpha \delta_n$ | Relative measurement error |
| $NE$  | Normalized error |
| $PAEE$ | Percent average estimation error |
| $SD$  | Standard deviation |
| $ME$  | Mean error |
| $MAE$ | Mean absolute error |
| $RMSE$ | Root mean squared error |
| $NRMSE$ | Normalized root mean squared error |
| $\bar{W}_{i, \text{est}}$ | Average computed source flux |
| $W_{i, \text{act}}$ | Actual source fluxes |
| $N_R$  | Number of realization |
| $K$    | Hydraulic conductivity |
| $O$    | Monitoring location |
| $S$    | Pollutant source |
| $SP$   | Stress period |
| $TF$   | Transfer function |
| $\alpha_L$ | Longitudinal dispersivity |
| $\alpha_T$ | Transverse dispersivity |
| $b$    | Saturated thickness |
| $\Delta x$ | Size of numerical cell grid in $x$ direction |
| $\Delta y$ | Size of numerical cell grid in $y$ direction |