Characterization of uncertainties of parameters with F-statistic for flows through porous media

Guo-Qiang Yang [a]

[a] *Department of Mathematics, Duke University, Box 90320, Durham, North Carolina 27708*

Abstract

The F-test (lack-of-fit) is applied to characterize the uncertainties in the estimation of parameters for flows through porous media. In the forward simulation, mixed finite element and second-order donor cell methods are used for the pressure-velocity equation and concentration equation respectively. The treatment of the wells are described. We show that F-test is flexible when handling the (ill-posed) inverse problem and gives the (exact) confidence regions for the unknown permeability field. Although the high dimensional confidence regions usually cannot be visualized, the simple evaluation of the F-statistic for each realization is desirable, as opposed to the usual Monte Carlo methods, which can only lead to approximate confidence levels with sufficient many samplings.

Key words: uncertainty, forward and inverse problems, mixed finite element, donor cell, F-test and lack-of-fit, confidence regions and confidence intervals, singular value decomposition

1 Introduction

The problem of flows through porous media is very important arising in many scientific and engineering fields, e.g., ground water hydrology, petroleum engineering, soil science, soil mechanics and chemical engineering.

In modeling a real groundwater system, two classes of problems, which are called forward and inverse, need to be solved. The former solves the flow

Email address: yanggq@math.duke.edu (Guo-Qiang Yang).

equations given model parameters of the groundwater system, while the latter determines unknown model parameters which are consistent with given observation values. A typical example is the estimation of some aquifer parameters, say, the hydraulic conductivity T, based on the observed hydraulic head data h at some wells possibly along with some field or laboratory estimates of the aquifer parameters, based on some known empirical models. For example, Darcy's law for unsteady flow can be described as

$$\frac{\partial h}{\partial t} - \nabla \cdot (T \nabla h) = Q \tag{1}$$

with appropriate initial and boundary conditions. Here Q is the injection rate ($Q > 0$) or production rate ($Q < 0$) at the wells.

The study of inverse problems is far more difficult than forward ones. Due to the ill-posedness of the inverse problems (NY79; TA77) in the sense of the lack of continuous dependence of the parameters on the measurements, the estimation of the parameters cannot be improved simply by improving the accuracy of forward simulations. Moreover, increasing the mesh refinement increases the ill-posedness. Also, since the observed data are often sparse and of varying quality, the estimation of the unknown parameters may not be unique or stable.

On the other hand, many theoretical and numerical methods for inverse problems and the corresponding methods have been widely applied in all science. Some books and many journal articles have appeared. Some selected publications on groundwater inverse problems are Yeh(Yeh86), Kuiper(Kuiper86), Ginn and Cushman(GC90), Sun(Sun94), and McLaughlin and Townley(MT96).

2 Formulation of two-dimensional pressure-concentration model

2.1 The model

In this work, we will consider the typical two-dimensional steady pressure-velocity equation

$$\begin{cases} \nabla \cdot v = q, \\ T^{-1} v = g - \nabla p, \end{cases} \tag{2}$$

and the corresponding concentration model

$$\frac{\partial c\phi}{\partial t} + \nabla \cdot (vc) = cq, \tag{3}$$

in the domain $\Omega \equiv [0,1] \times [0,1]$, where $T = K/\mu$ is the mobility (permeability/viscosity) which is positive (scalar or tensor), p is the pressure, q is the injection/production rate, c is the concentration, and ϕ is the porosity. We assume that μ is a constant, and the boundary condition of velocity and initial condition for tracer concentration are

$$v \cdot \nu = 0, \;\; x \in \partial\Omega, \tag{4}$$
$$c|_{t=0} = 0, \;\; x \in \Omega, \tag{5}$$

where ν is the outer normal unit vector of the boundary of Ω.

Although the concentration function may be discontinuous mathematically, the pressure function is continuous over the field under very weak assumption on $T(\vec{x})$ (see De Giorgi(Giorgi57), Nash(Nash58) and Moser(Moser60)).

Note that the continuity of the pressure field indicates that pressure data will give information about some average level of the permeability field. In contrast, the concentration field will be discontinuous if we ignore the small viscosity that may be involved.

3 Numerical methods

To identify the unknown mobility T, some forward solvers need to be developed. We shall use mixed finite element method for the pressure-velocity equation(2) and conservative difference scheme for the concentration equation (3).

4 Numerical methods for the forward model

4.1 Mixed finite element method for the pressure-velocity equation

First let us consider the pressure equation (2) with the zero velocity boundary conditions (4).

Let us define

$$\mathcal{H}(\mathrm{div};\Omega) = \{u \in (L^2(\Omega))^2 : \nabla \cdot u \in L^2(\Omega)\}, \tag{6}$$
$$\mathcal{V} = \{u \in \mathcal{H}(\mathrm{div};\Omega) : u \cdot \nu = 0 \text{ on } \partial\Omega\}, \tag{7}$$
$$\mathcal{P} = L^2(\Omega) \tag{8}$$

and denote the vector inner product on $(L^2(\Omega))^2$

$$(u, w) = \int_\Omega v \cdot w dx. \tag{9}$$

The variational form of (2) can be formulated as

$$\begin{cases} (g, u) - (T^{-1}v, u) + (p, \nabla \cdot u) = 0, \ \forall u \in \mathcal{V}, \\ (\nabla v, w) = (q, w), \qquad \forall w \in \mathcal{P}. \end{cases} \tag{10}$$

The finite element approximation to (10) requires appropriate finite-dimensional subspaces $\mathcal{V}_h \subset \mathcal{V}$ and $\mathcal{P}_h \subset \mathcal{P}$ to approximate $\mathcal{V}$ and $\mathcal{P}$ respectively. One convenient choice, called *Raviart-Thomas elements*, can be constructed as follows.

Choose meshes $\Delta = \Delta_x \times \Delta_y, \Delta_x : 0 = x_0 < x_1 < \cdots < x_I = 1$ and $\Delta_y : 0 = y_0 < y_1 < \cdots < y_J = 1$ and define the piecewise-polynomial space

$$\mathcal{M}_m^r(\Delta) = \{f \in C^m([0,1]) : f \text{ is a polynomial of degree} \leq r \text{ on each subinterval of } \Delta\}$$

where $m = -1$ refers to discontinuous functions.

Let $\mathcal{P}_h$ be the set of all piecewise constant functions on the grid cells formed by Δ_x and Δ_y and and

$$\mathcal{V}_h = \{\vec{u} = (u_x, u_y)^\top : \ u_x \text{ linear in } x \text{ and constant in } y; \ u_y \text{ constant in } x \text{ and linear in } y \ \}.$$

In the mixed finite element, we find functions $\vec{v} \in \mathcal{V}_h$ and $p \in \mathcal{P}_h$ such that

$$0 = \int_\Omega (\nabla \cdot \vec{v} - q) P_k d\Omega, \qquad \forall P_k \in \mathcal{P}, \tag{11}$$
$$0 = \int_\Omega \left(V_k \cdot \vec{g} - V_k \cdot T^{-1}\vec{v} + p\nabla \cdot V_k\right) d\Omega - \int_{\partial\Omega} p V_k \cdot \nu ds, \quad \forall V_k \in \mathcal{V}. \tag{12}$$

The above is equivalent to choose a basis for $\mathcal{P}_h$ and a basis for $\mathcal{V}_h$ that satisfy the systems. Define

$$\Omega_{ij} = \{(x,y) : x_{i-\frac{1}{2}} \le x \le x_{i+\frac{1}{2}}, y_{j-\frac{1}{2}} \le y \le y_{j+\frac{1}{2}}\}.$$

Our basis functions are

$$P_{ij}(x,y) = \begin{cases} 1, \ (x,y) \in \Omega_{ij} \\ 0, \ \text{ otherwise} \end{cases}, \quad i = 1, \cdots, I, \quad j = 1, \cdots, J;$$
$$V^1_{i-\frac{1}{2},j}(x,y) = V^1(\xi_{i-\frac{1}{2}}(x), \eta_j(y)), i = 1, \cdots, I, \quad j = 1, \cdots, J,$$
$$V^2_{i,j-\frac{1}{2}}(x,y) = V^2(\xi_i(x), \eta_{j-\frac{1}{2}}(y)), i = 1, \cdots, I, \quad j = 1, \cdots, J.$$

Here the canonical basis functions are

$$V^1(\xi,\eta) = \begin{bmatrix} \max\{0, 1-|\xi|\}\chi_{[0,1]}(\eta) \\ 0 \end{bmatrix}, \tag{13}$$

$$V^2(\xi,\eta) = \begin{bmatrix} \max\{0, 1-|\eta|\}\chi_{[0,1]}(\xi) \\ 0 \end{bmatrix}, \tag{14}$$

where $\chi_S(\cdot)$ is the characteristic function of set S, and the coordinate maps are

$$\xi_{i-\frac{1}{2}}(x) = \begin{cases} (x - x_{i-\frac{1}{2}})/(x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}), \ x \ge x_{i-\frac{1}{2}} \\ (x - x_{i-\frac{1}{2}})/(x_{i-\frac{1}{2}} - x_{i-\frac{3}{2}}), \ x < x_{i-\frac{1}{2}} \end{cases}, \quad \xi_i(x) = \frac{x - x_{i-\frac{1}{2}}}{x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}},$$
$$\eta_{j-\frac{1}{2}}(y) = \begin{cases} (y - y_{j-\frac{1}{2}})/(y_{j+\frac{1}{2}} - y_{j-\frac{1}{2}}), \ y \ge y_{j-\frac{1}{2}} \\ (y - y_{j-\frac{1}{2}})/(y_{j-\frac{1}{2}} - y_{j-\frac{3}{2}}), \ y < y_{j-\frac{1}{2}} \end{cases}, \quad \eta_j(y) = \frac{y - y_{j-\frac{1}{2}}}{y_{j+\frac{1}{2}} - y_{j-\frac{1}{2}}},$$

The equation (11) leads to

$$\int_\Omega qP_{ij}d\Omega = \int_{\Omega_{ij}} qP_{ij}d\Omega = q_{ij}\Delta x_i \Delta y_j = \int_{\Omega_{ij}} P_{ij}\nabla\cdot\vec{v}d\Omega = \int_{\partial\Omega_{ij}} \vec{n}\cdot\vec{v}ds$$
$$= (v_{i+\frac{1}{2},j} - v_{i-\frac{1}{2},j})\Delta y_j + (v_{i,j+\frac{1}{2}} - v_{i,j-\frac{1}{2}})\Delta x_i, \tag{15}$$

which is the discrete analog of $\nabla\cdot v = q$. For (12), there are four basis functions for V contributing to the ij-th cell:

$$
\begin{aligned}
0 =& \int_\Omega V^1_{i-\frac{1}{2},j}\cdot\vec{g} - V^1_{i-\frac{1}{2},j}\cdot T^{-1}\vec{v} + p\nabla\cdot V^1_{i-\frac{1}{2},j}]d\Omega - \int_{\partial\Omega} pV^1_{i-\frac{1}{2},j}\cdot\nu ds \\
=& \frac{1}{2}(g_{x,i-1,j}\Delta x_{i-1} + g_{x,ij}\Delta x_i)\Delta y_j - (p_{ij} - p_{i-1,j})\Delta y_j \\
& -\Delta x_{i-1}\Delta y_j\{(T^{-1}_{i-1,j})_{xx}[\frac{1}{6}v_{i-\frac{3}{2},j} + \frac{1}{3}v_{i-\frac{1}{2},j}] + (T^{-1}_{i-1,j})_{xy}[\frac{1}{4}v_{i-1,j-\frac{1}{2}} + \frac{1}{4}v_{i-1,j+\frac{1}{2}}]\} \\
& -\Delta x_i\Delta y_j\{(T^{-1}_{ij})_{xx}[\frac{1}{3}v_{i-\frac{1}{2},j} + \frac{1}{6}v_{i+\frac{1}{2},j}] + (T^{-1}_{ij})_{xy}[\frac{1}{4}v_{i,j-\frac{1}{2}} + \frac{1}{4}v_{i,j+\frac{1}{2}}]\}
\end{aligned}
$$

and similar relations with basis functions $V^1_{i+\frac{1}{2},j}$ or $V^2_{i,j\pm\frac{1}{2}}$ replacing $V^1_{i-\frac{1}{2},j}$ above. Of course, at the boundary of Ω, special modifications are needed. In summary, the mixed finite element method can be written as

$$
\begin{bmatrix} \mathbf{T}^{-1} & \mathbf{G} \\ \mathbf{G}^\top & \mathbf{0} \end{bmatrix}\begin{bmatrix} \mathbf{v} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} \mathbf{g} \\ \mathbf{q} \end{bmatrix}, \tag{16}
$$

where

$$
\mathbf{v} = \begin{bmatrix} (\mathbf{v})_{\cdot 1} \\ \vdots \\ (\mathbf{v})_{\cdot J} \\ (\mathbf{v})_{1\cdot} \\ \vdots \\ (\mathbf{v})_{I\cdot} \end{bmatrix}, (\mathbf{v})_{\cdot j} = \begin{bmatrix} v_{\frac{3}{2},j}\Delta y_j \\ \vdots \\ v_{I-\frac{1}{2},j}\Delta y_j \end{bmatrix}, (\mathbf{v})_{i\cdot} = \begin{bmatrix} v_{i,\frac{3}{2}}\Delta x_i \\ \vdots \\ v_{i,J-\frac{1}{2}}\Delta x_i \end{bmatrix}, \mathbf{p} = \begin{bmatrix} p_{11} \\ \vdots \\ p_{I1} \\ \vdots \\ p_{1J} \\ \vdots \\ p_{IJ} \end{bmatrix},
$$

$$
\mathbf{G} = \begin{bmatrix} \mathbf{I}_{J\times J}\otimes(\mathbf{G}_1)_{(I-1)\times I} \\ (\mathbf{G}_2)_{(J-1)\times J}\otimes\mathbf{I}_{I\times I} \end{bmatrix},
$$

$$
\mathbf{G}_1 = \begin{bmatrix} -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{bmatrix}_{(I-1)\times I}, \mathbf{G}_2 = \begin{bmatrix} -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{bmatrix}_{(J-1)\times J},
$$

$$\mathbf{T}^{-1} = \begin{bmatrix} (\mathbf{T}^{-1})_{\cdot 1} & & & | & & & \\ & \ddots & & | & & \mathbf{M} & \\ & & (\mathbf{T}^{-1})_{\cdot J} & | & & & \\ - & - & - & - & - & - & - \\ & & & | & (\mathbf{T}^{-1})_{1\cdot} & & \\ & \mathbf{N} & & | & & \ddots & \\ & & & | & & & (\mathbf{T}^{-1})_{I\cdot} \end{bmatrix},$$

$$(\mathbf{T}^{-1})_{\cdot j} = \begin{bmatrix} \alpha_{1j}+\alpha_{2j} & \beta_{2j} & & & & \\ \beta_{2j} & \alpha_{2j}+\alpha_{3j} & \beta_{3j} & & & \\ & \ddots & \ddots & \ddots & & \\ & & \beta_{I-2,j} & \alpha_{I-2,j}+\alpha_{I-1,j} & \beta_{I-1,j} & \\ & & & \beta_{I-1,j} & \alpha_{I-1,j}+\alpha_{I,j} \end{bmatrix},$$

$$(\mathbf{T}^{-1})_{i\cdot} = \begin{bmatrix} \xi_{i1}+\xi_{i2} & \eta_{i2} & & & & \\ \eta_{i2} & \xi_{i2}+\xi_{i3} & \eta_{i3} & & & \\ & \ddots & \ddots & \ddots & & \\ & & \eta_{i,J-2} & \xi_{i,J-2}+\xi_{i,J-1} & \eta_{i,J-1} & \\ & & & \eta_{i,J-1} & \xi_{i,J-1}+\xi_{iJ} \end{bmatrix},$$

$$\mathbf{M} = [\mathbf{M}_{ij}]_{i=1,\cdots,I;j=1,\cdots,J-1}, \quad \mathbf{N} = [\mathbf{N}_{ij}]_{i=1,\cdots,I-1;j=1,\cdots,J},$$

$$\mathbf{M}_{ij} = \frac{(T_{ji}^{-1})_{xy}}{4}(\mathbf{I}_{ij}+\mathbf{I}_{i-1,j}+\mathbf{I}_{i,j-1}+\mathbf{I}_{i-1,j-1}),$$

$$\mathbf{N}_{ij} = \frac{(T_{ij}^{-1})_{yx}}{4}(\mathbf{I}_{ij}+\mathbf{I}_{i-1,j}+\mathbf{I}_{i,j-1}+\mathbf{I}_{i-1,j-1}),$$

$$\alpha_{ij} = \frac{(T_{ij}^{-1})_{xx}\Delta x_i}{3\Delta y_j}, \beta_{ij} = \frac{\alpha_{ij}}{2}, \xi_{ij} = \frac{(T_{ij}^{-1})_{yy}\Delta y_j}{2\Delta x_i}, \eta_{ij} = \frac{\xi_{ij}}{2},$$

$$i = 1\cdots, I, \quad j = 1, \cdots, J,$$

$$\mathbf{q} = [q_{11}\Delta x_1\Delta y_1, \cdots, q_{I1}\Delta x_I\Delta y_1, \cdots, q_{1J}\Delta x_1\Delta y_J, \cdots, q_{IJ}\Delta x_I\Delta y_J]^\top,$$

and

$$\mathbf{g} = \begin{bmatrix} \mathbf{g}_x \\ \mathbf{g}_y \end{bmatrix},$$

$$\mathbf{g}_x = \frac{1}{2} \begin{bmatrix} g_{x,11}\Delta x_1 + g_{x,21}\Delta x_2 \\ \vdots \\ g_{x,I-1,1}\Delta x_{I-1} + g_{x,I1}\Delta x_I \\ \vdots \\ g_{x,1J}\Delta x_1 + g_{x,2J}\Delta x_2 \\ \vdots \\ g_{x,I-1,J}\Delta x_{I-1} + g_{x,IJ}\Delta x_I \end{bmatrix},$$

$$\mathbf{g}_y = \frac{1}{2} \begin{bmatrix} g_{y,11}\Delta y_1 + g_{y,12}\Delta y_2 \\ \vdots \\ g_{y,1,J-1}\Delta y_{J-1} + g_{y,1J}\Delta y_J \\ \vdots \\ g_{y,I1}\Delta y_1 + g_{y,I2}\Delta y_2 \\ \vdots \\ g_{y,I,J-1}\Delta y_{J-1} + g_{y,IJ}\Delta y_J \end{bmatrix},$$

and the (k,l)-th entry of the $I \times J$ matrix $\mathbf{I}_{ij}$ is defined as $\chi_{[(k,l)=(i,j),1\leq i<I,1\leq j\leq J]}$.

For simplicity, we make the following assumptions (a)-(c) for the unknown mobility field:

(a) if the tensor of the mobility field is symmetric, i.e., $T_{xy} = T_{yx}$, then the matrix $\mathbf{T}$ will be symmetric (and hence $\mathbf{N} = \mathbf{M}^\top$);

(b) if the tensor T is diagonal, i.e., $T_{xy} = T_{yx} = 0$, then $\mathbf{N} = \mathbf{M}^\top = \mathbf{0}$;

(c) if, in addition to (i) and (ii), T is isotropic, then $T(x,y) = \sigma(x,y)I$ and I is the (2×2) identity matrix.

In addition, instead of using $\sigma(x,y)$, we shall keep the notation $T(x,y)$ for the scalar function σ at (x,y). Note the different meaning of T in the following. In this case, the system can be rewritten as

$$\mathbf{v} = -\mathbf{T}^{-1}(\mathbf{G}\mathbf{p} - \mathbf{g}). \tag{17}$$

So we may eliminate $\mathbf{v}$ and obtain the linear system of $\mathbf{p}$:

$$(\mathbf{G}^\top \mathbf{T}^{-1} \mathbf{G})\mathbf{p} = (\mathbf{G}^\top \mathbf{T}^{-1} - \mathbf{I})\mathbf{g}, \tag{18}$$

where $\mathbf{I}$ is the identity matrix of order $(I-1)J + I(J-1)$.

In order to obtain a mixed element solver in which the above elimination of $\mathbf{v}$ can be done easily, we shall adopt a new version of mixed finite element method with the lowest-order in which a second-order trapezoidal approximation is adopted for the integrations involving permeability in the above deduction. Under such modification, $\mathbf{T}$ becomes diagonal and can be rewritten as

$$\begin{aligned}\mathbf{T} = \mathrm{diag}[&\gamma_{11} + \gamma_{21}, \cdots, \gamma_{I-1,1} + \gamma_{I1}, \cdots, \gamma_{1J} + \gamma_{2J}, \cdots, \gamma_{I-1,J} + \gamma_{IJ}, \\ &\gamma_{11} + \gamma_{12}, \cdots, \gamma_{1,J-1} + \gamma_{1J}, \cdots, \gamma_{I1} + \gamma_{I2}, \cdots, \gamma_{I,J-1} + \gamma_{IJ}],\end{aligned} \tag{19}$$

whose inverse can be obtained trivially. Note also that in this case, the matrix $\mathbf{G}^\top \mathbf{T}^{-1} \mathbf{G}$ becomes tridiagonal and the well-known *Thomas algorithm*(**?**) for tridiagonal matrix applies.

4.2 Well models and the pressure-velocity equation involving wells

There are mainly two types of well models, namely, cross-sectional and areal models, for the source term q in two-dimensional models (see Trangenstein and Bi (TB02), for example). Here we only consider the second one, for which

$$q_{ij} \equiv \int_{\Omega_{ij}} q dx dy = w_{ij}(p_{w,ij} - p_{ij}), \quad w_{ij} = \frac{2\pi T_{ij}}{\log(r_{e,ij}/r_{ij})},$$

where r is the well radius and r_e is the Peaceman (Peaceman78) effective well radius

$$r_{e,ij}^2 = \frac{2((\Delta x_i)^2 + (\Delta y_j)^2)}{e^\pi T_{ij}}.$$

Corresponding to the specification of well rate and pressure, some adjustments should be done for the system (18) of $\mathbf{p}$ and the new system can be rewritten as

$$\mathbf{A}\mathbf{p} = \mathbf{b}, \tag{20}$$

where, for the case we consider here, the entries of $IJ \times IJ$ matrix $\mathbf{A}$ are

$$A_{kl} = \begin{cases} (\mathbf{G}^\top \mathbf{T}^{-1} \mathbf{G})_{kl}, & (k,l) \neq (I,I) \\ (\mathbf{G}^\top \mathbf{T}^{-1} \mathbf{G})_{kl} + \omega_{I1} \Delta x_I \Delta y_1, & (k,l) = (I,I) \end{cases} \tag{21}$$

and the vector $\mathbf{b}$ is

$$\mathbf{b} = (\mathbf{G}^\top \mathbf{T}^{-1} - \mathbf{I})\mathbf{g} - \omega_{I1} p_{w,I1} \Delta x_I \Delta y_1 \cdot e_I. \tag{22}$$

4.3 Second-order donor cell method for the concentration equation

This subsection will give a description of the conservative difference scheme for the concentration equation (3) following the idea of Colella (**?**)).

First, the fact that for each cell Ω_{ij},

$$\begin{aligned} \int_{\Omega_{ij}} c(x,y,t^{n+1})\phi(x,y)d\Omega = & \int_{\Omega_{ij}} c(x,y,t^n)\phi(x,y)d\Omega \\ & - \int_{t^n}^{t^{n+1}} \int_{\partial\Omega_{ij}} cv \cdot \nu ds dt + \int_{t^n}^{t^{n+1}} \int_{\Omega_{ij}} cq d\Omega dt \end{aligned}$$

leads to a conservative difference scheme for (3)

$$\begin{aligned} c_{ij}^{n+1}\phi_{ij}\Delta x_i \Delta y_j = & c_{ij}^n \phi_{ij} \Delta x_i \Delta y_j \\ & - [f_{i+\frac{1}{2},j}^{n+\frac{1}{2}} - f_{i-\frac{1}{2},j}^{n+\frac{1}{2}}] - [f_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} - f_{i,j-\frac{1}{2}}^{n+\frac{1}{2}}] + Q_{ij}^{n+\frac{1}{2}}, \end{aligned}$$

where

$$f_{i+\frac{1}{2},j}^{n+\frac{1}{2}} = c_{i+\frac{1}{2},j}^{n+\frac{1}{2}} V_{i+\frac{1}{2},j}^{n+\frac{1}{2}}, f_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} = c_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} V_{i,j+\frac{1}{2}}^{n+\frac{1}{2}}, Q_{ij}^{n+\frac{1}{2}} = c_{ij}^{n+\frac{1}{2}} q_{ij}^{n+\frac{1}{2}} \Delta x_i \Delta y_j \Delta t^{n+\frac{1}{2}}.$$

In the above expressions, we choose

$$V_{i+\frac{1}{2},j}^{n+\frac{1}{2}} = v_{i+\frac{1}{2},j}^n \Delta t^{n+\frac{1}{2}} \Delta y_j, \quad V_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} = v_{i,j+\frac{1}{2}}^n \Delta t^{n+\frac{1}{2}} \Delta x_i.$$

In second-order version of the donor cell upwind scheme, we use a piecewise-linear reconstruction to provide better evaluations of the predictor fluxes. First we compute the limited cell increments

$$\begin{aligned} \Delta c_{x,ij}^n &= \text{muscl}(c_{ij}^n - c_{i-1,j}^n, c_{i+1,j}^n - c_{ij}^n), \\ \Delta c_{y,ij}^n &= \text{muscl}(c_{ij}^n - c_{i,j-1}^n, c_{i,j+1}^n - c_{ij}^n), \end{aligned}$$

where

$$\mathrm{muscl}(\delta_L,\delta_R) \equiv \begin{cases} \mathrm{sign}(\delta_L)\min\{2|\delta_L|, 2|\delta_R|, |\frac{1}{2}(\delta_L+\delta_R)|\}, & \delta_L\delta_R > 0 \\ 0, & \delta_L\delta_R \le 0 \end{cases}. \quad (23)$$

Define the cell pore volume

$$A_{ij} = \phi_{ij}\Delta x_i \Delta y_j.$$

Then we compute the first-order (in time) side concentrations

$$c^n_{i+\frac{1}{2},j} = \begin{cases} c^n_{ij} + \frac{1}{2}(1 - \frac{V^{n+\frac{1}{2}}_{i+\frac{1}{2},j}}{A_{ij}})\Delta c^n_{x,ij}, & V^{n+\frac{1}{2}}_{i+\frac{1}{2},j} \ge 0 \\ c^n_{i+1,j} - \frac{1}{2}(1 + \frac{V^{n+\frac{1}{2}}_{i+\frac{1}{2},j}}{A_{i+1,j}})\Delta c^n_{x,i+1,j}, & V^{n+\frac{1}{2}}_{i+\frac{1}{2},j} < 0 \end{cases},$$

$$c^n_{i,j+\frac{1}{2}} = \begin{cases} c^n_{ij} + \frac{1}{2}(1 - \frac{V^{n+\frac{1}{2}}_{i,j+\frac{1}{2}}}{A_{ij}})\Delta c^n_{y,ij}, & V^{n+\frac{1}{2}}_{i,j+\frac{1}{2}} \ge 0 \\ c^n_{i,j+1} - \frac{1}{2}(1 + \frac{V^{n+\frac{1}{2}}_{i,j+\frac{1}{2}}}{A_{i,j+1}})\Delta c^n_{y,i,j+1}, & V^{n+\frac{1}{2}}_{i,j+\frac{1}{2}} < 0 \end{cases}$$

and then the predictor flux time and side integrals

$$f^n_{i+\frac{1}{2},j} = c^n_{i+\frac{1}{2},j} V^{n+\frac{1}{2}}_{i+\frac{1}{2},j}, \quad f^n_{i,j+\frac{1}{2}} = c^n_{i,j+\frac{1}{2}} V^{n+\frac{1}{2}}_{i,j+\frac{1}{2}}.$$

Afterward, we determine the side concentration by

$$c^{n+\frac{1}{2}}_{i+\frac{1}{2},j} = \begin{cases} c^n_{ij} - \frac{f^n_{i,j+\frac{1}{2}} - f^n_{i,j-\frac{1}{2}}}{2A_{ij}}, & V^{n+\frac{1}{2}}_{i+\frac{1}{2},j} \ge 0 \\ c^n_{i+1,j} - \frac{f^n_{i+1,j+\frac{1}{2}} - f^n_{i+1,j-\frac{1}{2}}}{2A_{i+1,j}}, & V^{n+\frac{1}{2}}_{i+\frac{1}{2},j} < 0 \end{cases},$$

$$c^{n+\frac{1}{2}}_{i,j+\frac{1}{2}} = \begin{cases} c^n_{ij} - \frac{f^n_{i+\frac{1}{2},j} - f^n_{i-\frac{1}{2},j}}{2A_{ij}}, & V^{n+\frac{1}{2}}_{i,j+\frac{1}{2}} \ge 0 \\ c^n_{i,j+1} - \frac{f^n_{i+\frac{1}{2},j+1} - f^n_{i-\frac{1}{2},j+1}}{2A_{i,j+1}}, & V^{n+\frac{1}{2}}_{i,j+\frac{1}{2}} < 0 \end{cases}.$$

4.4 Treatment of well concentrations

Next let us consider vertical wells in the conservative law given by concentration equation.

For a producer, an upwind scheme would be

$$\frac{c_{ij}^{n+1}\phi_{ij} - c_{ij}^{n}\phi_{ij}}{\Delta t^{n+\frac{1}{2}}} + \frac{c_{i+1,j}^{n} v_{i+\frac{1}{2},j} - c_{i-1,j}^{n} v_{i-\frac{1}{2},j}}{\Delta x_i} + \frac{c_{i,j+1}^{n} v_{i,j+\frac{1}{2}} - c_{i,j-1}^{n} v_{i,j-\frac{1}{2}}}{\Delta y_j}$$
$$= \frac{c_{ij}^{n} + c_{ij}^{n+1}}{2}(-q)_{ij},$$
$$\frac{v_{i+\frac{1}{2},j} - v_{i-\frac{1}{2},j}}{\Delta x_i} + \frac{v_{i,j+\frac{1}{2}} - v_{i,j-\frac{1}{2}}}{\Delta y_j} = -q_{ij}.$$

Thus,

$$c_{ij}^{n+1} = \frac{c_{ij}^{n}[1 - \frac{q_{ij}\Delta t^{n+\frac{1}{2}}}{2\phi_{ij}}] - \frac{\Delta t}{\phi_{ij}}[\frac{c_{i+1,j}^{n} v_{i+\frac{1}{2},j} - c_{i-1,j}^{n} v_{i-\frac{1}{2},j}}{\Delta x_i} + \frac{c_{i,j+1}^{n} v_{i,j+\frac{1}{2}} - c_{i,j-1}^{n} v_{i,j-\frac{1}{2}}}{\Delta y_j}]}{1 + \frac{q_{ij}\Delta t}{2\phi_{ij}}}.$$

For an injector, an implicit upwind scheme would be

$$\begin{aligned}
&\frac{c_{ij}^{n+1}\phi_{ij} - c_{ij}^{n}\phi_{ij}}{\Delta t^{n+\frac{1}{2}}} \\
&+\frac{1}{2}\left[\frac{c_{ij}^{n+1} v_{i+\frac{1}{2},j} - c_{ij}^{n+1} v_{i-\frac{1}{2},j}}{\Delta x_i} + \frac{c_{ij}^{n+1} v_{i,j+\frac{1}{2}} - c_{ij}^{n+1} v_{i,j-\frac{1}{2}}}{\Delta y_j}\right. \\
&\left.+ \frac{c_{ij}^{n} v_{i+\frac{1}{2},j} - c_{ij}^{n} v_{i-\frac{1}{2},j}}{\Delta x_i} + \frac{c_{ij}^{n} v_{i,j+\frac{1}{2}} - c_{ij}^{n} v_{i,j-\frac{1}{2}}}{\Delta y_j}\right] \\
&= c_{ij}^{n+\frac{1}{2}} q_{ij}. \qquad (24)
\end{aligned}$$

It follows from (15) that

$$c_{ij}^{n+1} = \frac{c_{ij}^{n}\left(1 - \frac{q_{ij}\Delta t^{n+\frac{1}{2}}}{2\phi_{ij}}\right) + c_{ij}^{n+\frac{1}{2}}\frac{q_{ij}\Delta t^{n+\frac{1}{2}}}{\phi_{ij}}}{1 + \frac{q_{ij}\Delta t^{n+\frac{1}{2}}}{2\phi_{ij}}}.$$

In the special case where zero normal velocity is considered, both wells (the producer and injector) are located on the boundary of the domain. We may regard the four cells adjacent to a well as a bigger cell and treat the well concentration in the following way. At the producer

$$c_{I1}^{n+1} = \frac{c_{I1}^{n}[1 - \frac{4q\Delta t^{n+\frac{1}{2}}}{2\phi_{I1}}] + \frac{\Delta t}{\phi_{I1}}[\frac{-2c_{I-1,1}^{n} v_{I-\frac{1}{2},1}}{2\Delta x_I} + \frac{2c_{I2}^{n} v_{I,\frac{3}{2}}}{2\Delta y_1}]}{1 + \frac{4q\Delta t}{2\phi_{I1}}}, \qquad (25)$$

while at the injector,

$$c_{1J}^{n+1} = \frac{c_{1J}^{n}\left(1 - \frac{4q\Delta t^{n+\frac{1}{2}}}{2\phi_{1J}}\right) + c_{1J}^{n+\frac{1}{2}}\frac{4q\Delta t^{n+\frac{1}{2}}}{\phi_{1J}}}{1 + \frac{4q\Delta t^{n+\frac{1}{2}}}{2\phi_{1J}}}. \tag{26}$$

4.5 Sensitivities of pressure and concentration to the permeability field

From pressure equations (2), the sensitivity coefficients of pressure and velocity to the conductivity or permeability values can be calculated (McElwee87) from the following equations.

$$\nabla \cdot v_{T(x_0)} = 0, v_{T(x_0)} = -T\nabla p_{T(x_0)} - \delta(x - x_0)\nabla p, \tag{27}$$

where $v_{T(x_0)} = \partial v/\partial T(x_0), p_{T(x_0)} = \partial p/\partial T(x_0)$ and the symbol $\delta(x - x_0)$ represents the Dirac delta function. The boundary condition for the sensitivity equations can be obtained by differentiating the boundary conditions of the velocity and pressure equations with respect to $T(x_0)$. Note that the sensitivity equations in (27) are quite similar to those in (2) and thus we may apply mixed finite element methods described in subsection 4.1 in a similar fashion.

The equation of sensitivity coefficients for concentration can be represented as

$$\phi\frac{\partial c_{T(x_0)}}{\partial t} + v \cdot \nabla c_{T(x_0)} = q c_{T(x_0)} - v_{T(x_0)} \cdot \nabla c, \tag{28}$$

and the same solver for concentration in subsection 4.3 applies for (28) with some modification for the sources terms.

Remark 4.1 *In the numerical models for equations (27) and (28), we may choose different meshes for resolving the permeability field and evaluating pressure and concentration.*

5 Confidence region estimation for permeability field

5.1 One-dimensional problem as an example

To show the idea clearly, first we describe the uncertainties arising in estimating the unknown permeability field in a one-dimensional problem.

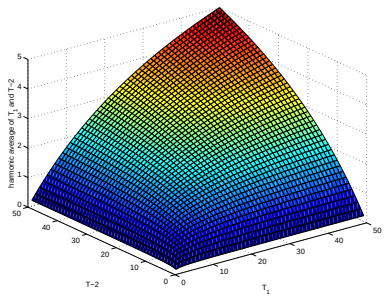

Fig. 1. Harmonic average of one-dimensional field when there are two blocks with permeability T_1 and T_2. The points on each contour curve of the surface give the same model output.

The one-dimensional steady state pressure-concentration model can be expressed as

$$\frac{\partial v}{\partial x} = q(x), \tag{29}$$

$$T^{-1}v = -\frac{\partial p}{\partial x}, \tag{30}$$

$$\frac{\partial c\phi}{\partial t} + \frac{\partial (vc)}{\partial x} = cq(x), \tag{31}$$

where $q(x) = 0$ except possibly at the injecting and producing wells. Assume that the wells are located in the ends of the domain. If we specify the injecting rate at the injector and the pressure at the producer, we have determined the injecting velocity v_0. Due to the incompressibility of the fluid, the velocity $v(x) = v_0$ is a constant. This can be obtained by integrating equation (29) with respect to x. Since the velocity is a known constant in this case, the concentration equation (31) is not useful in identifying the permeability field. In addition, if we only have the pressure data at the injector and the producer, from (30), we have

$$p_{\text{injector}} - p_{\text{producer}} = v_0 \int_{\text{injector}}^{\text{producer}} T^{-1}(\xi) d\xi, \tag{32}$$

where $\int_{\text{injector}}^{\text{producer}} T^{-1}(\xi) d\xi$ is the reciprocal of the harmonic average of $T(x)$ over the domain. In other words, all possible $T(x)$ that have the fixed harmonic average (Figure 4.1)will produce exactly the same observation data. Therefore it is not surprising that in the discrete numerical model, the confidence regions for the unknown permeability field are usually unbounded. However, we expect that in high-dimensional problems the confidence regions might become more intractable, even it is hard to find a statistic with a compact form corresponding to the harmonic average of $T(x)$ in one-dimensional case, since concentration data may be involved besides the pressure data.

5.2 Review of inference regions in nonlinear regression

Consider the nonlinear model

$$Y = \eta(\theta) + Z \tag{33}$$

with Z assumed to have a spherical normal distribution, i.e,

$$\mathbb{E}[Z] = \mathbf{0}, \quad \mathrm{Var}(Z) = \mathbb{E}[ZZ^\top] = \sigma^2\mathbf{I},$$

where $\mathbf{I}$ is the identity matrix with the appropriate dimension. The least squares estimator of θ is the parameter vector, denoted by $\hat{\theta}$, that minimizes the sum of the squares of the residuals, that is,

$$\hat{\theta} = \arg\min(Y - \eta(\theta))^\top(Y - \eta(\theta)) \equiv \arg\min R(\theta)^\top R(\theta). \tag{34}$$

In practice, the estimator $\hat{\theta}$ will not equal θ because of the random errors, Z, in the data. However, due to the fact that $\hat{\theta}$ is a random variable, it may be possible to indicate with some confidence level $1-\beta$ in what region about $\hat{\theta}$ we might reasonably expect θ to be. Such regions are known as $100(1-\beta)\%$ confidence regions. A joint confidence region for all of the parameters is defined using a function

$$CR_\beta : Y \rightarrow \text{ a region in } R^p \tag{35}$$

that satisfies

$$\Pr[\theta \in CR_\beta(Y)] = 1 - \beta. \tag{36}$$

Similarly, a confidence interval for an individual parameter θ_j is defined using a function

$$CI_{j,\beta} : \theta \rightarrow \text{ an interval in } R \tag{37}$$

that satisfies

$$\Pr[\theta_j \in CI_{j,\beta}(Y)] = 1 - \beta. \tag{38}$$

Many methods have been proposed for calculating confidence regions and intervals for parameters estimated by nonlinear least squares. These include the

linearization method, the likelihood method, and the lack-of-fit method, as well as the jackknife and bootstrap methods. Donaldson and Schnabel(DS87) examined three variants of the linearization method, the likelihood method, and the lack-of-fit method. Note that likelihood method confidence regions and intervals have the desirable property that they are constructed from contours of constant likelihood and that the regions and intervals are not affected by re-parameterization of the function η.

Next, we shall review several methods for obtaining joint confidence regions on θ, the parameters of (33) including one exact region (the lack-of-fit region) and two approximate regions (the likelihood ratio and linearized regions) and then decide which method should we select.

5.2.1 Exact regions

Let J be the sensitivity matrix

$$J(\theta) = \left[\frac{\partial \eta_i(\theta)}{\partial \theta_j}\right], \tag{39}$$

where θ_j is the j-th component of θ and $\eta_i(\theta)$ is the i-th component of $\eta(\theta)$, which is $\mathbb{E}[Y|\theta]$.

We assume here that J is full column rank. When J is not full column rank, then, as we will discuss in the section 4.5, singular value decomposition of J will produce a similar result but with a modification of the degrees of freedom of the F statistic.

Define a projection matrix

$$P(\theta) = J(\theta)(J(\theta)^\top J(\theta))^{-1} J(\theta)^\top, \tag{40}$$

which is easily seen to be symmetric idempotent, as is $I - P$. In fact,

$$\begin{aligned}
(P(\theta))^2 &= (J(\theta)(J(\theta)^\top J(\theta))^{-1} J(\theta)^\top)^2 \\
&= J(\theta)(J(\theta)^\top J(\theta))^{-1}(J(\theta)^\top J(\theta))(J(\theta)^\top J(\theta))^{-1} J(\theta)^\top \\
&= J(\theta)(J(\theta)^\top J(\theta))^{-1} J(\theta)^\top = P(\theta), \\
(I - P(\theta))^2 &= I - 2P(\theta) + (P(\theta))^2 = I - 2P(\theta) + P(\theta) = I - P(\theta).
\end{aligned}$$

The following two theorems are useful for the F-test for exact lack-of-fit confidence regions. The proofs can be found in Graybill(Graybill76).

Theorem 5.1 *Let the $n \times 1$ random vector X be distributed $N(x : \mu, I)$. Then the quadratic form $X^\top AX$ has a central chi-square distribution with K degrees of freedom if and only if A is a symmetric idempotent matrix of rank K.*

Theorem 5.2 *Let the $n \times 1$ random vector X be distributed $N(x : \mu, \Sigma)$, where Σ has rank n. If $A\Sigma B = 0$, then the two quadratic forms $X^\top AX$ and $X^\top BX$ are independent.*

If we choose $A = P(\theta), \Sigma = I$, and $B = I - P(\theta)$, then from $(P(\theta))^2 = P(\theta)$, we have $A\Sigma B = 0$. Further, let us choose $X = R/\sigma$, whose covariance matrix turns out to be I. Then it follows from theorems 4.3.1 and 4.3.2 that the quadratic forms

$$Q_1(\theta) = R(\theta)^\top P(\theta) R(\theta)/\sigma^2$$

and

$$Q_2(\theta) = R(\theta)^\top (I - P(\theta)) R(\theta)/\sigma^2$$

are independent chi-square random variables with p and $n - p$ degrees of freedom, respectively. Therefore a $(1 - \beta) \cdot 100\%$ exact confidence region for θ is given by the set Θ:

$$\Theta := \left\{ \dot{\theta} : \frac{Q_1(\dot{\theta})/p}{Q_2(\dot{\theta})/(n-p)} \leq F_\beta(p, n-p) \right\}. \tag{41}$$

5.2.2 Approximate regions

Linearization method. The simplest method for obtaining an approximation confidence region is the linearization method, which assumes that the solution locus is planar and that the coordinate grid is linear throughout the area to be covered by the confidence regions and confidence intervals. Despite the advantage of this method that the resulting confidence regions and confidence intervals are simple and easy to construct, it may produce results very far from the expected nominal coverage.

Likelihood Ratio Method. Besides the simplest linearization method, an approximate region may be constructed by using the likelihood ratio method, which is based on the fact that for large n,

$$\frac{[R(\theta)^\top R(\theta) - R(\hat{\theta})^\top R(\hat{\theta})]/(n-p)}{R(\hat{\theta})^\top R(\hat{\theta})/p} \tag{42}$$

has an approximate F distribution with p and $n-p$ degrees of freedom (see Rao(Rao73), pp.417-419).

5.2.3 What method shall we select?

In this work, we only apply the lack-of-fit method in (41). There are at least two reasons for our choice. First, lack-of-fit method is the only method that can give the exact confidence region which we expect to lead to better result. In particular, as we pointed out before, the linearization method seems not desirable here due to the strong (and even unrealistic) assumptions. Second, in our case, the model is described by partial differential equations and it is usually not possible to obtain the explicit analytical solution. Therefore, it is essentially impossible to write an explicit formula for the operator $\eta(\theta)$. Thus we have to resort to numerical methods for partial differential equations, i.e., the forward models, which often have expensive cost. Hence, we would like to avoid the global optimization problem by computing all possible outputs from all possible realizations of the unknown permeability field, which is the key step in likelihood ratio method. Moreover, if the maximum likelihood set is a submanifold of the parameter space of dimensional greater or equal to 1, as is usually the case in groundwater inverse problem, it would not be possible to adopt likelihood ratio method.

5.3 Confidence region estimation for permeability field with lack-of-fit F-test

In section 4, we have obtained the sensitivity coefficients of pressure and concentration at each grid cell. Only those sensitivity coefficients locating at the producing well are used in computing the lack-of-fit F-statistic.

Suppose that discrete values for permeability are denoted by $T_{kl}, k = 1, \cdots, m_x$, $l = 1, \cdots, m_y$, and, as before, the discrete values for pressure and concentration are defined as $p_{ij}, c_{ij}, i = 1, \cdots, I, j = 1, \cdots, J$. Usually, $m_x \leq I$ and $m_y \leq J$ and in this work, we assume the mesh for T is a (coarser) sub-mesh of the original grid mesh $(x_i, y_j), i = 1, \cdots, I, j = 1, \cdots, J$.

Define

$$
\begin{aligned}
J(T_{kl})^{(c)} &= \left[\frac{\partial \log c_w^{1,\mathrm{cal}}}{\partial T_{kl}}, \cdots, \frac{\partial \log c_w^{N,\mathrm{cal}}}{\partial T_{kl}}\right]^\top = \left[\frac{1}{c_w^{1,\mathrm{cal}}}\frac{\partial c_w^{1,\mathrm{cal}}}{\partial T_{kl}}, \cdots, \frac{1}{c_w^{N,\mathrm{cal}}}\frac{\partial c_w^{N,\mathrm{cal}}}{\partial T_{kl}}\right]^\top, \\
J(T_{kl}) &= \begin{bmatrix} \frac{\partial \log p_w^{\mathrm{cal}}}{\partial T_{kl}} \\ J(T_{kl})^{(c)} \end{bmatrix} = \begin{bmatrix} \frac{1}{p_w^{\mathrm{cal}}}\frac{\partial p_w^{\mathrm{cal}}}{\partial T_{kl}} \\ J(T_{kl})^{(c)} \end{bmatrix}, \\
J(T) &= \left[J(T_{11}), \cdots, J(T_{1,m_y}), \cdots, J(T_{mx,1}), \cdots, J(T_{m_x,m_y})\right], \\
r_p(T) &= \log p_w^{\mathrm{cal}} - \log p_w = \log \frac{p_w^{\mathrm{cal}}}{p_w}, \\
r_c^n(T) &= \log \sqrt{c_w^{n,\mathrm{cal}}(1-c_w^{n,\mathrm{cal}})} - \log \sqrt{c_w^n(1-c_w^n)} = \frac{1}{2}\log \frac{c_w^{n,\mathrm{cal}}(1-c_w^{n,\mathrm{cal}})}{c_w^n(1-c_w^n)}, \forall n, \\
R(T) &= [r_p(T), r_c^1(T), \cdots, r_c^N(T)]^\top, \\
S(T) &= R(T)^\top R(T), \\
P(T) &= J(T)[J(T)^\top J(T)]^{-1} J(T)^\top.
\end{aligned}
$$

We assume here that $r^n(T), \forall k, l$ are normal, iid random variables with mean 0 and variance $\dot{\sigma}^2$.

Based on the fact that

$$Q_1(T) = R(T)^\top P(T) R(T)/\dot{\sigma}^2$$

and

$$Q_2(T) = R(T)^\top (I - P(T)) R(T)/\dot{\sigma}^2$$

are independent chi-squared random variables with $(m_x m_y)$ and $(N + 1 - m_x m_y)$ degrees of freedom, respectively, we have (Donaldson and Schnabel(DS87), Graybill(Graybill76))

$$\frac{Q_1(T)/(m_x m_y)}{Q_2(T)/(N+1-m_x m_y)} = \frac{(N+1-m_x m_y) R(T)^\top P(T) R(T)}{(m_x m_y) R(T)^\top (I - P(T)) R(T)} \tag{43}$$

is distributed as $F_{m_x m_y, N+1-m_x m_y}$ and hence an exact $100(1-\beta)\%$ confidence region (here interval) consists of all values θ such that

$$\frac{R(T)^\top P(T) R(T)}{R(T)^\top (I - P(T)) R(T)} \leq \frac{m_x m_y}{N+1-m_x m_y} F_{m_x m_y, N+1-m_x m_y}(1-\beta). \tag{44}$$

It should be remarked that it may be difficult to save all elements of $R(T)$ in computer memory simultaneously because usually we do not know how big N

ought to be to give acceptable results. In practice, some sophisticated strategy will be adopted (Trangenstein(**?**)). Since $\tilde{\sigma}^2 Q_1(T)$ can be rewritten as

$$Q_1(T) = V(T)W(T)^{-1}V(T)^\top, \quad Q_2(T) = R(T)^\top R(T) - Q_1(T), \tag{45}$$

where

$$V(T) = R(T)^\top J(T), \quad W(T) = J(T)^\top J(T).$$

The procedure for computing $V(T)_{1\times(m_x m_y)}$ and $W(T)_{(m_x m_y)\times(m_x m_y)}$ can be formulated as the following pseudo-FORTRAN routine. Note that in the FORTRAN code, we express $V(T)$ and $W(T)$ as $(1:mx, 1:my)$ and $(1:mx, 1:my, 1:mx, 1:my)$ arrays.

(1) Initialize $R^\top R = 0$;
(2) Set $V(k,l) \leftarrow 0$ and $W(k_1,l_1,k_2,l_2) \leftarrow 0$, for $k, k_1, k_2 = 1, \cdots, m_x$ and $l, l_1, l_2 = 1, \cdots, m_y$;
(3) Solve pressure equation and save the values of the pressure and the velocity field, denoted as p_T and v_T;
(4) Compute pressure residual $r_p \leftarrow p_w^{\rm cal} - p_w^{\rm obs}$ and set $R^\top R \leftarrow R^\top R + r_p$;
(5) Set $V(k,l) \leftarrow V(k,l) + r_p * p_{T,w}(k,l)$, for $k = 1, \cdots, m_x$ and $l = 1, \cdots, m_y$;
(6) Set $W(k_1,l_1,k_2,l_2) \leftarrow W(k_1,l_1,k_1,l_2) + p_{T,w}(k_1,l_1) * p_{T,w}(k_2,l_2)$, for $k_1, k_2 = 1, \cdots, m_x$ and $l_1, l_2 = 1, \cdots, m_y$;
(7) Solve sensitivity equation of pressure and velocity to the sampled permeability field and save the sensitivity coefficients;
(8) Set time $t \leftarrow 0$;
(9) Initialize concentration values and store in array $c(1:I, 1:J)$;
(10) Initialize sensitivity of concentration to permeability and store in array $c_T(1:I, 1:J)$;
(11) Do while $(t < t_{\max})$
  $t \leftarrow t + \Delta t$;
  Solve concentration equation using the concentration values at lower time level and save the value in array $c(1:I, 1:J)$;
  Compute residual $r_c \leftarrow c_w^{\rm cal} - c_w^{\rm obs}(t)$ and set $R^\top R \leftarrow R^\top R + r_c$;
  Solve sensitivity equation of concentration to the permeability field and save the sensitivity coefficients;
  Set $V(k,l) \leftarrow V(k,l) + r_c * c_{T,w}(k,l)$, for $k = 1, \cdots, m_x$ and $l = 1, \cdots, m_y$;
  Set $W(k_1,l_1,k_2,l_2) \leftarrow W(k_1,l_1,k_1,l_2) + c_{T,w}(k_1,l_1) * c_{T,w}(k_2,l_2)$, for $k_1, k_2 = 1, \cdots, m_x$ and $l_1, l_2 = 1, \cdots, m_y$;
(12) End of do while;
(13) Invert W;
(14) $\dot{\sigma}^2 Q_1 \leftarrow V * W^{-1} * V^\top$;
(15) $\dot{\sigma}^2 Q_2 \leftarrow R^\top R - \sigma^2 Q_1$;

(16) The statistic $F = \frac{\dot{\sigma}^2 Q_1(T)/(m_x m_y)}{\dot{\sigma}^2 Q_2(T)/(N+1-m_x m_y)}$.

5.4 What if $J^\top J$ is ill-conditioned or singular?

In inverse processes, the sensitivity coefficients are often zero or not independent so that the matrix $J^\top J$(W in the routine in last subsection) will be ill-conditioned (singular or nearly singular), which makes it difficult to use the theorems in Section 4.3. However, we may adopt the singular value decomposition (SVD) of $J^\top J$ and only invert it "partially" as follows.

First, the symmetric nonnegative definite matrix $J^\top J$ has SVD in the form:

$$J^\top J = VDV^\top, \tag{46}$$

where D is the diagonal matrix with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{m_x^2 m_y^2}$ of $J^\top J$ as the diagonal entries and V is an orthogonal matrix with the eigenvector corresponding to λ_i as the $i-$th column. If $\lambda_1 \geq \cdots \geq \lambda_r \gg 0$ while $\lambda_{m_x^2 m_y^2} \leq \cdots \leq \lambda_{r+1} \approx 0$, then we replace the inverse of $J^\top J$ with

$$V \cdot \mathrm{diag}(\lambda_1^{-1}, \cdots, \lambda_r^{-1}, 0, \cdots, 0) \cdot V^\top. \tag{47}$$

The following theorem guarantees the matrices P and Q after this treatment are still orthogonal projections. To our knowledge, there is no similar treatment in the parameter estimation in groundwater problems yet in the literature.

Theorem 5.3 *For $m \times n$ nonzero matrix J, after the treatment stated in the above remark, the matrix P is still a projection matrix. In other words, there exists a matrix J^*, such that $(J^*)^\top J^*$ is invertible (better conditioned) and*

$$P = J^*((J^*)^\top J^*)^{-1}(J^*)^\top. \tag{48}$$

Proof: Suppose the matrix $J_{m\times n}$ has a singular value decomposition $J_{m\times n} = U_{m\times m} S_{m\times n} V^\top_{n\times n}$, where U and V are orthogonal matrices, and

$$S_{m\times n} = \begin{bmatrix} \Sigma_{r\times r} & 0_{r\times(n-r)} \\ 0_{(m-r)\times r} & 0_{(m-r)\times(n-r)} \end{bmatrix}.$$

where Σ is a diagonal matrix with the diagonal entries the nonzero eigenvalues of S (see, for example, Trangenstein(**?**)). With loss of generality, we assume

the absolute values of the diagonal entries of Σ are in decreasing order. (In fact, we can always modify the order of the diagonal entries of Σ by multiplying a permutation matrix $(P_1)_{m\times m}$ to U from the left and another permutation matrix $(P_2)_{n\times n}$ correspondingly to V from the right and take P_1U as U and VP_2 as V here).

Also assume that

$$S_{m\times n} = \begin{bmatrix} Z_{p\times p} & 0_{r\times(n-p)} \\ 0_{(m-p)\times p} & E_{(m-p)\times(n-p)} \end{bmatrix} \equiv [(S_1)_{m\times p}, (S_2)_{m\times(n-p)}], \tag{49}$$

where the diagonal entries of Z are far from 0 and the diagonal entries of E are 0 or close to 0. Note that $S_1^\top S_2 = 0$. Then

$$J^\top J = V \begin{bmatrix} S_1^\top \\ S_2^\top \end{bmatrix} U^\top U \begin{bmatrix} S_1 & S_2 \end{bmatrix} V^\top = V \begin{bmatrix} S_1^\top S_1 & 0 \\ 0 & S_2^\top S_2 \end{bmatrix} V^\top. \tag{50}$$

In our treatment,

$$\begin{aligned} P &= USV^\top \left(V \begin{bmatrix} (S_1^\top S_1)^{-1} & 0 \\ 0 & 0 \end{bmatrix} V^\top \right) VS^\top U^\top = US \begin{bmatrix} (S_1^\top S_1)^{-1} & 0 \\ 0 & 0 \end{bmatrix} S^\top U^\top \\ &= US_1(S_1^\top S_1)^{-1} S_1^\top U^\top = (US_1)((US_1)^\top (US_1))^{-1}(US_1)^\top \\ &= J^*((J^*)^\top J^*)^{-1}(J^*)^\top, \end{aligned} \tag{51}$$

where

$$J^* = US_1.$$

Thus we have proved that after our treatment, the matrix P is still a projection matrix and hence so is $Q = I - P$. □

Remark 5.4 *"Partial inversion" procedure has several advantages. First, it generalizes the classical results on characterizing uncertainties arising in nonlinear parameter estimation with F lack-of-fit so that some illposed problems can be dealt with as well. Second, by ignoring unimportant "factors", it produces a new projection matrix projecting the output on important "factors", reconciling the analytical one-dimensional case, in which only harmonic average is important. For example, in one-dimensional one-injector and one-producer model, the sensitivity of concentrations with respect the permeability is zero constantly if we fix the injecting rate, that is the concentration data are unimportant in this case.*

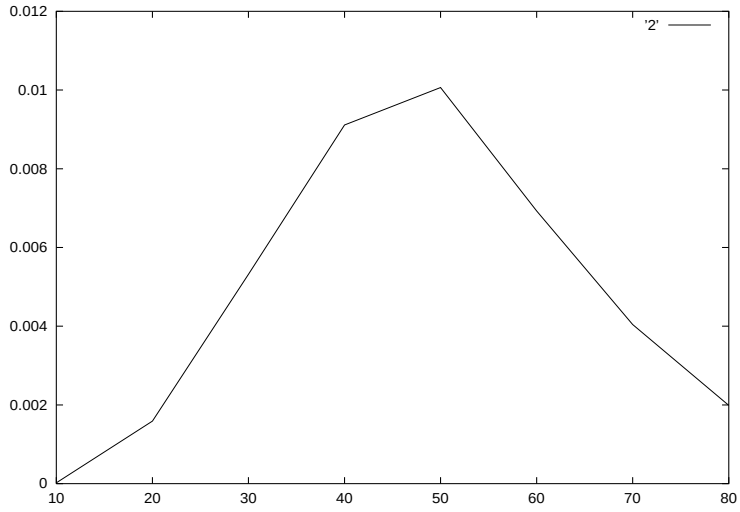

Fig. 2. Profile of tracer concentrations
at the producing well

5.5 Numerical results for lack-of-fit

The concentration data profile at the producer is shown in Figure 2. Since the time lag for different concentration observations is relatively big, our assumption of the independence of concentration at different time is acceptable. The pressure at the producer is seen as 0.00097.

Unfortunately, to our knowledge, it has not been possible to visualize the high-dimensional confidence regions efficiently. We hope further study in computer graphics can shed light on this in the future. However, we can calculate the cdf values of the corresponding F-distribution for some realizations of the permeability field. Some possible permeability field ands the corresponding F-values are shown in Figure 3. The values in each block correspond to the realization of the permeability field. With the cdf values, we can draw conclusions about the confidence levels.

For a constant permeability field, we have shown a picture representing the likelihood of possible realizations and the confidence regions/intervals in Figure 4. Due the nonlinearity of the model, we can see that the confidence regions/intervals may be disjoint.

6 Conclusions, remarks and further study

In this work, we have developed the characterization of uncertainties in estimating the unknown permeability field based on the observations of pressure and concentration at the producing well. Due to lack of data, the problem is

.2393899895E+01	.2671204571E+01		$F(0.8249, 2, 7) = 0.5232.$
.2387692630E+01	.7006188253E+01		
.3111063635E+00	.2086426079E+01		$F(0.1130, 1, 8) = 0.2546.$
.2539489827E+01	.2504055877E+01		
.1013946844E+01	.2127017212E+01		$F(2.2020, 1, 8) = 0.8239.$
.5931052055E-01	.1055052673E+01		
.5386798117E+00	.6050530125E+00		$F(0.5193, 1, 8) = 0.5083.$
.1194135608E+01	.2761065169E+01		
.5113829917E+00	.5429181119E+01		$F(0.0253, 1, 8) = 0.0011.$
.3219212494E+01	.7172266162E+00		
.1027649248E+01	.1190103919E+01		$F(0.0133, 1, 8) = 0.0890.$
.4531196218E+01	.1421775254E+01		
.7516754450E+00	.1373307984E+01		$F(0.0580, 1, 8) = 0.1843.$
.3240046694E+00	.5643336931E+01		
.3221349492E+00	.5147041582E+00		$F(0.0913, 1, 8) = 0.2298.$
.1952786119E+00	.1749958387E+01		
.2086426079E+01	.1055052673E+01	.5386798117E+00	
.2504055877E+01	.1013946844E+01	.1194135608E+01	$F(2.0425e-04, 1, 8) = 0.0111.$
.3111063635E+00	.5931052055E-01	.2127017212E+01	
.6158561309E+00	.2383077391E+00	.1093151823E+01	
.6050530125E+00	.1855643055E+01	.3357232178E+00	$F(0.0879, 1, 8) = 0.2256.$
.2761065169E+01	.6615927652E+00	.3112003655E+01	
.3219212494E+01	.5429181119E+01	.1421775254E+01	
.6887050120E+00	.7172266162E+00	.1027649248E+01	$F(0.0011, 1, 8) = 0.0257.$
.3048397020E+00	.5113829917E+00	.4531196218E+01	
.7297854614E+00	.1610627993E+01	.5011987122E+00	
.4046235019E+00	.1931860854E+00	.7376256845E+00	$F(0.2210, 1, 8) = 0.3492.$
.9977806328E+00	.8197411953E+00	.1246337934E+01	
.2403977954E+01	.3111063635E+00	.2086426079E+01	
.4236138744E+00	.2539489827E+01	.2504055877E+01	$F(0.0876, 1, 8) = 0.2252.$
.1013946844E+01	.2127017212E+01	.5386798117E+00	
.5931052055E-01	.1055052673E+01	.1194135608E+01	$F(1.2347, 1, 8) = 0.7012.$
.6051909922E+01	.1172397739E+01	.9526627004E+00	
.4151448315E+01	.5925907251E+00	.5403163559E+00	$F(0.0601, 1, 8) = 0.1875.$

Fig. 3. The realizations of the unknown permeability field and the corresponding F values.

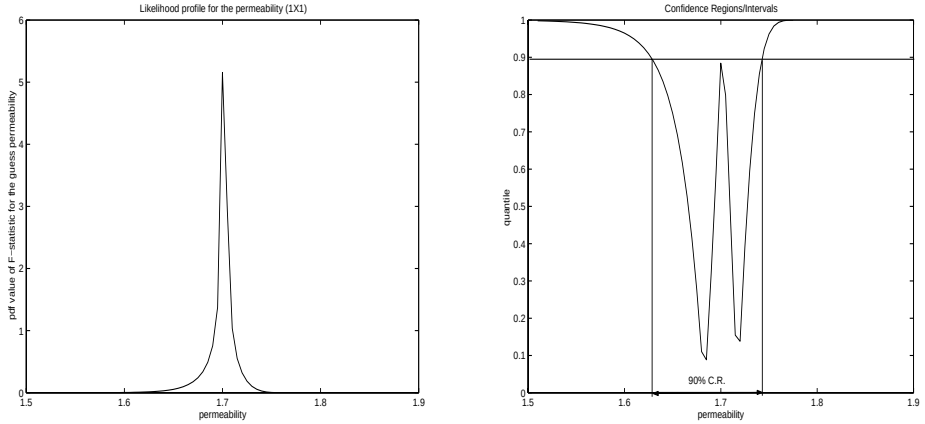

Fig. 4. Results for constant permeability model: the left is the likelihood profile of the permeability, whose level sets correspond to highest likelihood confidence region; the right shows the equi-tailed confidence regions, which may be disjoint.

highly ill-posed. Even in the one dimensional case, we have seen that usually all points in a certain sub-manifold have maximum likelihood. This makes it impossible to "reconstruct" the field (even approximately). However, it is possible to characterizing the uncertainties by calculating some statistics of the field. With mixed finite element and second order donor cell methods for pressure and concentration equations respectively, we have computed the output of possible realizations of the unknown permeability field and the sensitivity matrix of the output against the realization, then by assuming that the error have i.i.d. log-normal distribution and based on the classical theory of lack-of-fit in nonlinear regression, we have obtained the F-statistic of possible realizations. The F-statistic leads to conclusions about the confidence levels of a given realization. To our knowledge, we are the first to have noticed the flexibility of F-test with SVD.

Our method has some advantages. First, although we have only considered the two-dimensional problem with a single injector and a single producer, the procedure can be generalized to three-dimensional cases with possibly more wells. Next, one can see that the result we have obtained is consistent with the known result in the one-dimensional case, which tells us that the harmonic average of the unknown permeability field is the only key statistic when estimating the permeability given the well observations. This contrasts with some results arguing "reconstructing" the field based on limited data. Third, beyond the fact that it provides the seemingly only exact confidence regions, the lack-of-fit method that we selected is flexible to deal with the highly ill-posed problem here. With the singular value decomposition of the sensitivity matrix, a very small number of independent statistics of the permeability field are kept, even if they are not in an explicit form. This, as mentioned before, reconciles the analytical theory in one-dimensional problem. Fourth, the evaluation of the F-statistic for a given realization is straightforward in the sense that it does not depend upon other realizations. This differs from the popular Monte Carlo methods, in which *many* samples have to be applied to the model to obtain the *approximate* pdf or cdf, i.e., the inference of a single realization relies upon the statistic(s) of large number of samples which is(are) expected to be close to the true statistic(s) of the parameters. Finally, we would like to mention that this method can be applied in a Bayesian scenario as well if we are given prior knowledge about the field.

On the other hand, there are disadvantages in our methods. For example, it may be hard to determine the exact number degrees of of freedom based on eigenvalues of the sensitivity matrix as a consequence of possible improper scaling of the quantities. Also, it is hard to visualize the usually high-dimensional F function and hence the confidence regions. Moreover, the improper assumption of the error structure may lead to unreasonable F-values (e.g., very big numbers). Although this may be avoided by modifying the degrees of freedom appropriately, this undermines the efficiency of the method.

Finally, there are some open problems that need to be studied more intensively. First, are there any explicit key statistics in high-dimensional cases? Or at least are there approximate ones reconciling known perturbation results and the conclusion in this thesis? Second, it there an efficient way to visualize high-dimensional functions or regions? Third, could the result from MCMC (LHBFW02) be combined with the lack-of-fit result we have obtained here to obtain a "posterior" F-test lack-of-fit method? Finally, we also noticed that our choice of degree of freedoms in "lack-of-fit" is more or less subjective. A more reasonable way would be to treat the degrees of freedom as a smooth function of the parameters instead of only discrete integers. The interesting idea of Buja *et al* (BHT96; Breiman96) could shed light in this direction.

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