Galerkin Finite Element Solution of Free-Boundary Groundwater Contaminant Model

by

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OUTLINE

1. Introduce free-boundary Groundwater Model tracking Contaminant Dynamics in Groundwater flowing through fissures (cracks) in rock matrix via schematic diagram.

2. Present coupled PDE (Partial Differential Equation) representing model.

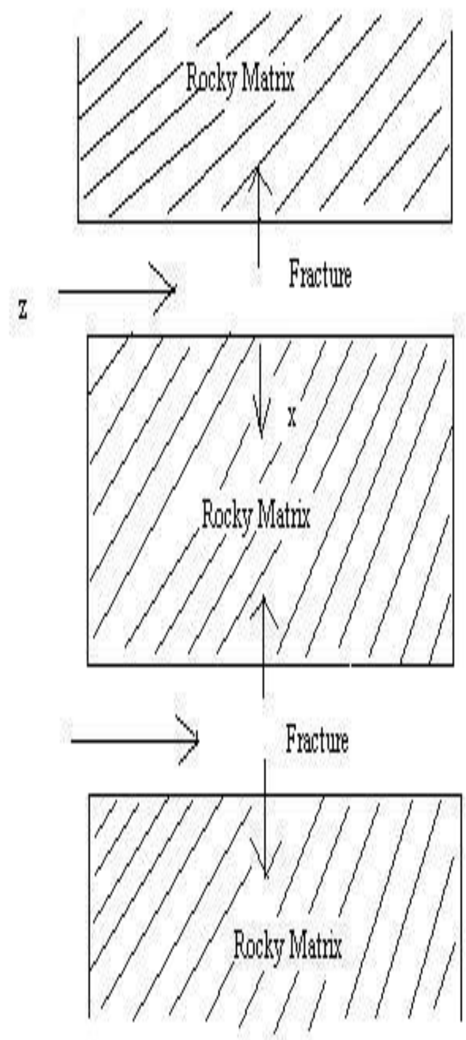
3. Describe terms and parameters in PDE model.

4. Describe Galerkin finite element method to numerically estimate model solution.

5. Present graphical illustrations.

6. Discuss advantages of using OSCER Condor Pool and OSCER Sooner Supercomputing Facilities in obtaining numerical results, computationally.

SCHEMATIC DIAGRAM



PDE MODEL

$$\begin{cases} \partial_t C + \alpha^* \partial_z C = \beta^* \partial_z^2 C - \lambda^* C + I_R^* \Gamma(z) \\ \partial_t M = \gamma^* \left[\partial_x^2 + \partial_z^2 \right] M - \lambda^* M + A_R^* \mathrm{C}\, \Gamma(x) \\ C(0, z) = C^0(z) \\ M(0, x, z) = M^0(x, z) \end{cases}$$

where

$$(t, x, z) \in [0, T_{max}] \times [0, x_{max}] \times [0, z_{max}].$$

PARAMETERS

$$\alpha^* = \frac{v}{1 + K_F/b}$$

$$\beta^* = \frac{D_W + \alpha_L v}{R_F}$$

$$\gamma^* = \frac{\theta D_W}{1 + \rho_b K_M/\theta}$$

Let

$$T = \frac{t}{T_{max}},\ X = \frac{x}{x_{max}},\ Z = \frac{z}{z_{max}}$$

to get

$$\begin{cases} \kappa_1 \partial_T C + \kappa_2 \alpha^* \partial_Z C = \kappa_2^2 \beta^* \partial_z^2 C - \lambda^* C + I_R^* \Gamma(Z) \\ \kappa_1 \partial_t M = \gamma^* \left[\kappa_3^2 \partial_x^2 + \kappa_2^2 \partial_z^2 \right] M - \lambda^* M + A_R^* \mathrm{C}\, \Gamma(X) \\ C(0, Z) = C^0(Z) \\ M(0, X, Z) = M^0(X, Z) \end{cases}$$

where

$$\kappa_1 = \frac{1}{T_{max}},\ \kappa_2 = \frac{1}{z_{max}}, \kappa_3 = \frac{1}{x_{max}}$$

and

$$(t, x, z) \in [0,\ 1]^3.$$

FINITE ELEMENT METHOD

Define weak solution as follows:

$$\begin{cases} \langle \kappa_1 \partial_T C + \kappa_2 \alpha^* \partial_Z C = \kappa_2^2 \beta^* \partial_z^2 C - \lambda^* C + I_R^* \Gamma(Z), \phi \rangle \\ \langle \kappa_1 \partial_t M = \gamma^* \left[\kappa_3^2 \partial_x^2 + \kappa_2^2 \partial_z^2 \right] M - \lambda^* M + A_R^* \mathrm{C}\, \Gamma(X),\ \psi \rangle \end{cases}$$

together with initial conditions

$$\begin{cases} C(0, Z) = C^0(Z) \\ M(0, X, Z) = M^0(X, Z) \end{cases}$$

where

ϕ piece-wise differentiable on $[0,\ 1]$

and

ψ piece-wise differentiable on $[0,\ 1]^2$

NON-UNIFORM FINITE ELEMENT GRID

$$Z_0 = 0,\ Z_1 = \omega_Z$$

$$Z_j = Z_{j-1} + \rho_Z\left(Z_{j-1} - Z_{j-2}\right) \ \text{ for } \ j = 2, \cdots, ZDIM$$

and

$$X_0 = 0,\ X_1 = \omega_X$$

$$X_i = X_{i-1} + \rho_X(X_{i-1} - X_{i-2}) \ \text{ for } \ i = 2, \cdots, XDIM$$

FINITE ELEMENT APPROXIMATION

$$C(T,\ Z) = \sum_{i=0}^{ZDIM} \alpha_i(T)\, \varphi_i(Z)$$

and

$$M(T,\ X,\ Z) = \sum_{i=0}^{ZDIM} \sum_{j=0}^{XDIM} \beta_{ij}(T) \varphi_i(Z) \omega_j(X)$$

where $\{\varphi_i\}_{i=0}^{ZDIM}$ and $\{\omega_j\}_{j=0}^{XDIM}$ represent linear spline functions acting as approximating elements on $[0,\ 1]$.

COMPUTATIONAL PROBLEM

$$\begin{cases} (\dot{\vec{\alpha}}) = F(T,\ \vec{\alpha}) \\ \vec{\alpha}(0) = \overrightarrow{(\alpha_0)} \end{cases}$$

and

$$\begin{cases} (\dot{\vec{\beta}}) = G(T,\ \vec{\beta}) \\ \vec{\beta}(0) = \overrightarrow{(\beta_0)} \end{cases}$$

Solved using *CVODE* from SUNDIALS from Lawrence Livermore National Laboratories (LLNL) with following values:

T_{max}	x_{max}	z_{max}	$XDIM$	$ZDIM$
1, 2, 3, months	10 meters	10 meters	14	14

ρ_X	ρ_Z	ω_X	ω_Z
0.95	0.95	0.1	0.1

GRAPHICAL ILLUSTRATIONS

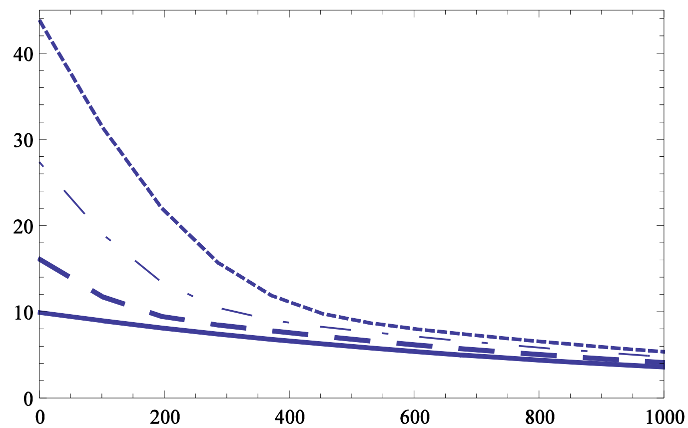


Figure 1: z versus C with no decay

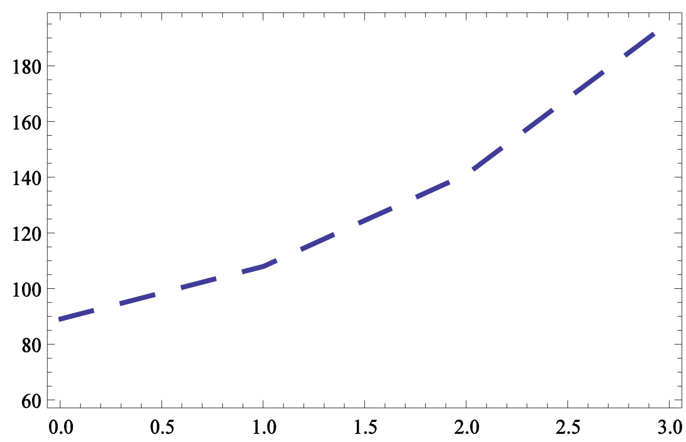


Figure 2: t versus Total C - no decay

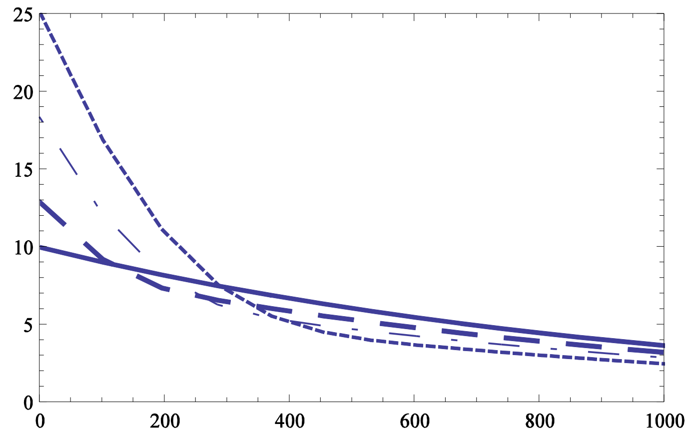


Figure 3: z versus C with decay

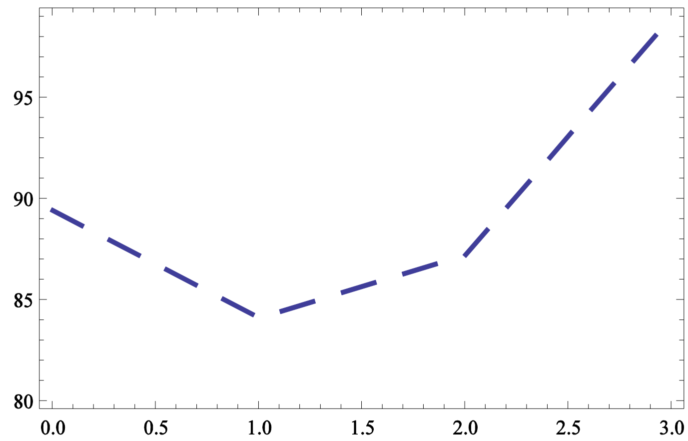


Figure 4: t versus Total C with decay

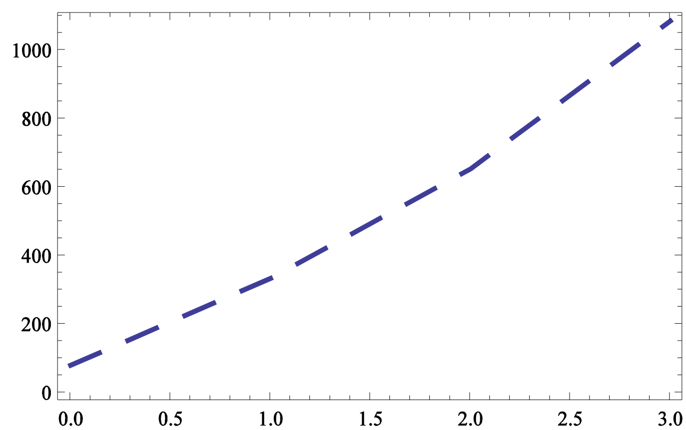


Figure 5: t versus total M with no decay

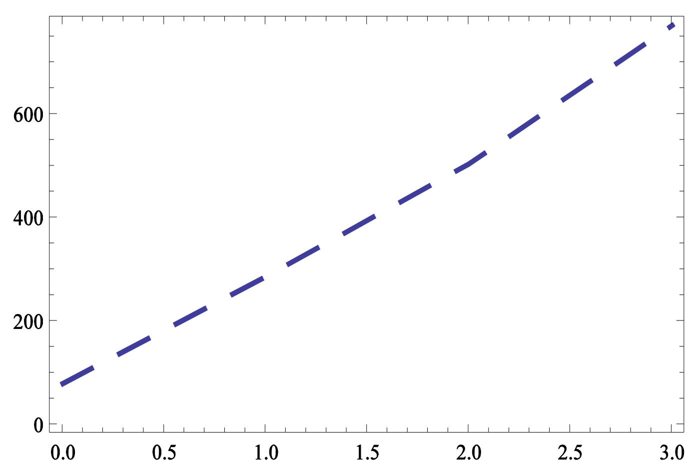


Figure 6: t versus total M with decay

COMPARISON OF COMPUTATION TIME

ECU UNIX	OSCER CONDOR	OSCER SOONER
5 min	2 sec	2 sec
10 hours	3 hours	32 min

SUPERCOMPUTING IS AMAZING!!

REFERENCES

[1] E. A. Sudicky & E. O. Frind, *Contaminant Transport in Fractured Porous Media: Analytic Solutions For a System of Parallel Fractures*, Water Resources Research **18(6)**, 1982.

[2] R. L. Drake & J. Chen, *Contaminant Transport in Parallel Fractured Media: Sudicky and Frind Revisited,* Submitted for Publication, 2003.

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