



**Galerkin Finite Element Solution  
of  
Free-Boundary  
Groundwater Contaminant Model**

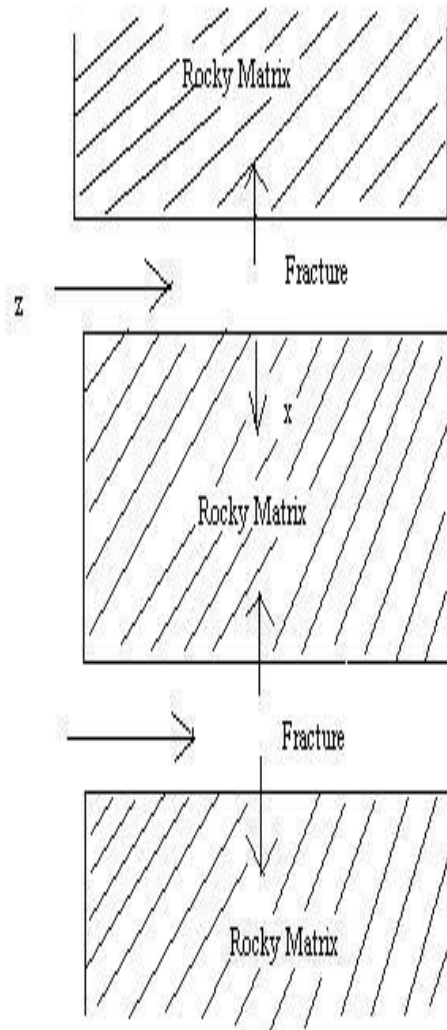
**by**

**Robert Ferdinand  
East Central University, Ada, OK  
[rferdand@ecok.edu](mailto:rferdand@ecok.edu)**

## 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

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

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

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

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:

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

together with initial conditions

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

where

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

and

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

## **NON-UNIFORM FINITE ELEMENT GRID**

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

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

and

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

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

## **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**

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

and

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

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

$\rho_x$	$\rho_z$	$\omega_x$	$\omega_z$
0.95	0.95	0.1	0.1



# GRAPHICAL ILLUSTRATIONS

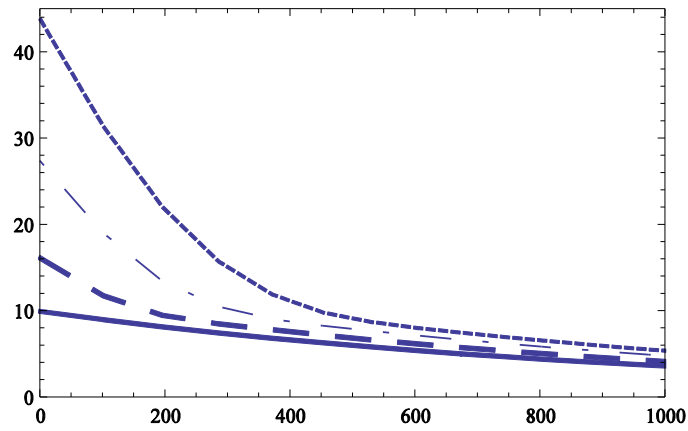


Figure 1: z versus C with no decay

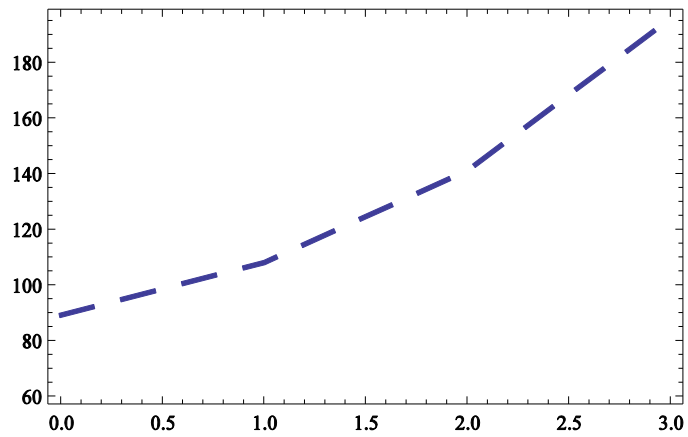


Figure 2: t versus Total C - no decay

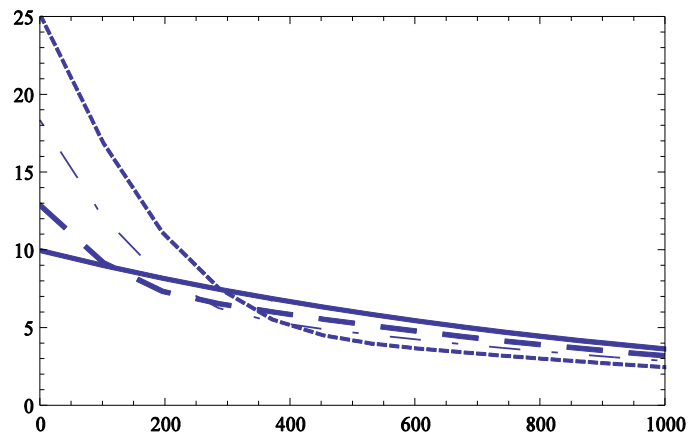


Figure 3: z versus C with decay

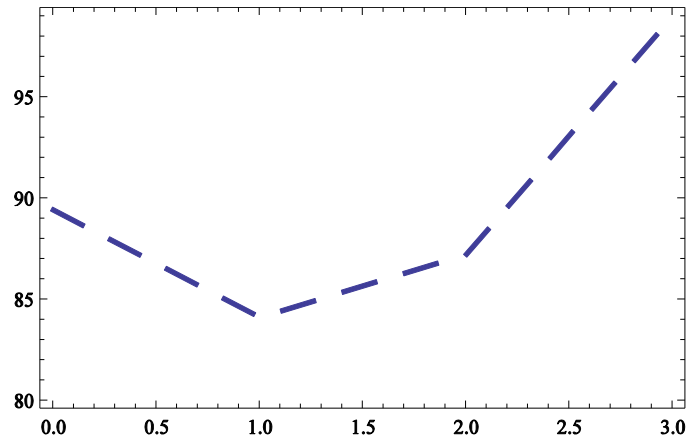


Figure 4: t versus Total C with decay

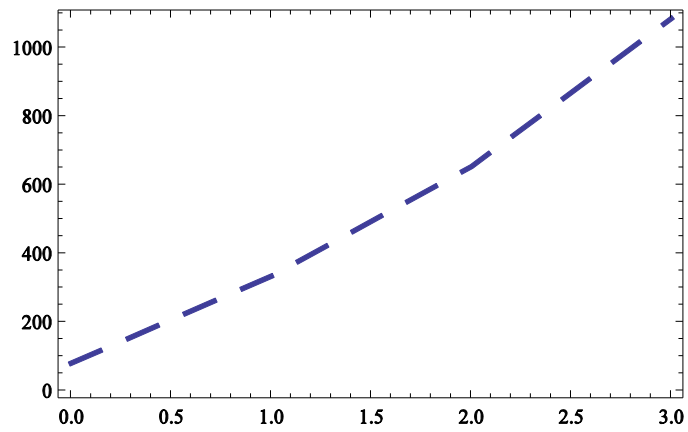


Figure 5: t versus total M with no decay

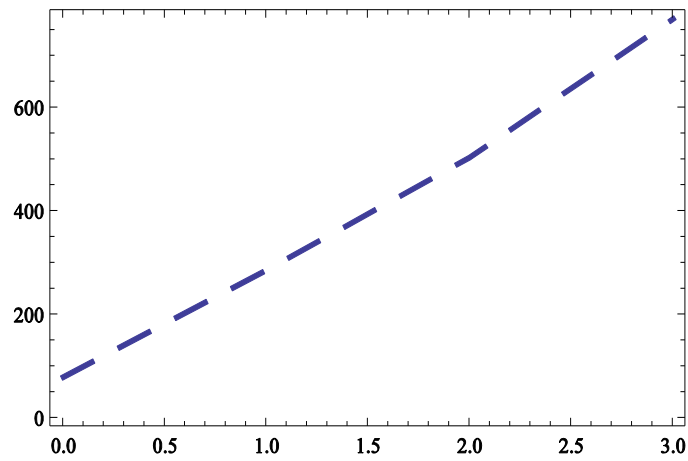


Figure 6: t versus total M with decay

## **COMPARISON OF COMPUTATION TIME**

<b>ECU UNIX</b>	<b>OSCER CONDOR</b>	<b>OSCER SOONER</b>
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.

## **ACKNOWLEDGMENTS**

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