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YUCCA MOUNTAIN PROJECT

U.S. Department of Energy
Office of Civilian Radioactive Waste Management

Diffusive Conductance for Bifurcation of Diffusive Flux From a Single Continuum to a Dual Continuum

Presented to:
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TSPA Model Design/Analysis
Performance Assessment Strategy and Scope

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Outline

- Conceptual model of single to dual continuum diffusive transport
- Calculation of effective diffusive conductance
- Approximation by an interface cell
- GoldSim model using effective diffusive conductances (exact)
- GoldSim model using interface cell (approximate)
- Calculation comparison of exact versus approximate treatment of diffusive flux

Conceptual Model

- Engineered Barrier System in the Total System Performance Analysis for License Application (TSPA-LA) for the Yucca Mountain Project
- Bifurcation of diffusive flux occurs between the single continuum invert cell and the dual continuum (fracture/matrix) unsaturated zone (UZ) cells

Diffusion Parameters

Determination of diffusive flux transport between cells requires

- A = diffusive area of cell
- L = diffusive length of cell
- D = effective diffusivity of cell
- Θ = water content of cell

Note diffusive area is assigned as a cell property to better describe domain geometry

Diffusive Conductance

Diffusive flux between two cells (single continuum case) is the diffusive conductance times the concentration difference between cells

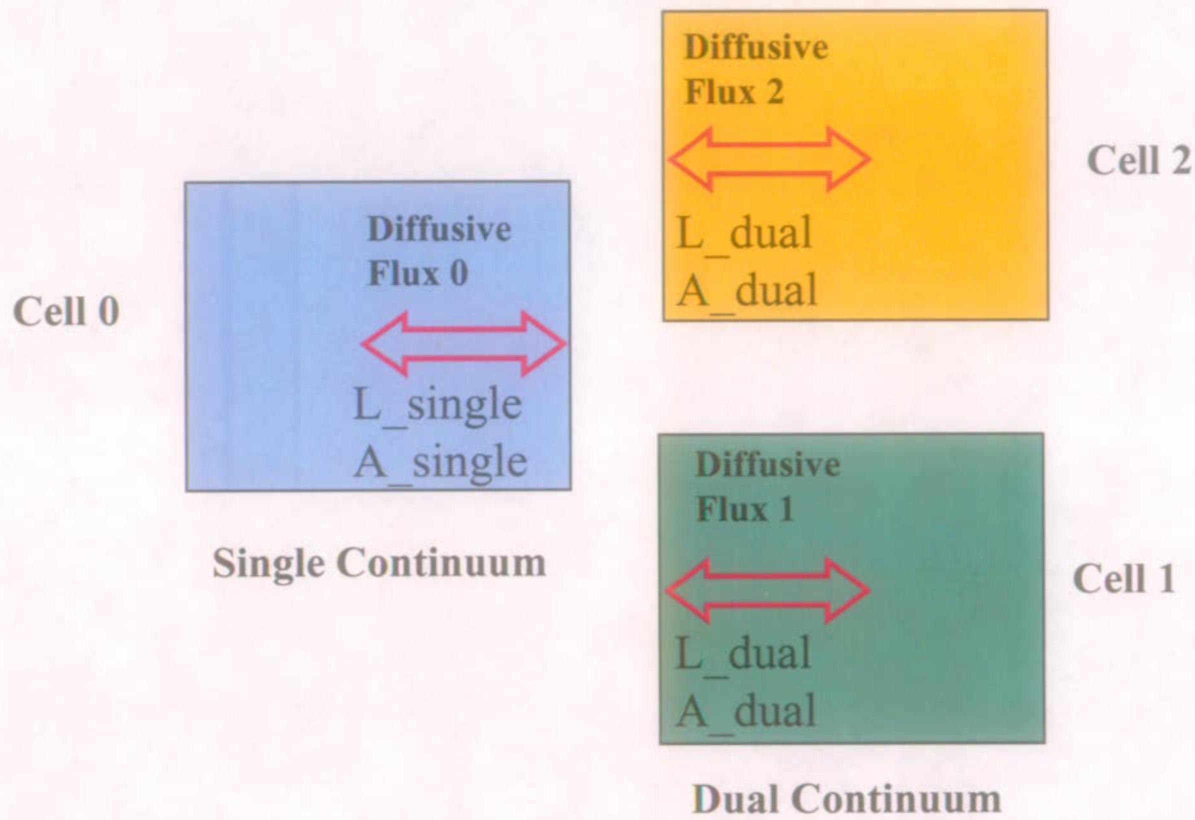
$$\text{Diffusive Flux} = - D_c(c_2 - c_1)$$

Determination of Diffusive Conductance

- The diffusive conductance between cells is determined by imposing flux continuity at the cell interface and results in the harmonic average of $\theta AD/2L$ or

$$D_c = \frac{1}{\dfrac{L_1}{\theta_1 D_1 A_1} + \dfrac{L_2}{\theta_2 D_2 A_2}}$$

Continuity of Diffusive Flux for Transport from Single to Dual Continua



Diffusive Flux 0 = Diffusive Flux 1 + Diffusive Flux 2

Exact or Pseudo-Flux Method for Single Cell to Dual Cell Transport

$$F_1 = D_{c\_0/1}\left(c_0 - c_1\right) + D_{c\_1/2}\left(c_2 - c_1\right)$$

$$F_2 = D_{c\_0/2}\left(c_0 - c_2\right) - D_{c\_1/2}\left(c_2 - c_1\right)$$

The second term in these expressions appears to be a diffusive flux between cells 1 and 2, but is a pseudo-flux arising from the dependence of the diffusive fluxes on all three concentrations. Transport from cell 0 to cells 1 and cell 2 requires defining three diffusive conductances

Diffusive Conductance Between Cell_0 and Cell_1 and Cell_0 and Cell_2

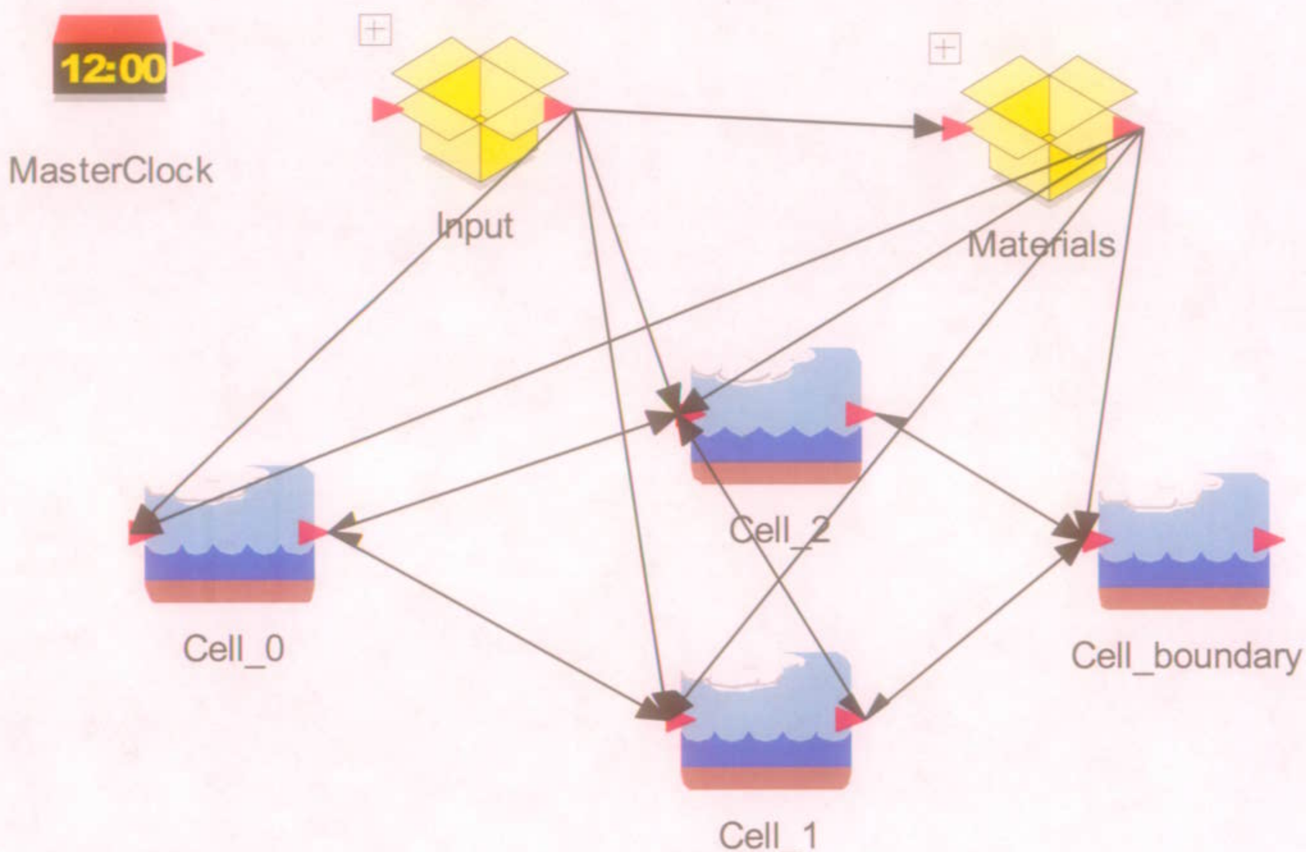
$$D_{c\_0/1} = \frac{1}{\dfrac{L_{single}}{\theta_0 D_0 A_{single}\left[\dfrac{\theta_1 D_1}{\theta_1 D_1 + \theta_2 D_2}\right]} + \dfrac{L_{dual}}{\theta_1 D_1 A_{dual}}}$$

$$D_{c\_0/2} = \frac{1}{\dfrac{L_{single}}{\theta_0 D_0 A_{single}\left[\dfrac{\theta_2 D_2}{\theta_1 D_1 + \theta_2 D_2}\right]} + \dfrac{L_{dual}}{\theta_2 D_2 A_{dual}}}$$

Pseudo Diffusive Conductance Between Cell_1 and Cell_2

$$D_{c\_1/2} = \frac{1}{\dfrac{L_{dual}}{\theta_1 D_1 A_{dual}\left[\dfrac{\theta_2 D_2 A_{dual} L_{single}}{\theta_2 D_2 A_{dual} L_{single} + \theta_0 D_0 A_{single} L_{dual}}\right]} + \dfrac{L_{dual}}{\theta_2 D_2 A_{dual}}}$$

Diffusion Bifurcates from Single Continuum, Cell_0, to Dual Continuum Represented by Cell_1 and Cell_2

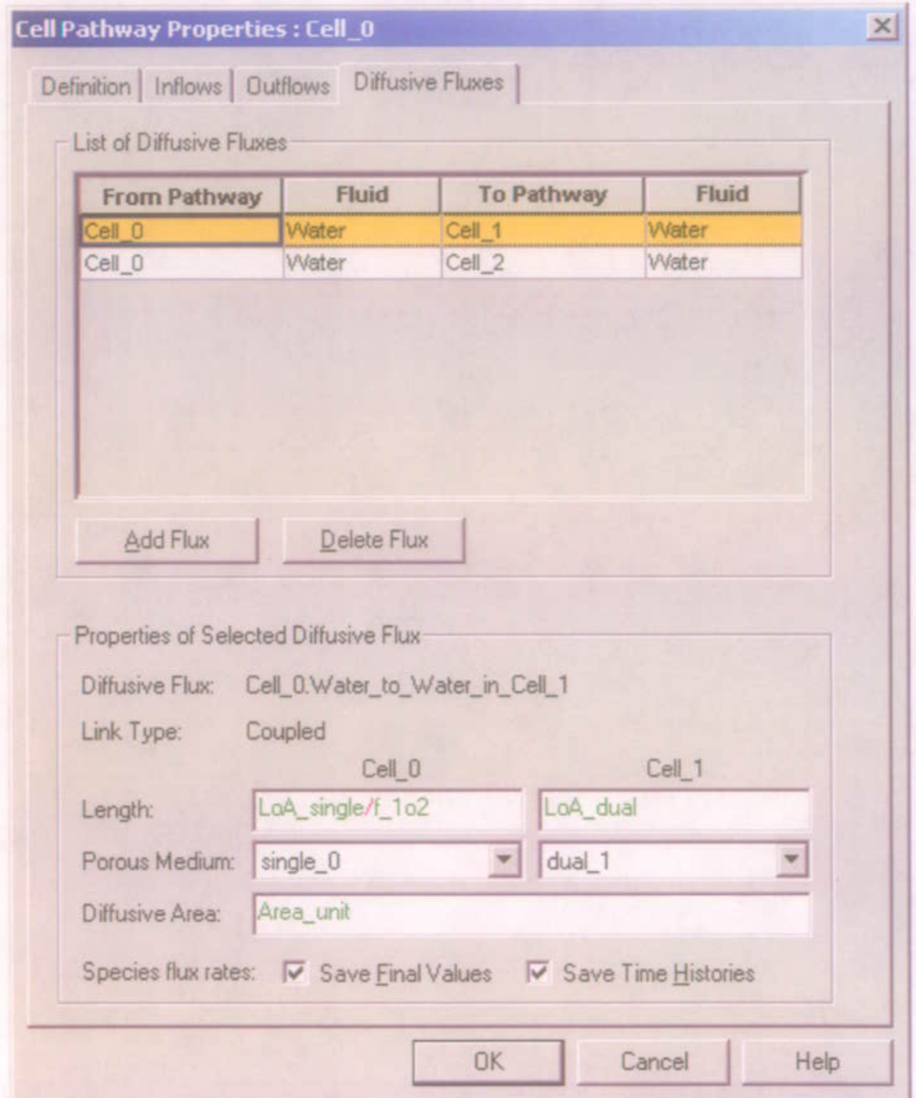


This model has only diffusive transport. 1 gm solute is released at time 0 in cell_0. Boundary condition at Cell_boundary is zero concentration

Assignment of Diffusive Flux Links in GoldSim

Diffusive Flux tab on the Cell pathway editing dialog requires:

- For both cells
  1) Diffusive Flux Length
  2) Porous Medium
- Interface Diffusive Area



Exact or Pseudo-Flux Method

Assignment of Diffusive Lengths and Area, Cell_0 to Cell_1

$$D_{c\_0/1} = \frac{1}{\dfrac{L_{single}}{\theta_0 D_0 A_{single}\left[\dfrac{\theta_1 D_1}{\theta_1 D_1 + \theta_2 D_2}\right]} + \dfrac{L_{dual}}{\theta_1 D_1 A_{dual}}}$$

$$Length(Cell\_0) = \frac{L_{single}}{A_{single}\left[\dfrac{\theta_1 D_1}{\theta_1 D_1 + \theta_2 D_2}\right]}$$

$$Length(Cell\_1) = \frac{L_{dual}}{A_{dual}}$$

$$Diffusive\_Area = 1$$

Exact or Pseudo-Flux Method
Assignment of Medium Properties

$$Porosity(Cell\_0) = \theta_0$$
$$Porosity(Cell\_1) = \theta_1$$
$$Porosity(Cell\_2) = \theta_2$$

$$tortuosity(Cell\_0) = \frac{D_0}{D_{free\_water}}$$
$$tortuosity(Cell\_1) = \frac{D_1}{D_{free\_water}}$$
$$tortuosity(Cell\_2) = \frac{D_2}{D_{free\_water}}$$

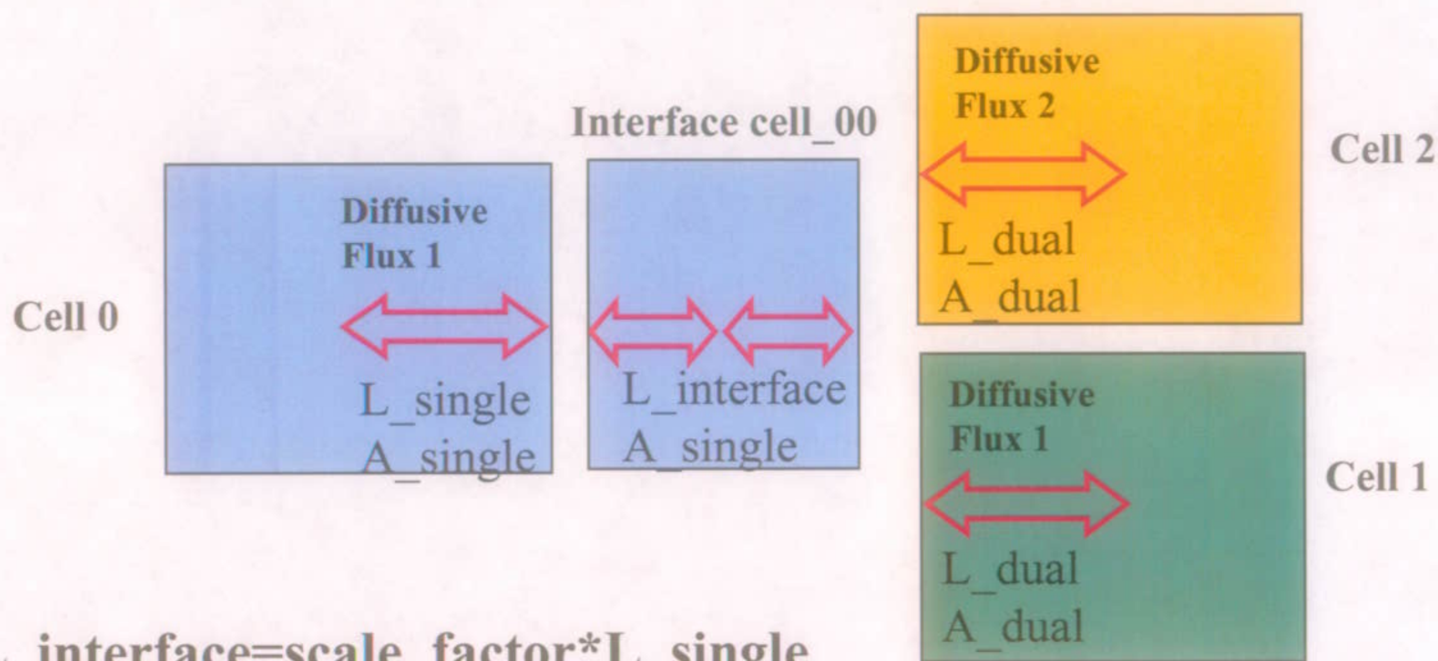
Approximate or Interface Cell Method

- Exact pseudo-flux method requires a non-physical diffusive flux link between the two dual continuum cells (Cells 1 and 2). This could be confused in the model with the physically-based matrix diffusion link.
- An alternative to the nonphysical pseudo-flux method is to use an additional cell at the interface between Cell 0 and Cells 1 and 2, which allows GoldSim to solve for the interface concentration, instead of having to *a priori* solve for the interface concentration.

Approximate or Interface Cell Method
(continued)

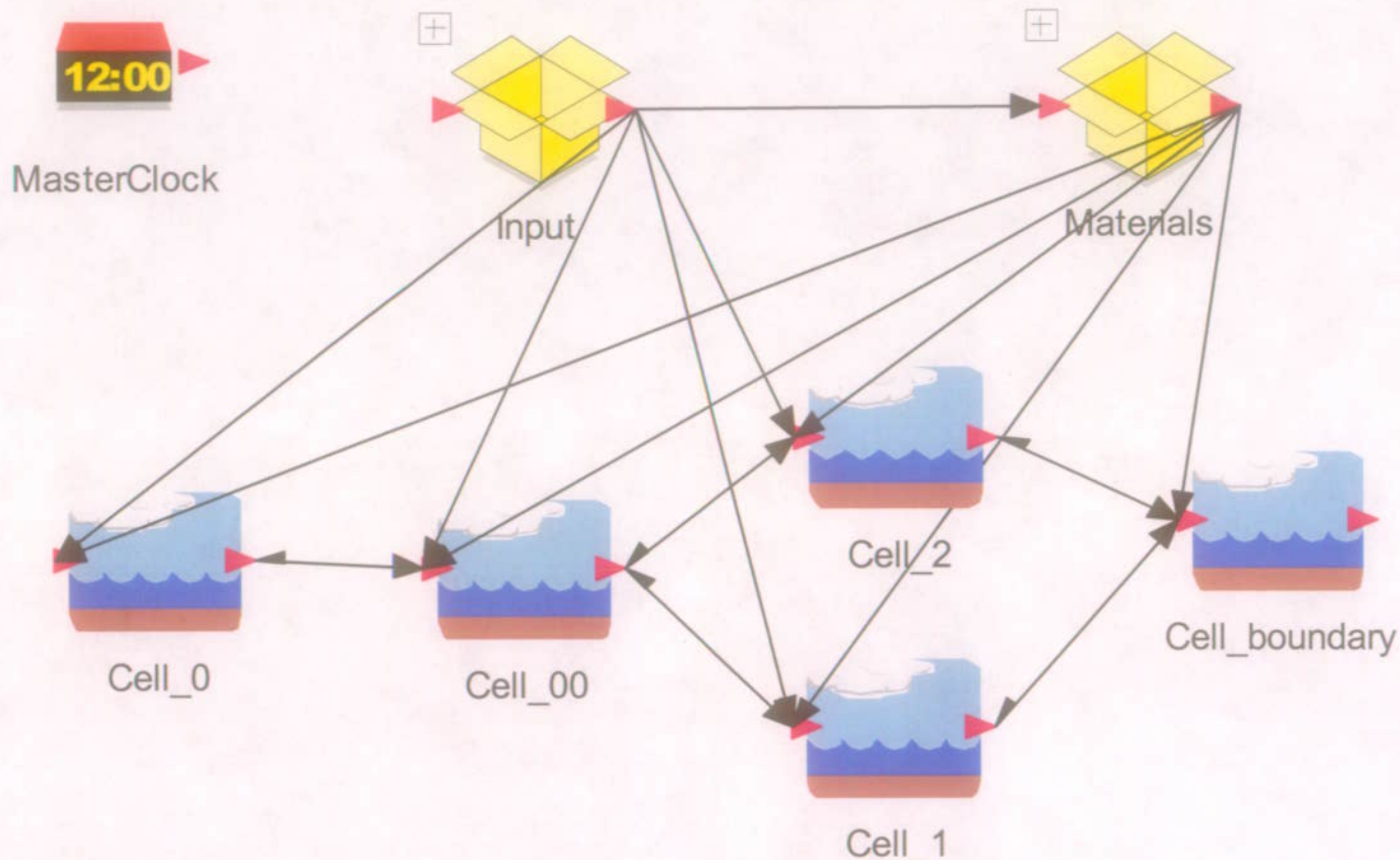
- An interface cell representing a thin slice of the single continuum cell at the interface location can approximate the exact diffusive fluxes by effectively decoupling concentrations and properties in the two dual continuum cells
- This is useful because the approximate interface concentration is sufficient to calculate the diffusive fluxes from the interface cell to the dual continuum cells using only two diffusive conductances, which avoids the nonphysical pseudo-flux term and its associated diffusive conductance

Introduce Interface Cell



L_interface=scale_factor*L_single

Diffusion Bifurcates from Single Continuum Interface Cell_00, to Dual Continuum, Cell_1 and Cell_2



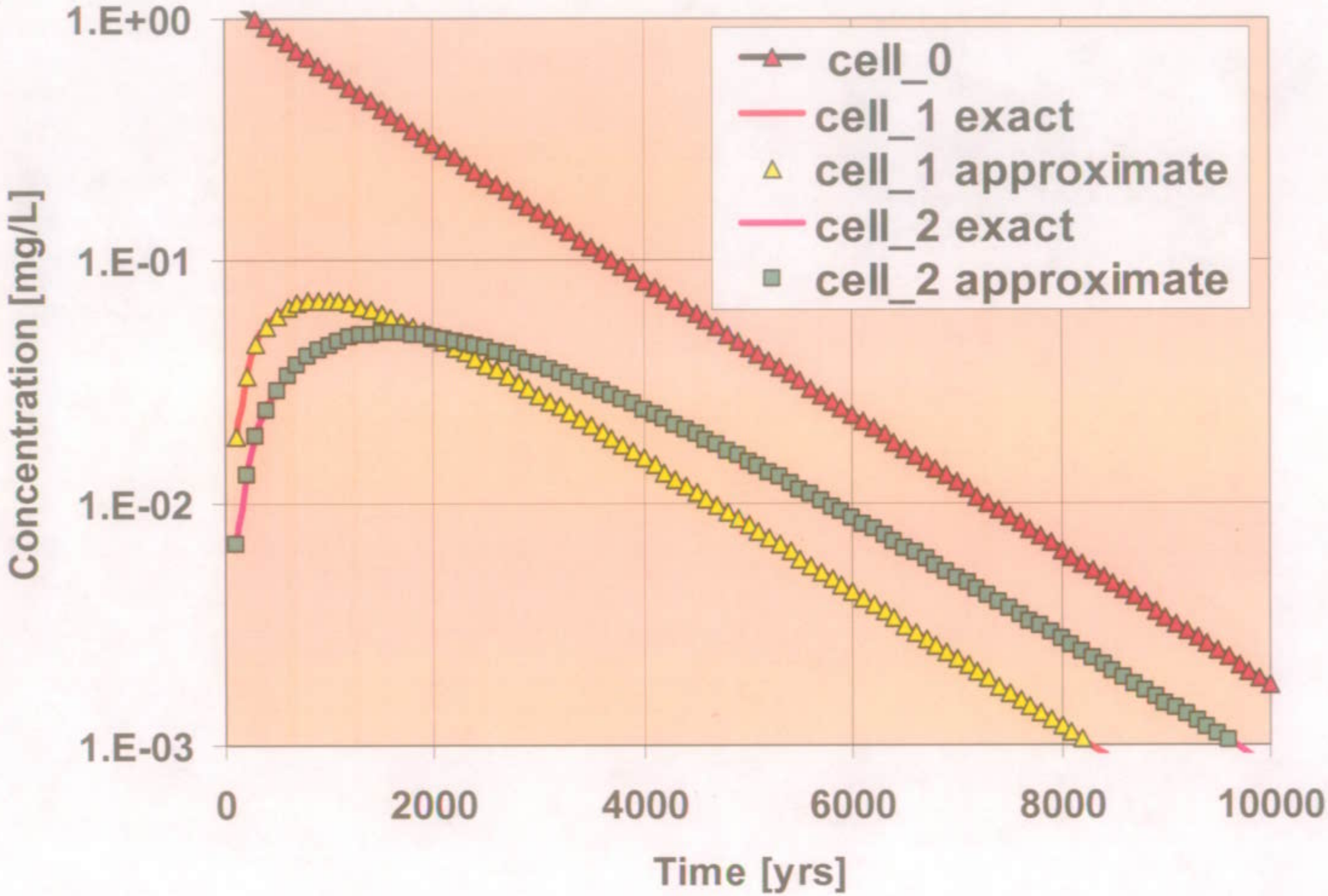
This model has only diffusive transport. 1 gm of solute is released at time 0 in Cell_0. Boundary condition at Cell_boundary is zero concentration

Interface Cell Method
Diffusive Conductances Cell_0 to Cell_1 and Cell_0 to Cell_2

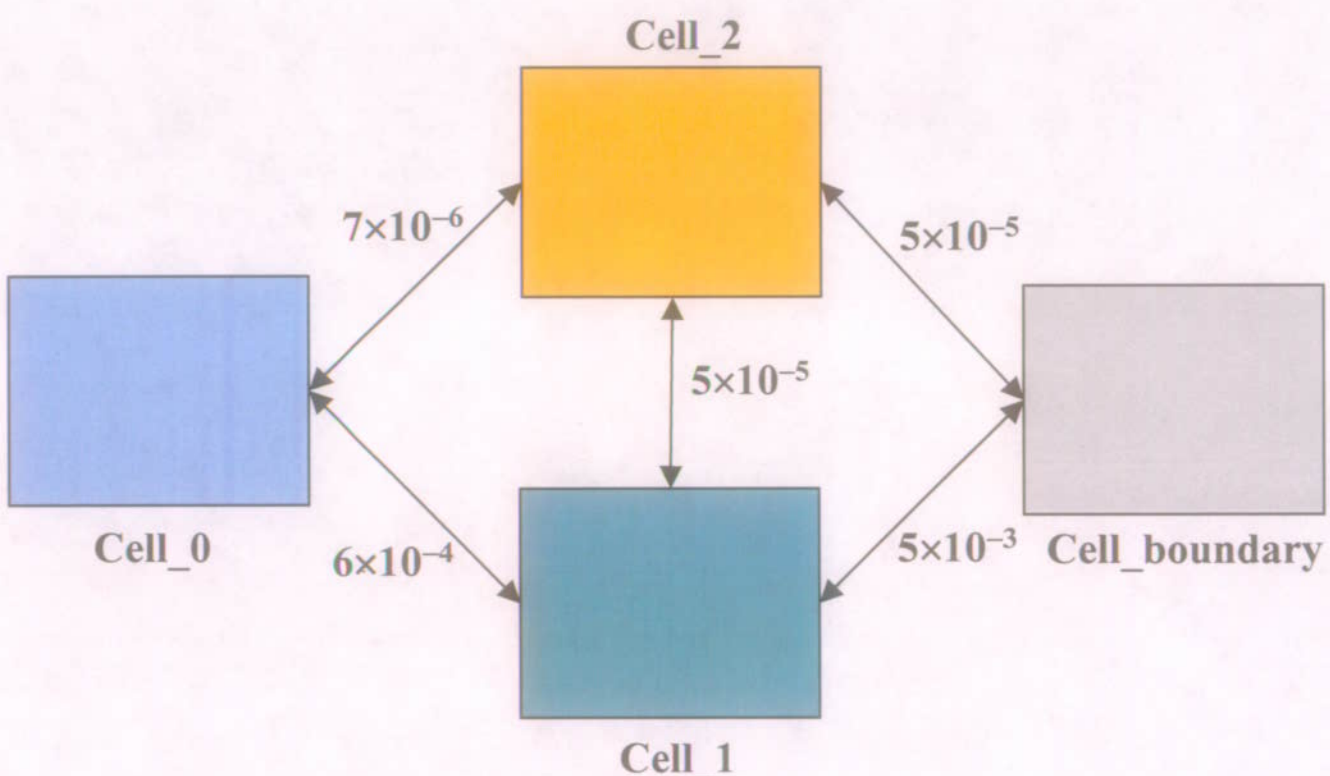
$$D_{c\_0/1} = \frac{1}{\dfrac{L_{single}}{\theta_0 D_0 A_{single}} + \dfrac{L_{dual}}{\theta_1 D_1 A_{dual}}}$$

$$D_{c\_0/2} = \frac{1}{\dfrac{L_{single}}{\theta_0 D_0 A_{single}} + \dfrac{L_{dual}}{\theta_2 D_2 A_{dual}}}$$

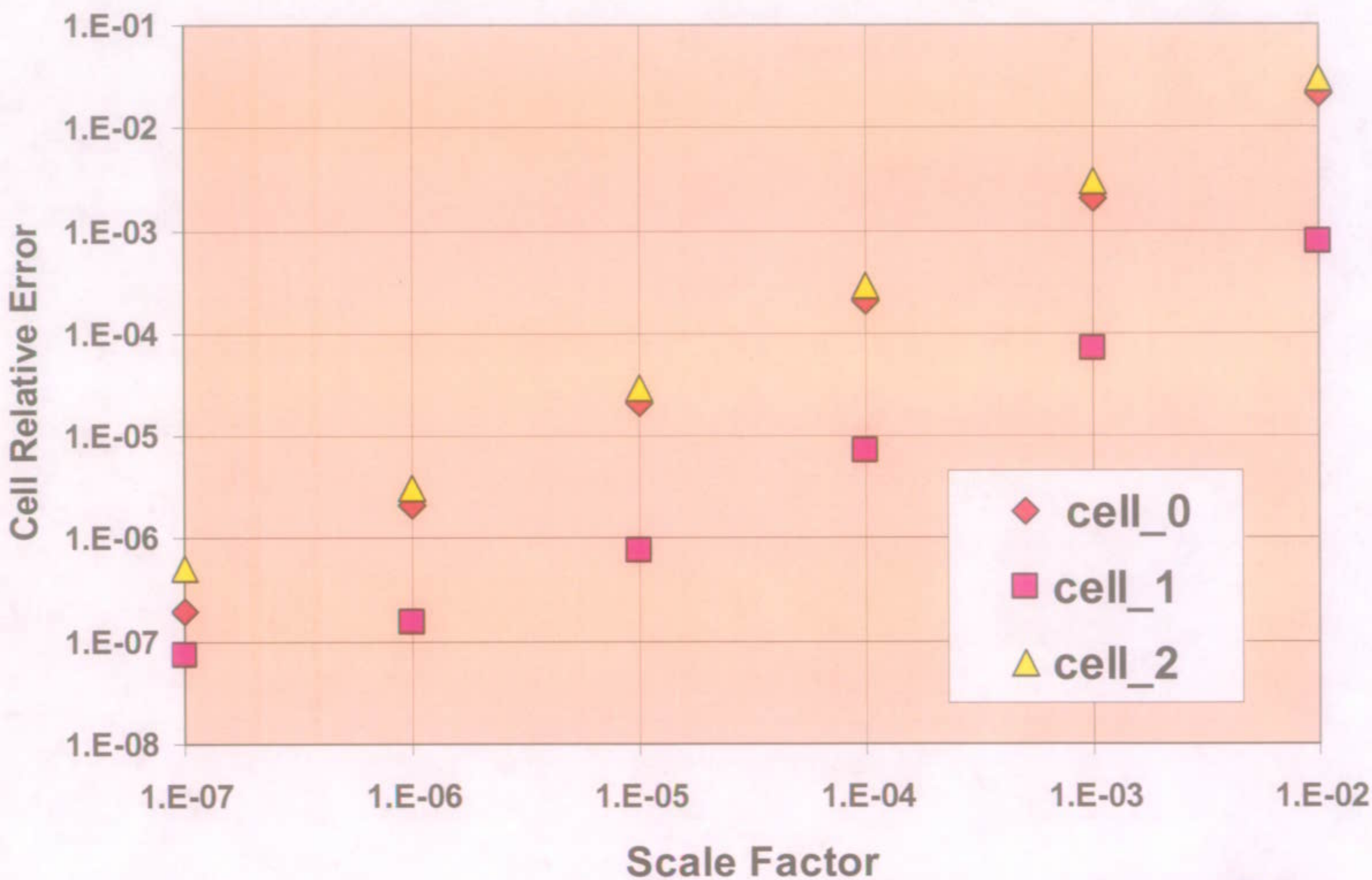
Comparison of Exact and Approximate Concentrations in the Two Dual Continuum Cells with Scale Factor = 1.E-06



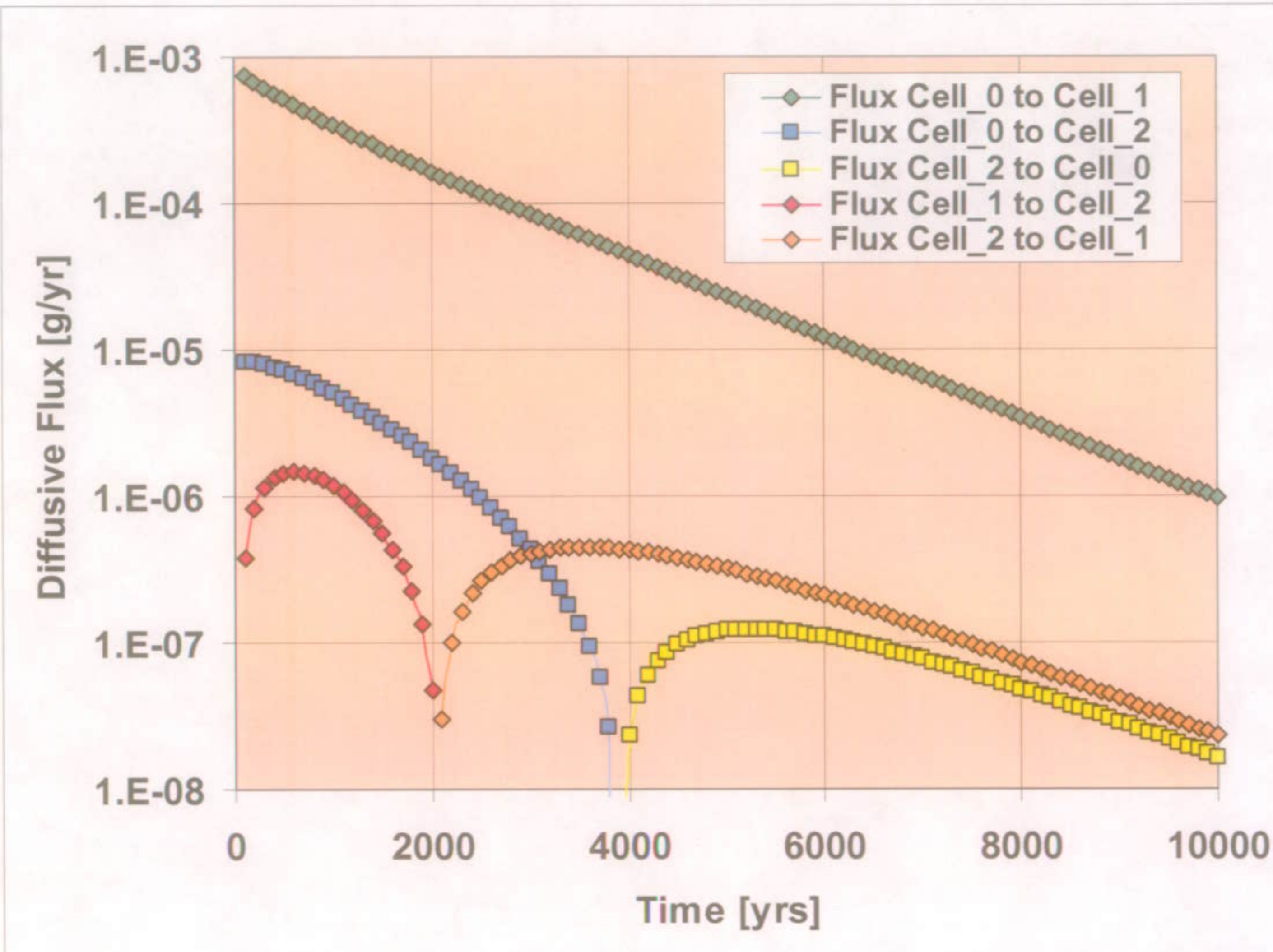
Cell Network Diffusive Conductances [m^3/yr]



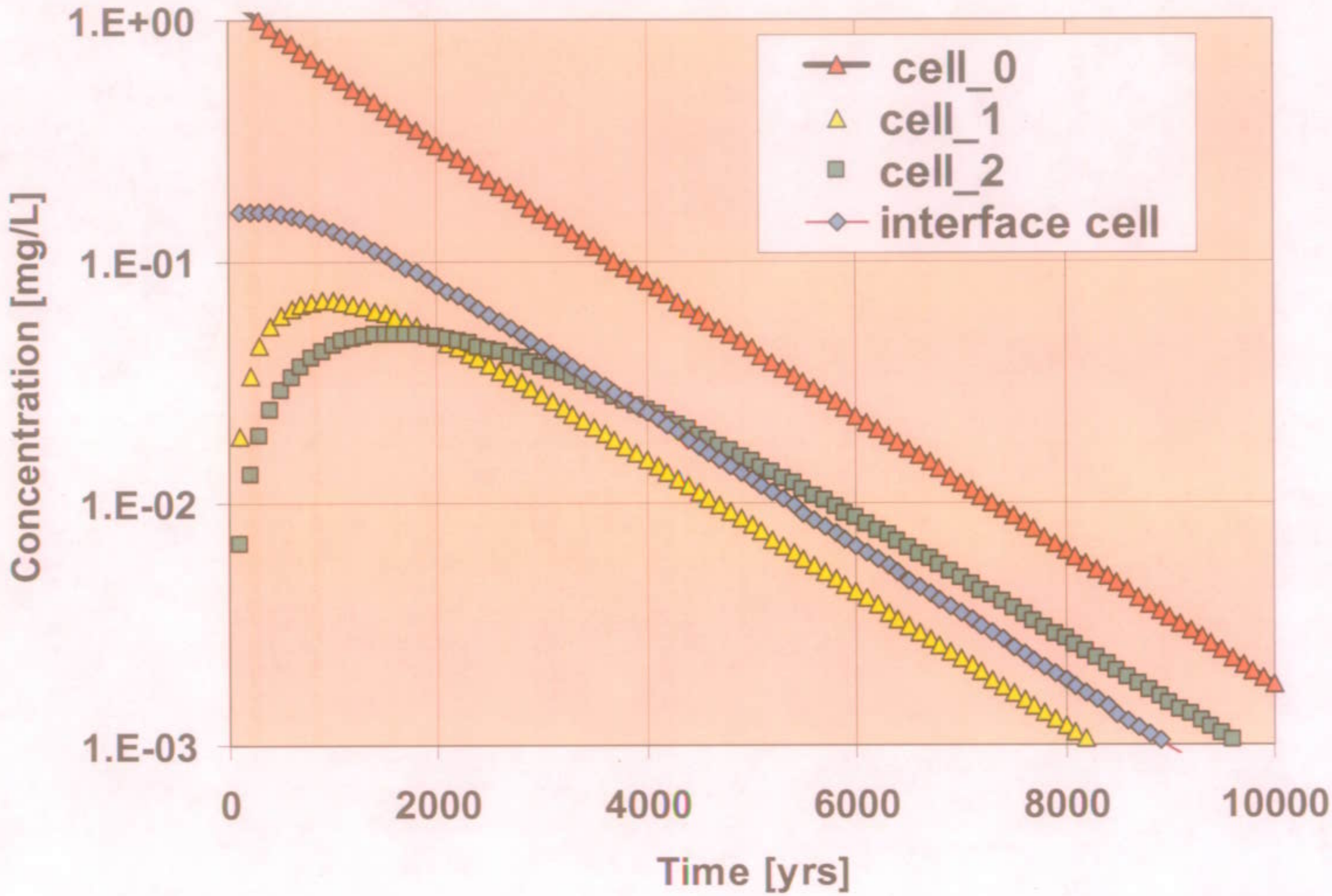
Relative Errors in Concentration Between Exact and Approximate Solutions at Time = 2000 yrs



Diffusive Fluxes



Concentrations



Conclusions

- Two methods for calculating diffusion across an interface between a single continuum and a dual continuum
- Exact or pseudo-flux method requires an additional diffusive flux expression between dual continuum cells and introduces complexity to the coupled diffusive conductances
- Approximate or interface cell method requires an additional cell, but with uncoupled diffusive conductances
- Approximate method converges to the exact method with respect to the interface cell scale factor
- With interface cell scale factor of 1×10^{-6}, the interface cell method provides a very good approximate solution to the diffusive transport
- The TSPA-LA model requires a fracture/matrix mass transfer, which is a real physical transport. The cell interface method was implemented in TSPA-LA, so that this physical diffusive flux is not confused with the pseudo-flux introduced in the exact method