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Interactive Comment

# *Interactive comment on* "Time dependent dispersivity behavior of non-reactive solutes in a system of parallel fractures" *by* G. Suresh Kumar et al.

#### G. Suresh Kumar et al.

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#### Reply to the Comments of Referee # 2

The authors' thank the reviewer for his comments and suggestions. The replies to the reviewer's comments are provided below:

**Referee's Concern 1:** How are effective parameters calculated from spatial moments. If the authors apply their procedure to derive effective CDE parameters from spatial moments of a concentration profile that is simulated using a 1-D CDE (Equation 1 with q=0) and the boundary conditions used in Eq. 3, would they obtain exactly the same effective parameters as the ones they used to simulate the concentration profile?



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**Authors' Response:** The spatial moments are obtained for the concentration in fracture using a similar approach adopted by Guven et al. (1984). The zeroth moment  $(M_o)$  is proportional to the total aqueous mass of solute in the fracture, the first spatial moment  $(X_1)$  describes the displacement of the center of mass of the tracer and the second spatial moment  $(X_{11})$  describes the spread around the center of the mass. The following are the expressions for these moments using the fracture concentrations:

$$M_{o} = \int_{0}^{l'} c(x)dx; \quad M_{1} = \int_{0}^{l'} xc(x,t)dx; \quad M_{2} = \int_{0}^{l'} x^{2}c(x,t)dx$$

and

$$X_1(t) = \frac{M_1}{M_0}; \quad X_{11}(t) = \frac{M_2}{M_o} - \left(\frac{M_1}{M_o}\right)^2$$

From these moments, the effective properties of the solute velocity, the macrodispersion coefficient and the dispersivity can be obtained using the following expressions:

$$V(t) = \frac{d\{X_1(t)\}}{dt}; \quad D(t) = \frac{1}{2}\frac{d\{X_{11}(t)\}}{dt}; \quad \alpha(t) = \frac{1}{2}\frac{dX_{11}(t)}{dX_1(t)}$$

The above expressions are valid for a concentration pulse source. Since a constant continuous source is applied as a boundary condition at the inlet of the fracture, a first spatial derivative of the concentration in the fracture is used to obtain an equivalent pulse in order to use the above expressions.

In 1-D CDE, meant for a classical porous system, the concentration profile corresponds to a single unit, i.e., to the whole system. There are no two different continuous media namely high permeability fracture and low permeability rock matrix. But, in a fracture-matrix coupled system, represented by a set of 2 equations, the concentration profiles from which spatial moments have been computed correspond to the concentration history along the fracture. However, when the coupling term q = 0, the simulation

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studies yield the initial values of water velocity, dispersivity and/or dispersion coefficient and these results have already been explained in Figs. 2 and 3 (Suresh Kumar and Sekhar, 2005).

From the Figs. 2 and 3, when the matrix diffusion coefficient,  $D_m$ , is very low, i.e., when the rock matrix term is negligible (or ignored), the simulation yields the initial values of water velocity and dispersion coefficient.

#### Reference:

Suresh Kumar, G., and M. Sekhar. (2005). Spatial Moment Analysis for Transport of Nonreactive Solutes in Fracture-Matrix System. Journal of Hydrologic Engineering, v. 10(3), pp. 192-199.

**Referee's Concern 2:** How are the transport equations solved. Was this done numerically or using analytical solutions?

**Authors' Response:** In this study, the system is described by two sets of coupled partial differential equations, each set containing one equation for the high permeability fracture and one for the low permeability rock matrix, both formulated in a one-dimensional framework. The system is solved numerically using a second-order central-difference finite-difference scheme. To satisfy the continuity at the fracture-matrix interface, the solution is iterated in each time step.

The convective and the dispersive parts of Eq. (1) and the diffusive transport described by Eq. (2) are solved using the finite-difference method. The coupling between the fracture and matrix in solute transport involves iterations. The discretization of the hyperbolic coupling term (first-order PDE) representing the last term on the right-hand side in Eq. (1),  $\left(\frac{\partial c_m}{\partial y}\right)\Big|_{y=b}$ , involves the difference in the matrix concentrations over the fracture-matrix interface between the second and first nodes within the rock matrix.

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Now, the coupling term in Eq. (1) is discretized as:

$$\left(\frac{\partial c_m}{\partial y}\right) = \frac{\left(C_{m_2}^{m+1} - C_{m_1}^{m+1}\right)}{\Delta y}$$

Here, the concentration at the first node in the rock matrix becomes equal to the corresponding fracture concentration perpendicular to the rock matrix satisfying the boundary condition (Eq. (4)),

that is,  $C_{m_1}^{n+1} = C_{f_1}^{n+1}$ 

Because the concentration of the second node in the rock matrix,  $C_{m_2}^{n+1}$ , is known only at the initial time, i.e. at t=0, and is unknown at the next time level, i.e.  $(n+1)^{th}$ , its value is assumed and iterated until convergence. Thus, using Thomas' algorithm solver (Huyakorn and Pinder, 1983), the three unknowns that are solved are the concentrations in the fracture at the  $I^{th}$  node,  $(I-1)^{th}$  node and  $(I+1)^{th}$  node, at  $(n+1)^{th}$ time level. The fourth additional unknown, the concentration at the second node of the matrix at  $(n+1)^{th}$  level is not involved in the solver and hence its value is assumed at  $(n+1)^{th}$  level and is iterated until convergence.

The grid size in the fracture is maintained uniform whereas a non-uniform grid size is adopted in the rock matrix; it is to be noted that the grid size does not change with time. A smaller grid size is used at the fracture–matrix interface to accurately simulate concentration flux into the matrix. The simulations are carried out starting with small time steps to ensure the accuracy of the initial results. The time steps are then increased, with their magnitude limited by a maximum Courant number of 0.5 (Heath, 2002).

References:

Heath, M.T., 2002. Scientific Computing: An Introductory Survey, second ed. McGraw-Hill, New York. 3, S1017–S1026, 2006

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Huyakorn, P.S., Pinder, G.F., 1983. Computational Methods in Subsurface Flow. Academic Press, 473 p.

**Referee's Concern 3:** For the case of parallel multiple fractures with varying apertures, it is not clear how the pore water velocities in the fracture were related to fracture aperture. If  $v_f$  is different in different neighboring fractures, then the boundary condition in Eq. 4 at half of the fracture spacing (which I have to guess because it is actually not defined in Eq. 4) does not hold. Analytical solutions, which rely on this boundary condition, do not apply for this situation.

**Authors' Response:** In the present study, the multiple fractures are assumed to be parallel, while the thickness of the fracture aperture is constant throughout the fracture length. However, the fracture aperture is different for each of these fractures in the multiple fracture case. Hence, the boundary conditions meant for a single fracture is still assumed to be applicable for each fracture of the multiple fracture system, however with a different value of fracture aperture. The fracture spacing is kept constant among the fracture sets. The present study explores the sensitivity of the mixing characteristics of parallel fracture apertures with respect to its influence on the characteristics of the solute front.

The water velocity  $v_f$  is different in each of the neighboring fractures as the fracture aperture "b" is not the same. The boundary condition in Eq.4 at half fracture spacing still remains the same and is valid. The solution is obtained numerically, which poses no difficulty.

**Referee's Concern 4:** Why do the authors focus on the non-asymptotic behaviour of the dispersivity? I would assume that in the pre-asymptotic region, the concentration profiles and breakthrough curves will be highly skewed in fractured media so that they cannot be described by a convection dispersion model.

Authors' Response: In a fracture-matrix coupled system, the mixing/dispersion behavior is mainly due to significant variation in velocity of the solute, while getting trans3, S1017–S1026, 2006

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ported along the high permeability fracture. Dispersivity, essentially, being a measure of variations in velocity, its behavior during pre-asymptotic regime becomes critical. It is to be noted that during asymptotic regime, the fracture and the matrix act as a single entity, while it acts as a distinct fracture and matrix during pre-asymptotic regime, and the variations in solute velocity arise basically from the interplay between fracture and matrix.

**Referee's Concern 5:** Why do the authors use spatial moments and not temporal moments? There are two arguments in favour of using temporal moments. It is practically impossible to determine spatial moments of concentrations in a fracture experimentally whereas breakthrough curves can be measured more easily. Relatively simple relations between the convection dispersion equation (CDE) parameters and the spatial moments of a solute plume are only obtained in infinite media. For their simulations, the authors define a boundary condition and for boundary condition problems or transport in semi-infinite media the relation between spatial moments and CDE parameters becomes far more complex.

**Authors' Response:** Spatial moments of point concentration data (Taylor 1953; Aris 1956; Horn and Kipp 1971) provide an integrated measure of the concentration field over the extent of the solute plume. The method is useful for assessing the dispersive transport model formulations (Freyberg 1986). Field observations have shown (Sauty 1978) that, on the scale in question (at the scale of a single fracture), the macrodispersivity clearly dominates the molecular diffusion; de Marsily (1986) highlighted that such field values were likely to be due to the heterogeneity of the velocity between the fracture and the reservoir matrix. On a larger scale, however, in a tracer experiment over a longer distance and time, the coefficients of solute dispersion reach an asymptotic value, but this has not been experimentally confirmed (de Marsily 1986). In addition to the longitudinal dispersion in the fracture, the present study involves the mixing/dispersion characteristics arising from matrix diffusion, and therefore the time-dependent analysis of various solute transport parameters becomes vital for deducing

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the dominant factors in the transport behavior of solutes in a fractured geothermal reservoir.

In the present model, the convective transport and spreading characteristics are considered by characterizing the spatial moments of the concentration distribution (Fischer et al. 1979; Gelhar 1993) along the fracture. This approach is suitable for numerical simulations in the sense that all concentrations in space are available at a given time. Field experiments require a dense network of observation points, and for obvious economical reasons such facilities are rare and proposed only for specific experimental sites. The advantage of the front spatial analysis is to permit characterization of the effective dispersion on the basis of the temporal evolution of the concentration spatial moments.

References:

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de Marsily, G. \_1986\_. Quantitative hydrogeology, Academic, Orlando, Fla.

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Gelhar, L. W. \_1993\_. Stochastic subsurface hydrology, Prentice-Hall, New York.

Freyberg, D. L. \_1986\_. "A natural gradient experiment on solute transport in a sand aquifer. II: Spatial moments and the advection and dispersion of non-reactive tracers." *Water Resour. Res.*, 22(13), 2031–2046.

Horn, F. J. M., and Kipp Jr., R. L., Jr. \_1971\_. "Induced transport in pulsating flow." *AIChE J.*, 17, 621.

Sauty, J. P. \_1978\_. "Identification des parameters due transport hydrodispersif dans les aquiferes par interpretation de tracages en ecoulement cylindrique convergent ou

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divergent." J. Hydrol., 39, 69-103 \_in French\_.

Taylor, G. E. \_1953\_. "Dispersion of soluble matter in solvent flowing slowly through a tube." *Proc. R. Soc. London, Ser. A*, 219, 186–203.

**Referee's Concern 6:** Just after the start of the solute injection, the bulk mass is in the fractures so that the effective velocity derived from the spatial moments of concentrations in the fracture is equal the pore water velocity in the fractures. At later stages, due to mixing of solutes between fractures and matrix, the overall velocity of the tracer plume will be equal to the water flux divided by the total porosity and will be much smaller (depending on the ratio of the fracture volume to the total pore volume) than the velocity in the fracture. Therefore, I do not understand the statement that the time behaviour of the first spatial moment is linear. I think that this cannot be the case. I suggest that the authors also pay attention to the behaviour of the first spatial moment of the solute plume.

**Authors' Response:** The temporal behavior of the first and second spatial moments is nonlinear even for a single fracture system, which can be observed from the Figs 2 and 3 shown above while replying to the "concern # 1". The statement made in the paper in Page 905 – lines 7 and 8 is incorrect in that respect. However, here it is meant to indicate that a linear relation between these quantities is observed during early time when the effect of matrix diffusion has not yet resulted on the system. It is to be read as – "It is observed from the figures that the effective dispersivity has a linear relationship with both space and time at pre-asymptotic stage up to 0.2 day".

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Figure 1: Temporal variation of solute mobility along the fracture.

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Figure 2: Temporal variation of solute variance along the fracture.