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Finite Analytic Methods for Simulation of Advection-Dominated and Pure Advection Solute Transport With Reaction in Porous Media

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ABSTRACT: The transport of dissolved contaminants in groundwater is usually described by the advection dispersion equation with reaction. Several numerical methods for solving the one-dimensional are available including finite difference methods, finite volume methods, and finite element methods. Stringent conditions, such as small Peclet (Pe) and Courant (Cr) numbers, must be satisfied to ensure the accuracy and stability of the numerical solutions. The practical finite analytic (PFA) method was applied to the solution of two solute transport problems: 1- One-dimensional advection–dispersion equation with reaction under advection-dominated conditions, and 2- One-dimensional pure advection equation with reaction. A triangular explicit PFA (EPFA) spatial-temporal computational molecule was developed. The EPFA solutions were compared with solutions from the quadratic upwind differencing (QUICK) scheme. For both cases, the EPFA solution gives accurate results as long as the Courant (Cr) was close to one. Stability analysis shows that the EPFA molecule is always stable for high Pe number.

Key words: Advection-dominated transport, Explicit practical finite analytic methods (*EPFA*), *QUICK* scheme, Refined *QUICK* solution (*RQS*)

INTRODUCTION

The transport of dissolved contaminants in porous media is usually described by the advection dispersion equation with and without reaction (*ADE* and *ADER*). Several numerical methods for solving the one-dimensional *ADER* are available including finite difference methods (*FD*), finite volume methods (*FV*), and finite element methods (*FE*). Oscillations, dissipations and numerical dispersion are the main problems correspond to numerical methods (Ataie *et al.*, 1996, Ataie *et al.*, 1999, Batu, 2006, Dehghan, 2004, Morton, 1996). More importantly, many of the numerical schemes, including explicit and implicit approaches, used in these methods fail to produce monotonic solutions when there is a sharp discontinuity in the physical solution (Leer, 1973, Leonard, 1979, Versteeg and Malalasekera, 2007). Accurate explicit methods such as Lax-Wendroff (LW) and McCormack method, which are based on two predictor-corrector steps (Anderson *et al.*, 1984, Thommen, 1966), and accurate implicit methods such as implicit Petrov Galerkin and implicit Taylor Galerkin usually suffer from oscillations and numerical dispersion, particularly at large *Pe* and need correction approaches (Finlayson, 1992). For example Li and Jackson (2007) used correction methods for two explicit and implicit *FD* schemes including the McCormack and Salvey method to solve advection-dominated problems in surface water. Arbogast and Wheeler (1995) proposed the characteristic mixed *FE* method (*CMFE*) to improve the accuracy of the *FE* method. This method is theoretically based on local mass conservation, but the ability to ensure mass conservation in numerical solution is uncertain. Douglas and Russell (1982) combined the *FE* method with the method of characteristics (*MOC*) to decrease truncation error, but this method is difficult to apply for flux boundary conditions (*BC*). Ataei *et al.*, (1996, 1999) proposed a correction scheme to remove numerical dispersion in *ADER*, but did not apply this method for advection-dominated problems. In most flow simulations, the main source of problems in simulating the *ADER* is the advection term and using high resolutions may not be a good remedy for this problem. Discretization of advection terms in the *ADER* has extensively documented (Asensio *et al.*, 2007, Finlayson, 1992, Wang *et al.*, 1999, Henao *et al.*,

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2010, Leonard, 1979). Proper treatment of the advection terms becomes more important in advection-dominated flows. However, excessive computational time and limited accuracy due to overshoot or numerical dissipation are still the most important disadvantages of the proposed solutions for advection-dominated problems (Wang *et al.,* 1999). Stringent conditions, such as small Peclet (*Pe*) and Courant (*Cr*) numbers, must be satisfied to ensure the accuracy and stability of the numerical solutions. A novel approach called the practical finite analytic (*PFA*) method, for solving partial differential equations was proposed by Civan (1995, 2008). In this method, an analytical solution based on power series is developed to solve *ADER* for nodes of an arbitrary molecule (in this study a triangular molecule was selected). These analytical solutions are functions of spatial space, *x*, time, *t*, velocity, V_x, dispersion, D_x, and reaction term, *K*. These analytical solutions construct a set of algebraic equations. If the determinant of the matrix of coefficients corresponding to the algebraic equations is set to zero, the relationship between the nodes of a computational molecule can be determined. These relationships give the coefficients used for the all grid nodes unless the spatial discretization or time step are not uniform. Since the *PFA* method does not rely on Taylor series approximations of the derivatives, it does not suffer from numerical dispersion and spurious oscillations. In addition, this method applies a universal procedure regardless of the types of boundary conditions involved in the differential equations and also without sacrificing the accuracy in the implementation of the boundary conditions (Civan, 2008). However, the *PFA* method has chiefly been applied to heat conduction problems (Fukuyo, 2005, Fukuyo, 2004) and simulation of the *ADER* by the *PFA* method has not been fully investigated. The main objective of this study is to extend the *PFA* method that was previously developed by Civan (1995) to simulation of the *ADER*. This is the first time that the application of this method has been evaluated for advection-dominated problems with inclusion of reaction.

In this study advection-dominated transport with reaction in porous media with several reaction terms is considered. A computational *PFA* molecule, triangular explicit *PFA* (*EPFA*), is considered. The von Neumann stability analysis is used to determine the stable range of Courant number, *Cr*, dispersion number, *Ds*, and sink/source number, *Sr*. Finally, the results of the triangular explicit molecule were compared with a *QUICK* scheme with the same discretizations and with a refined *QUICK* solution (*RQS*) obtained using the high resolution *QUICK* scheme with very fine time and space discretizations.

MATERIALS & METHODS

The one dimensional *ADER* is:

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} - V_x \frac{\partial C}{\partial x} - KC \qquad (1)$$

where *C* is the concentration, V_x is the velocity in x direction, D_x is the dispersion coefficient, and *K* is the first-order reaction rate coefficient. Note that and D_x are considered to be positive and constant values for this study. The general solution of equation (1) can be represented by a time-space power series as:

$$C(x,t) = \sum_{p=0}^{UB} \sum_{q=0}^{p} a_{q,p} x^{p-q} t^q \qquad (2)$$

where $a_{q,p}$ the recurrence relationship and *UB* is the upper bound of the series and usually the greater the *UB* value, the more accurate is the result. Applying equation (2) to equation (1), a recurrence relationship can be derived:

$$a_{q,p} = \frac{D_x (p-q+2)(p-q+1) a_{q-1,p+1} - V_x (p-q+1) a_{q-1,p} - K\, a_{q-1,p-1}}{q} \qquad (3)$$

Substituting equation (3) into equation (2) results in:

$$C(x,t) = \sum_{m=1}^{UB} b_m B_m(x,t) \qquad (4)$$

where b_m and $B_m(x,t)$ denote the new unknown coefficients and the basis functions, respectively. As mentioned by Civan (1995, 2008), there is no need to calculate the unknown coefficients. In this study, the *PFA* molecule has four nodes and therefore requires three basis functions (*BFs*) (Table 1). The order of

Table 1. The respective basis function for the triangular *EPFA*

BF_1	$1 - Kt + \frac{1}{2} K^2 t^2 - \frac{1}{6} K^3 t^3$
BF_2	$x - V_x t - Kxt + K V_x t^2 + \frac{1}{2} K^2 x t^2 - \frac{1}{2} K^2 V_x t^3$
BF_3	$2 D_x t + x^2 - 2 V_x x t + \left(-2 K D_x + V_x^2\right) t^2 - K x^2 t + 2 K V_x x t^2 + \left(\frac{1}{3} D_x K^2 - \frac{1}{3} K \left(-2 K D_x + V_x^2 \right) - \frac{2}{3} V_x^2 K \right) t^3$

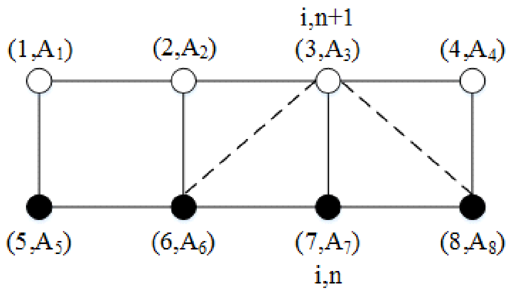


Fig. 1. The general computational molecule including triangular *EPFA* and *QUICK* scheme

accuracy for this stencil (the triangular molecule) would be zero to third order in time and space.

Fig. 1 demonstrates the general computational molecule used in this paper. The *EPFA* computational molecule is based on explicit technique. The triangular *EPFA* uses four nodes including 3 and 6 to 8. A_i represents the coefficients correspond to each node. For this molecule, A_1, A_2, A_4 and A_5 are equal to zero.

Applying equation (4) with the aforementioned basis functions to the triangular four point molecule produces a system of linear algebraic equations for interior nodes, i = 1: *Nx*-1, which leads to the final expression as below:

$$A_3C_i^{n+1} = A_6C_{i-1}^n + A_7C_i^n + A_8C_{i+1}^n \tag{5}$$

where *Nx* is the number of discretization in x domain, *n* is the time index and *i* is the space index. Since the *PFA* molecules are being tested for advection-dominated problems, the results are compared with the *QUICK* method which is a robust scheme based on a *FD* approach. All nodes in Fig. 1 used for the *QUICK* scheme. The *QUICK* scheme was obtained as follows (Leonard, 1979):

$$\begin{aligned}\frac{C_i^{n+1}-C_i^n}{\Delta t} &= \frac{D_x}{2\Delta x^2} \\ &\left(C_{i+1}^{n+1}-2C_i^{n+1}+C_{i-1}^{n+1}+C_{i+1}^n-2C_i^n+C_{i-1}^n\right)-\frac{V_x}{2\Delta x} \\ &\left(\begin{aligned}&\frac{C_{i+1}^{n+1}-C_{i-1}^{n+1}}{2}+\frac{C_{i+1}^n-C_{i-1}^n}{2}-\frac{C_{i+1}^{n+1}-3C_i^{n+1}+3C_{i-1}^{n+1}-C_{i-2}^{n+1}}{6} \\ &-\frac{C_{i+1}^n-3C_i^n+3C_{i-1}^n-C_{i-2}^n}{6}\end{aligned}\right) \\ &-\frac{K}{2}\left(C_i^{n+1}+C_i^n\right)\end{aligned} \tag{6}$$

The temporal weighting for the implicit *QUICK* scheme was equal to 0.5. For the *QUICK* molecule, the linear algebraic equation used for i = 2: *Nx*-1 would be:

$$\begin{aligned}&A_1C_{i-2}^{n+1}+A_2C_{i-1}^{n+1}+A_3C_i^{n+1}+A_4C_{i+1}^{n+1}= \\ &A_5C_{i-2}^n+A_6C_{i-1}^n+A_7C_i^n+A_8C_{i+1}^n\end{aligned} \tag{7}$$

In the *QUICK* scheme, in order to avoid using artificial *BC*, the following approximation was used for i = 1, which is identical to the central difference method:

$$\begin{aligned}\frac{C_i^{n+1}-C_i^n}{\Delta t} &= \frac{D_x}{2\Delta x^2} \\ &\left(C_{i+1}^{n+1}-2C_i^{n+1}+C_{i-1}^{n+1}+C_{i+1}^n-2C_i^n+C_{i-1}^n\right) \\ &-\frac{V_x}{2\Delta x}\left(C_i^{n+1}-C_{i-1}^{n+1}+C_i^n-C_{i-1}^n\right) \\ &-\frac{K}{2}\left(C_i^{n+1}+C_i^n\right)\end{aligned} \tag{8}$$

The stencil used for the first node, i = 1, includes nodes 2 to 4 and 6 to 8. The values of these coefficients are shown in Tables 2-3 in terms of dimensionless variables including Courant number (*Cr*), Dispersion number (*Ds*), and sink and source number (Sr) defined as the following:

$$Cr = \frac{V_x\Delta t}{\Delta x} \tag{9}$$

$$Ds = \frac{D_x\Delta t}{(\Delta x)^2} \tag{10}$$

$$Sr = K\Delta t \tag{11}$$

When the value of *UB* in equation (4) decreases, the number of terms in the coefficients will also decrease but less complex basis functions will result in less complex coefficients with lower order of accuracy. Gaussian elimination technique for matrix inversion was used to solve the final form of ***Rx* = *b*** where ***R*** is the matrix of coefficients, ***b*** is representative of *BCs* and concentration of previous time step, and ***x*** is the concentration vector.

The one dimensional *AER* is:

$$\frac{\partial C}{\partial t} = -V_x\frac{\partial C}{\partial x} - KC \tag{12}$$

In this case, the pure advection equation with reaction was considered. When the ratio of advection to dispersion numbers is very large, the behaviour of *ADER* equation changes from a parabolic equation to a wave equation which needs a special attention (advection-dominated problems in extreme cases, i.e. D_x=0). Therefore, it is reasonable to check the results of the triangular molecule for these types of equations as well. The basis functions and relevant coefficients of the triangular *EPFA* in this case are similar to the section 2.1 except the dispersion number is equal to zero. This also holds for the respective coefficients of the *QUICK* scheme. The stability criteria for the *PFA* method can be determined using von Neumann's method (Duffy, 2006). Although, this method is a local stability type, it gives helpful information about the

Table 2. The coefficients used for the triangular *EPFA* molecule

A_2	0
A_3	-2
A_4	0
A_6	$Sr\,Cr-\frac{1}{2}Sr^2\,Cr+2\,Ds\,Sr-\frac{2}{3}Ds\,Sr^2+Cr^2\,Sr-Cr-2\,Ds-Cr^2$
A_7	$-4\,Ds\,Sr+\frac{4}{3}Ds\,Sr^2-2\,Cr^2\,Sr-2+2\,Sr-Sr^2+\frac{1}{3}Sr^3+4\,Ds$ $+2\,Cr^2$
A_8	$-Sr\,Cr+\frac{1}{2}Sr^2\,Cr+2\,Ds\,Sr-\frac{2}{3}Ds\,Sr^2+Cr^2\,Sr+Cr-2\,Ds$ $-Cr^2$

Table 3. The coefficients used for the implicit *QUICK* scheme

	QUICK scheme for node *i* = 1	*QUICK* scheme for node *i* = 2:*Nx*-1
A_1	0	$\frac{Cr}{12}$
A_2	$-\frac{1}{2}(Cr+Ds)$	$-\frac{1}{2}(Cr+Ds)$
A_3	$\frac{1}{2}(2+Cr+2Ds)$	$\frac{1}{2}(2+2Ds+\frac{Cr}{2}+Sr)$
A_4	$-\frac{Ds}{2}$	$\frac{1}{2}(-Ds+\frac{Cr}{3})$
A_5	0	$-\frac{Cr}{12}$
A_6	$\frac{1}{2}(Cr+Ds)$	$\frac{1}{2}(Cr+Ds)$
A_7	$\frac{1}{2}(2-Cr-2Ds)$	$\frac{1}{2}(2-2Ds-\frac{Cr}{2}-Sr)$
A_8	$\frac{Ds}{2}$	$\frac{1}{2}(Ds-\frac{Cr}{3})$

stability criteria. In von Neumann's method a general one-step scheme for an initial value problem in vector form is:

$$\vec{B}^{n+1}=G\vec{B}^{n} \quad n\geq 0 \tag{13}$$

where G is an amplification factor and B is a function. In order to reach a stable condition, one must satisfy the inequality:

$$\vec{B}^{n+1} \leq \vec{B}^{n} \tag{14}$$

or:

$$|G|\leq 1 \tag{15}$$

The amplification factor for the stencils is:

$$G=\left|\frac{[(A_6+A_8)\cos(\beta\Delta x)+A_7]+i[(A_8-A_6)\sin(\beta\Delta x)]}{[(A_2+A_4)\cos(\beta\Delta x)+A_3]+i[(A_4-A_2)\sin(\beta\Delta x)]}\right| \tag{16}$$

where $\beta\Delta x$ is the phase angle. For all molecules G can be calculated based on the relevant coefficient for that molecule. Equation (14) can be solved for $|G|$ as a function of $\beta\Delta x$, given a constant *Cr*, *Ds* and *Sr* numbers. This equation is stable if the calculated curve is confined in the unit circle. This study focuses on advection-dominated problems which is characterized by high Pe number, i.e. *Pe*>10. *Pe* is defined by the ratio of *Cr* to *Ds* number:

$$Pe=\frac{Cr}{Ds}=\frac{V_x\Delta x}{D_x} \tag{17}$$

The results of the stability analysis for $0<Cr\leq 1$, $0<Ds\leq 1$ and $0<Sr\leq 2.5$ for the triangular *EPFA* are demonstrated in Fig. 2. The stability analysis shows that the triangular *EPFA* is always stable for high *Pe* numbers. However, when the *Ds* increases, i.e. the transport mechanism is mostly due to dispersion than advection, the yielded results may become unstable. As can be seen by Fig 2, to find stable area, all three curves, *Cr-Sr*, *Cr-Ds* and *Ds-Sr* should be considered simultaneously.

Although Fig 2 demonstrates the stable area for triangular *EPFA*, for high *Pe* numbers, this molecule produce an undershoot/overshoot after the front for *Cr*<1 and has no oscillations for $Cr\approx 1$ or *Cr* = 1.

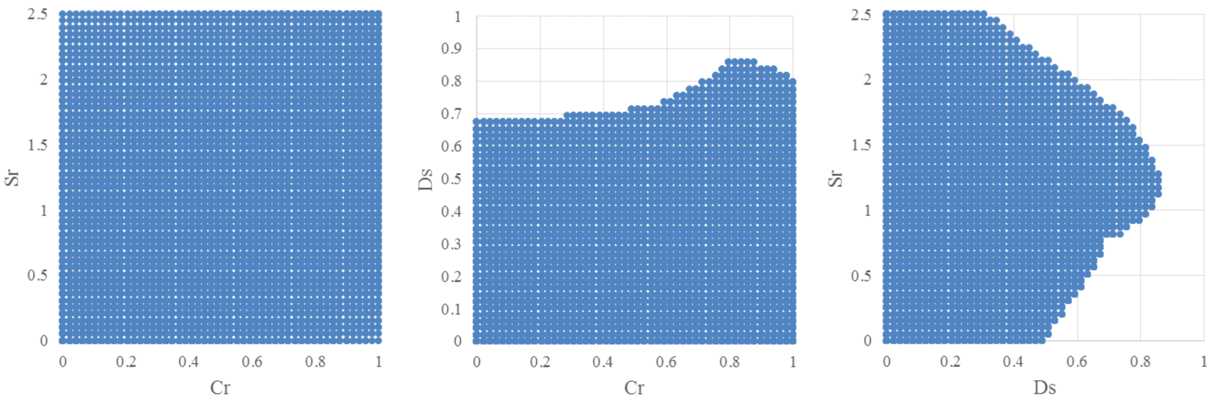


Fig. 2. The stable region (blue area) for the triangular *EPFA* molecule for $0 < Cr \le 1$, $0 < Ds \le 1$ and $0 < Sr \le 2.5$

Table 4. Domain and physical parameters used in case 1

Domain length	$X_0 = 500 \quad (m)$
Velocity in *x* direction	$V_x = 1.5 \quad (m/d)$
Dispersion coefficient	$D_x = 0.01 \quad (m^2/d)$
Initial concentration	$C_{IC} = 0 \quad (mg/l)$
Concentration at the left boundary	$C_0 = 1 \quad (mg/l)$
Final time	$T = 100 \ (d)$

Table 5. Solution of *ADER*, space and time discretizations for different numerical methods

K	Stencil	*Nx*	*Nt*	*Pe*	*Cr*	*Sr*
0.001	*EPFA and QUICK methods*	600	183	125	0.99	5.5×10^{-4}
	RQS	2500	1800	30	0.42	5.5×10^{-5}
0.01	*EPFA and QUICK methods*	600	183	125	0.99	5.5×10^{-3}
	RQS	2000	1800	37.50	0.34	5.5×10^{-4}
0.1	*EPFA and QUICK methods*	50	15	1500	1.07	0.71
	RQS	200	50	375	1.22	0.21

RESULTS & DISCUSSION

Since the exact solutions are not accurate for problems at high *Pe* numbers, the performance of the triangular *EPFA* molecule for high *Pe* numbers was compared with the *RQS*.

Numerical results were compared with the *RQS* obtained by the high resolution *QUICK* scheme for the following initial and boundary conditions:

$$C(x,0) = C_{IC} \tag{18}$$

$$C(0,t) = C_0 \tag{19}$$

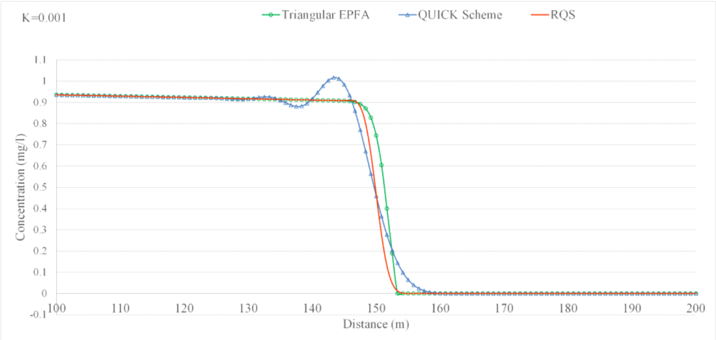
$$\frac{\partial C}{\partial x}(\infty, t) = 0 \tag{20}$$

where C_{IC} denotes initial concentration (*IC*). The parameters chosen for this example are listed in Table 4.

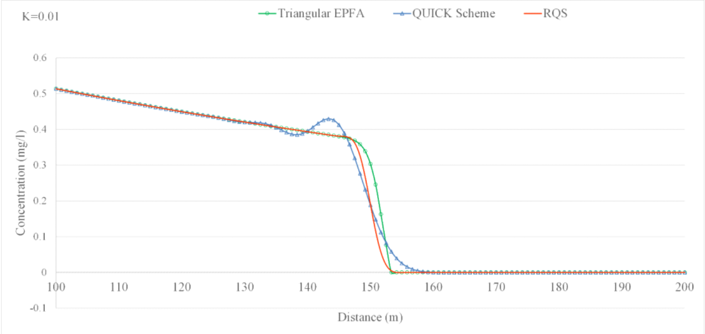
Table 5 demonstrates the various space and time discretizations, i.e. *Nx* and *Nt*, used to investigate the behaviour of the triangular *EPFA*. These are the minimum *Nx* and *Nt* that triangular *EPFA* molecule requires to yield accurate results with no oscillations. In addition, different reaction terms *K* was chosen to test the *PFA* method. To compare the results of the triangular *EPFA* with the *QUICK* scheme, the same value of *Nx* and *Nt* are used for both numerical methods. However, obtained results (Figs 3 and 4) show that the *Nx* and *Nt* should be increased. Therefore, to test the triangular molecule for higher *Pe* numbers, it was compared with the *RQS* which is based on high resolution *QUICK* scheme. Since the *Pe* number in this study is only changing due to a change in Δx (velocity and dispersion do not change), the triangular molecule can be compared with the *RQS*.

To compare the numerical methods accurately, the results are shown only after and before the shock front. As can be seen by Figs 3a and 3b, the triangular *EPFA* does not have oscillations while the *QUICK* scheme yields unstable results for the corresponding *Pe* number. According to Figs 3a and 3b, there is a phase mismatch between the triangular *EPFA* and *RQS* which can be removed by selecting finer mesh (e.g. the Nx = 1200, Nt = 367 and Cr = 0.99 which is half of the Nx, and one sixth of Nt corresponding to *RQS*). The reaction term K stabilizes the solution and as this term increases, the *QUICK* solution yields results with fewer oscillations (Compare Figs 3a with 3b and Figs 3b with 3c). There is not much difference between the results of the numerical methods for large value of K (Fig 3c). However, like the solutions of *ADER* with K = 0.001, 0.01, the triangular *EPFA* yields results with smaller values of Nx and Nt.

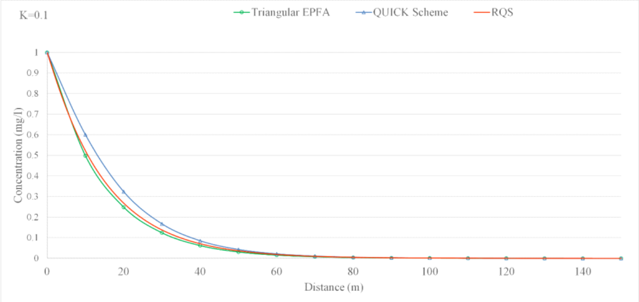
The domain and physical parameters and numerical parameters used in this case are listed in Tables 4 and 6 respectively. The *BCs* and *IC* are the same as the section 3.1 (equations 22-24). As mentioned earlier, the importance of this section is to check the behaviour of the triangular *EPFA* under extreme cases, i.e. pure advection cases. The results are compared with different values of reaction terms. As expected, the front of the respective curves (Figs 4a and 4b) in this case is sharper because of the absence of the dispersion. Like section 3.1, the results of triangular *EPFA* are obtained with smaller Nx and Nt compared to the *RQS*. However, for larger values of K, the results of



(3a)



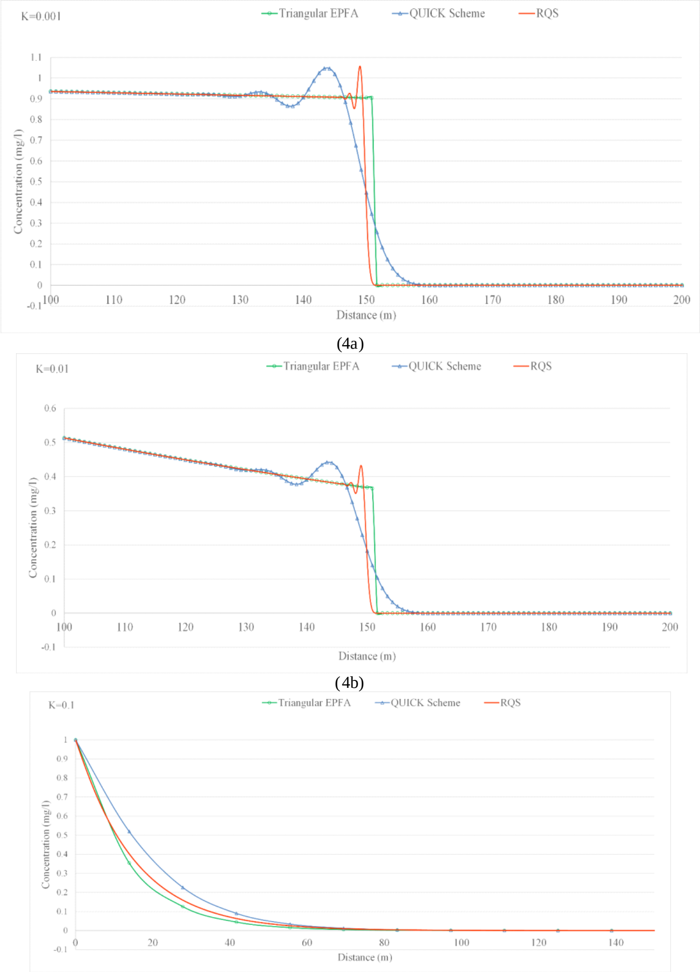
(3b)



(3c)

Fig. 3. Case 1; solution of *ADER*, the triangular *EPFA* result compared to the *QUICK* scheme and *RQS* for different values of *K*

all numerical schemes are roughly similar. It has been determined that for larger values of *K* such as 0.1 and greater, the results of other numerical schemes like Crank-Nicolson centred in dispersion and upwind in advection terms is also accurate for high *Pe* numbers. This phenomenon corresponds to the effect of reaction term on *AER* or *ADER* solutions. Therefore, there is not much difference between the results of triangular *EPFA*, *QUICK* scheme and *RQS* for *K* = 0.1 (see Fig.4c). However, as can be seen by Fig. 4c, the results of the triangular *EPFA* and *RQS* are more similar. The oscillations of the *QUICK* scheme decreases when the reaction term increases (compare Figs 6 and 7). In addition, according to Figs 4a and 4b, the *RQS* never reach stable results even in large discretizations given in Table 6. It has been determined that the triangular molecule yields results of free oscillations for smaller discretizations (e.g. *Nx* = 400 and *Nt*



(4a)

(4b)

(4c)

Fig. 4. Case 2; solution of *AER*, the triangular *EPFA* result compared to the *QUICK* scheme and *RQS* for different values of *K*

Table 6. Solution of *AER*, space and time discretizations for different numerical methods

K	Stencil	*Nx*	*Nt*	*Cr*	*Sr*
0.001	*EPFA and QUICK methods*	600	181	1	5.6×10^{-4}
	RQS	7500	3000	0.75	3.33×10^{-3}
0.01	*EPFA and QUICK methods*	600	181	1	5.6×10^{-3}
	RQS	7500	3000	0.75	3.33×10^{-4}
0.1	*EPFA and QUICK methods*	36	11	1.08	1
	RQS	130	35	1.14	0.29

=121 and *Nx* = 200 and *Nt* = 61 with *Cr* = 1). Like previous section, there is a phase mismatch between the results of triangular *EPFA* and *RQS* which can be eliminated for higher number of discretizations. In both cases, the results obtained by the triangular *EPFA* are free of oscillations when $Cr \approx 1$ (See Tables 5 and 6). In addition, the difference between the *PFA* solution and *RQS* can be resolved by choosing the following ways: 1- selecting finer mesh; 2- selecting more accurate basis functions, i.e. the order of accuracy with respect to *x* and *t* will increase; 3- selecting molecules with more nodes such as a rectangular molecule (nodes 2-4 and 6-8) or a trapezoidal molecule (nodes 2-3 and 6-8). The aforementioned cases show that the triangular *EPFA* is able to capture a fully sharp profile with no smearing. It is noteworthy that this molecule uses an explicit stencil and the numbers of time and space steps used by this molecule are much smaller than the implicit *RQS*.

CONCLUSIONS

This study is focused on the solution of advection-dominated transport with inclusion of reaction phenomenon in porous media. The explicit *PFA* method based on a power series, and the *QUICK* scheme, which is a robust numerical method for solution of *ADER* at high *Pe* numbers, were used to solve a problem with dirichlet *BCs*. The results show that the triangular *EPFA* molecule has a good behaviour for different values of reaction terms at high *Pe* numbers as long as *Cr* number is almost equal to one, i.e. corresponding results are free of overshoots or undershoots. This is significant because of the simplicity in explicit approaches and the accuracy with coarse time and space discretization. In addition, stability analysis shows that the triangular *EPFA* molecule is always stable for *Cr* numbers less than unity for high *Pe* numbers, i.e. small values of *Ds*.

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