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EVALUATION OF A FINITE DIFFERENCE METHOD FOR FILTRATION

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INTRODUCTION

The present paper is concerned with numerical analysis of a general form of the partial differential equations describing one dimensional depth filtration. For this purpose it is convenient to express the equations in dimensionless forms (in order to minimize the number of parameters appearing therein). An appropriate dimensionless set of differential equations and boundary and initial conditions can be written as (see, for instance, Tien, 1989)

\[
(N_2 \phi_1 - N_4 \phi_2) \partial_c + q \partial_c = N_3 \partial_c(D \partial_c c)
\]

\[
N_1(1 - N_4 \phi_2)M,
\]

\[
\partial_c = N_1 M e(0, z) = e_0 e(z, 0) = 0
\]

\[
s(z, 0) = 0
\]

\[
(1a,b,c,d,e)
\]

Eq. 1a expresses the filtrate mass balance while Eq. 1b expresses the filter mass balance. Eq. 1c indicates that the filter entrance is subjected to a time dependent dust concentration (challenge) after the process begins and Eqs. 1d and 1e state that both the filter and the filtrate are clean before the process begins. In Eqs. 1a,b the parameters

\[
N_1 = \frac{3 L}{2}
\]

\[
N_2 = \frac{\bar{L}}{(qT)}
\]

\[
N_3 = \frac{D_1}{(qL)}
\]

\[
N_4 = \frac{\bar{c}}{c_0}
\]

are dimensionless numbers which provide respective characterizations of the attachment/detachment rate, the transient completion time, the diffusivity, and the filtrate particulate concentration. The functions \( \phi_1(0), \phi_2(0), D_1, e_0, D, c_0, c, M, \) and \( c_0(0) \) must be specified in each case to render the problem determinate. In Eqs. 1a,b,c,d and 2a,b,c,d L is the filter length, \( T \) is the characteristic process time, \( \lambda \) is the characteristic inverse filtration length, and \( \bar{c}, \bar{D}, e_0, \bar{\phi} \) are respective characteristic values of concentration, diffusivity, superficial velocity, and porosity. Also, \( z \) denotes position (ratios to \( L \)), \( t \) denotes time (ratios to \( T \)), \( c \) denotes concentration (ratios to \( \bar{c} \)), \( x \) denotes specific deposit (ratios to \( \bar{D} \)), \( e_0 \) denotes inlet concentration (ratios to \( \bar{c} \)), \( e_0 \) denotes initial porosity (ratios to \( e_0 \)), \( D \) denotes diffusivity (ratios to \( \bar{D} \)), \( M \) denotes attachment/detachment rate (ratios to \( \bar{D} \)), \( \lambda \) and \( \bar{c} \) denotes superficial velocity (ratios to \( \bar{c} \)).

Eqs. 1a,b,c,d,e constitute a rather general formulation of the problem of depth filtration. Arbitrary forms of the equations describing the initial porosity distribution, the challenge and superficial velocity histories, and the diffusivity and attachment/detachment rate functions are allowed for. As such, Eqs. 1a,b,c,d,e encompass a multitude of filtration applications. Specificity is created through appropriate characterizations of the quantities mentioned above. For the purposes of the present paper, it is helpful to work with the general forms of Eqs. 1a,b,c,d,e. In this way, the maximum level of generality can be maintained in the numerical method to be discussed next.

NUMERICAL METHOD

In their most general forms, Eqs. 1a,b are nonlinear and coupled. Therefore, closed form solutions to these equations are unlikely and numerical procedures are required. Many existing computer codes employ a finite difference approach for the solution of transport equations. It is, therefore, logical to investigate the applicability of this methodology to Eqs. 1a,b.

In the present work the following finite difference scheme is employed to discretize Eqs. 1a,b. Two point backward difference quotients are used to represent the \( t \) derivatives and three point central difference quotients are used to represent the \( z \) derivatives. The computation starts with initial conditions at \( t = 0 \) and marches forward in time. At each time a system of nonlinear algebraic equations must be solved to determine the \( z \) distributions of \( c \) and \( x \). An iteration procedure is employed for this purpose. At each iteration an equivalent linear system of algebraic equations (the linearization being effected by representing some quantities by their values from the previous iteration) must be solved. These equations have a tridiagonal form and can be solved by Potter’s method.
variables which can be determined by a forward sweep in the $c$ direction. Then the physical variables can be found from a corresponding backward sweep. This process avoids the need for matrix inversion. Iteration is continued until convergence is obtained at a given time. Then the procedure moves forward to the next time. Without going into the details of commercially available Computational Fluid Dynamics (CFD) computer codes, it is interesting to note that, while obtained in a somewhat different way, the final discrete equations associated with the procedure employed herein are equivalent to those appearing in such codes as FLUENT, SIMPLE, and PHOENIX (Patakas, 1980). The methodology has become standard over the past three decades and, therefore, the details will not be repeated here. It is logical to assume that widely available CFD codes will be applied to filtration simulations. It is of interest to ask whether any peculiarities of Eqs. 1a,b,c,d,e might interfere with a straightforward forward application of CFD codes to filtration predictions by users treating them as black boxes. Attention will be focused on this question in the present work.

It is helpful to have some exact solutions to use as standards of comparison for the numerical procedure. This is the subject of the next section.

CLOSED FORM SOLUTIONS

In order to facilitate the process of obtaining closed form solutions, a seem-infinite region is considered and all solutions are based on the special case

$$N_4 = 0, D = 1, c_i = 1, c_j = 1, q = 1, M = c - N_2/N_1$$

for which Eqs. are simplified to read

$$N_2 \frac{\partial^2 c}{\partial z^2} + \frac{\partial c}{\partial z} = N_2 \frac{\partial^2 c}{\partial z^2} + N_2 s - N_1 c, \frac{\partial s}{\partial z} = N_1 c - N_2 s$$

These equations are linear and can be solved by Laplace transform methods. Eqs. have the respective meanings that the filtrate concentration is small, the is constant, the initial porosity is constant, the superficial velocity is constant, and the attachment/detachment rate function is assumed to he of the linear "chromatography like" form (with the dimensionless parameter $N_1$ characterizing the attachment rate and the dimensionless parameter $N_2$ characterizing the detachment rate).

While Eqs. 4a,b,c,d,e can be used to model a variety of practical filtration problems, that is not the main point of their use herein. Instead, it is desired to create problems having closed form solutions which can be used both as standards of comparison for the numerical method and as vehicles to illustrate some of the effects of diffusivity. Several special cases of Eqs. 4a,b,c,d,e fulfill these requirements. Three of these special cases will be discussed below.

A relatively simple exact solution is possible for the special case of $N_2 = 0$ (no detachment). In this case, Eq. 4a is uncoupled from Eq. 4b and its solution has the form:

$$c = \exp \left(-\left((1 + 4N_1N_3)^{1/2} - 1\right)c/(2N_1)\right)$$

$$\text{erfc} \left(((1 + 4N_1N_3)/\left(N_2N_3\right))^{1/2}(N_2z - t)/2 \right) + \exp \left((1 + 4N_1N_3)^{1/2}z/N_3\right)$$

$$\text{erfc} \left(((1 + 4N_1N_3)/\left(N_2N_3\right))^{1/2}(N_2z + t)/2 \right)$$

(5)

For $N_3 = 0$ (no diffusivity), Eq. 5 reduces to

$$c = \exp \left(-N_1z\right)H \left(t - N_2z\right)$$

(6)

where $H$ is the unit step function. For small amounts of diffusivity ($N_3 << 1$), the discontinuity exhibited by Eq. 6 at $\pm 4N_2$ is replaced by a narrow continuous transition layer. The corresponding solution for $s$ can be written as

$$s = N_1 \int_0^z c (z', t')dz'$$

(7)

For the special case in which both $N_1 = 0$ and $N_2 = 0$ (no attachment or detachment), Eq. 4a becomes a simple convection/diffusion equation and there is no collection ($s = 0$). Eqs. 5 and 6 are valid here with $N_1$ equated to zero. This leads to the respective results

$$c = \exp \left((N_2z - t)/(2(N_2N_3)^{1/2})\right) + \exp \left((N_2z + t)/(2(N_2N_3)^{1/2})\right)$$

$$\text{erfc} \left((N_2z - t)/(2(N_2N_3)^{1/2})\right)/2$$

(8)

and

$$c = H \left(t - N_2z\right)$$

(9)

This problem (due to the lack of attachment and detachment) is not really within the realm of filtration but the associated solutions are, nevertheless, useful as standards of comparison for the numerical method. An alternative interpretation of Eqs. 8 and 9 (which is relevant to filtration) will be given below.

An exact solution exists to the complete form of Eqs. 4a,b but it involves integrals which must be evaluated numerically (see Adin and Rajagopalan, 1989, for the special case of $N_1 = 0$). In the present work, it was decided to employ the method of Rasmussen (1975) to obtain a simpler approximate solution valid for moderate and large times which can more easily be used to illustrate certain points below. This has the form:

$$c = \exp \left(\text{erfc} \left(((N_1 + N_2N_3)N_2/(N_1 + N_3(N_1 + N_2N_3)^2))^{1/2}((N_1 + N_2N_3)^2c)/(N_1 + N_3(N_1 + N_2N_3)^2)\right) \right)$$

$$\left(N_1 + N_2N_3\right)^{1/2}/2$$

(10)

which reduces to
\begin{equation}
\begin{aligned}
c &= (\text{erfc} \left( (N_1 + N_2 N_3) N_5 / (N_1 r) \right)/2 \\
&\quad + \exp \left( (N_1 + N_2) z N_5 \right)/2) + \exp \left( (N_1 + N_2) r N_5 \right)/2)
\end{aligned}
\end{equation}

for \( N_3 = 0 \). In this case the corresponding expression for \( s \) is

\begin{equation}
\begin{aligned}
s &= (N_1 c + N_2 \partial_c c + \partial_c c - N_2 \partial_c c) N_5
\end{aligned}
\end{equation}

Eqs. 5 and 6 are respective special cases of Eqs. 10 and 11 found by equating \( N_5 \) in the latter to zero. The solutions reported above are for the fully dynamic situation (\( N_2 \neq 0 \)). In each case the corresponding quasistatic solutions can be obtained by formally equating \( N_2 \) (the measure of the transient completion time) to zero.

An interesting special case of Eqs. 10, 11, 12 occurs when the attachment and detachment rates are large and of comparable magnitudes. This is brought about by assuming \( N_2 \gg 1, N_5 \gg 1 \) with \( N_1 / N_5 = 0 \). Then Eq. 12 can be approximated by

\begin{equation}
\begin{aligned}
s &= N_1 c / N_5
\end{aligned}
\end{equation}

which can be recognized as characteristic of a quasiequilibrium situation. The respective corresponding limits of Eqs. 10 and 11 are

\begin{equation}
\begin{aligned}
c &= (\text{erfc} \left( (N_2 + N_1 N_3) z / 2 \right) + \exp (z N_5) \\
&\quad - \exp ((N_2 + N_1 N_3) z + t) / 2(\exp (N_2 z) - 1)) / 2)
\end{aligned}
\end{equation}

and

\begin{equation}
\begin{aligned}
c &= H (t - (N_2 + N_1 N_3) z)
\end{aligned}
\end{equation}

Comparing Eqs. 14 and 15 with Eqs. 8 and 9 shows that the latter with \( N_2 \) replaced by \( N_2 + N_1 N_3 \) are identical to the former. Thus, the quasiequilibrium limits of Eqs. 10 and 11 are formally identical to solutions of the simple convection/diffusion equation. This provides an alternate interpretation of Eqs. 8 and 9.

In the next two sections a number of numerical solutions are presented graphically. Unless otherwise noted on the figures the corresponding numerical calculations were carried out using step sizes of \( \Delta r = 0.001 \) and \( \Delta t = 0.001 \).

**NUMERICAL METHOD EVALUATION**

Some of the closed form solutions discussed in the previous section were used as standards of comparison for the results computed by the numerical method. A selection of such comparisons is discussed in this section. Most filtration solutions are carried out neglecting diffusion (\( N_3 = 0 \) in Eq. 4a). In this case Eq. 4a is first order in space and only one boundary condition is needed. It is imposed at the filter entrance (Eq. 4c). Most standard CFD codes, on the other hand, are set up to solve partial differential equations which are second order in the space variables. To make Eq. 4a compatible with such codes requires the retention of the diffusion term (\( N_3 \neq 0 \)) and imposition of two boundary conditions. In order to facilitate comparisons of solutions predicted with and without diffusion in a meaningful way, it is desired that the filter exit be a nonreflecting boundary. Analytically this can be achieved by finding a solution in a semi-infinite region and applying it only over the length of the filter (\( 0 \leq z \leq 1 \)). The closed form solutions presented thus far are to be interpreted in this way.

For finite difference computations, on the other hand, a finite computational domain is required. One can either choose a computational length \( z \gg 1 \) to approximate a semi-infinite region and use the computed solution only in the region \( 0 \leq z \leq 1 \) or directly impose a nonreflecting boundary condition at the filter exit \( z = 1 \). All the finite difference solutions to be discussed have been computed using the standard nonreflecting simple outflow boundary condition

\begin{equation}
\begin{aligned}
\partial_c c (1,t) = 0
\end{aligned}
\end{equation}

in addition to Eqs. 4c,d,e. To verify Eq. 16 some solutions were computed in a long region in which the concentration was assumed to vanish at \( z \approx 1 \). It was then shown that in the region \( 0 \leq z \leq 1 \) these solutions agreed quantitatively with the corresponding results computed using Eq. 16. This work will not be presented for sake of brevity. In the absence of diffusion (\( N_3 = 0 \)) Eq. 16 is dropped.
Fig. 1 pertains to the special case of Eq. 4a corresponding to $N_1 = N_5 = 0$. As mentioned previously, this can be interpreted either as an absence of attachment and detachment or as a quasiequilibrium between attachment and detachment. For the present purposes the physical interpretation is not as important as the fact that Eqs. 8 and 9 provide relatively simple standards of comparison for the numerical work.

If there is no diffusivity ($N_3 = 0$), the exact solution is a simple step function (Eq. 9). For small amounts of diffusivity the discontinuity exhibited by Eq. 9 turns into a smooth continuous narrow transition layer as shown by Eq. 8. Fig. 1 reports the exact and finite difference solutions corresponding to $N_1 = 0.001$. To the scale of the figure no difference can be detected between the numerical and exact solutions.

![Figure 2](image)

**Figure 2.** Concentration vs. Position (Finite Difference)

Most standard CFD codes allow for the use of artificial diffusivity as an aid to convergence. Such artificial diffusivity is often introduced by using two point backward difference quotients (rather than three point central difference quotients as employed herein) to discretize convection terms appearing in the transport equations. This is called upwind differencing. The existence of the exact solutions Eqs. 8 and 9 provides an opportunity to evaluate the influence of the artificial diffusivity associated with upwind differencing. It can be shown by a standard calculation that use of the most straightforward upwind differencing of the convection term of Eq. 4a in connection with a constant spatial step size $\Delta z$ is equivalent to the addition of a constant artificial diffusivity $\Delta z/2$ to the real diffusivity. If there is no real diffusivity, $N_3 = \Delta z/2$. Thus, the exact solution reported in Fig. 1 can be used as a standard of comparison for the numerical solution of Eq. 4a with $N_1 = N_3 = N_5 = 0$ using a step size of $\Delta z = (2)(0.001) = 0.002$ (501 points) and a straightforward upwind difference of the convection term. The exact solution is Eq. 9 as mentioned earlier. It can be seen that even for this small step size there is considerable diffusion of the discontinuity and that this effect increases with time. The corresponding numerical solution is shown in Fig. 2. It can be seen that in this case the finite difference process itself introduces no additional error.

Figs. 3 - 6 are associated with the special case of Eqs. 4a,b found by requiring $N_3$ to vanish. In this case the attachment rate is directly proportional to the concentration and there is no detachment. Again, the physical interpretation is not as important herein as the utility of Eqs. 5 and 6 as standards of comparison for the numerical work. In the absence of diffusivity the exact solution for the concentration is Eq. 6. Fig. 3 presents the exact and finite difference solutions for $C$. To the scale of the figure there is no difference between the numerical and exact solutions. Fig. 4 presents the associated numerical predictions for $\Delta z = 0.002$. Fig. 5 shows the specific deposit predictions corresponding to Fig. 3 and Fig. 6 reports the corresponding numerical solution for $\Delta z = 0.002$.

![Figure 3](image)

**Figure 3.** Concentration vs. Position (Exact and Finite Difference)

Again it is possible to infer some information about the effect of artificial diffusivity from Figs. 3 - 6. In the absence of real diffusivity the solution for $s$ in Eq. 6 and the corresponding solution for $s$ is

$$
S = N_1 (t - N_2 z) \exp (-N_1 z) (t - N_2 z)
$$

(17)

The exact solutions shown in Figs. 3 and 5 can be used as standards of comparison for numerical solutions of Eqs. 4a,b with $N_3 = N_5 = 0$ using 501 spatial points ($s = 0.002$) and straightforward upwind differencing of the convection term in
Eq. 4a. It can be seen that the discontinuities are again diffused with the effect being more apparent in Fig. 3 than in Fig. 5. The amount of smearing of discontinuities again increases with time. The actual numerical solutions are shown in Figs. 4 and 6. As before, it can be seen that the finite difference process itself introduces no additional smearing.

**Figure 4.** Concentration vs. Position (Finite Difference)

**Figure 5.** Specific Deposit vs. Position (Exact Finite Difference)

**Figure 6.** Specific Deposit vs. Position (Finite Difference)

**Figure 7.** Concentration vs. Position (approximate)
Figure 8. Concentration vs. Position (Approximate)

Figure 9. Concentration vs. Position (Finite Difference)

Figure 10. Concentration vs. Position (Finite Difference)

Figure 11. Specific Deposit vs. Position (Finite Difference)
result from either the use of a nonlinear form of $M$ or the existence of large concentrations. The latter effect was considered herein. Thus, Eq. 3a was dropped while Eqs. 3b,c,d,e,f were retained to yield

\begin{align*}
(N_2 - N_{12}) \partial c + \partial_z c &= N_2 \partial_z c \\
+ (1 - N_{12})(N_{12} - N_1c) \\
\partial_z s &= (1 - N_{12})(N_{12}c - N_{12}s)
\end{align*}

(18a)

(18b)

In order to illustrate the capabilities of the program, solutions were computed for an initial concentration of $N_1 = 0.5$ (several orders of magnitude higher than realistic for most situations). Some typical results of these simulations, together with reference predictions computed with $N_2 = 0$, are reported in Figs. 9 - 12.

Figs. 9 and 10 and 11 and 12 show the respective related concentration and specific deposit solutions obtained by the finite difference method for a small amount of diffusivity. The two sets of results differ significantly for the larger times. These solutions were obtained without numerical difficulties, illustrating the ability of the method to deal with nonlinear situations. It can be seen that the specific deposit has nearly reached its saturation value $s = N_1/N_2 = 0.2$ at the entrance at $t = 1$.

CONCLUSION

In the present paper a numerical method based on finite difference concepts was developed to solve a general form of the exact one dimensional depth filtration equations. The method was verified by comparison with exact solutions available for an approximate form of the equations and then employed to determine new solutions to the exact equations. It was observed that this methodology may require large computer times to deal with problems involving small or zero diffusivity (a common situation in filtration applications). This suggests that many existing commercial CFD codes are not well suited to the solution of filtration problems.

LITERATURE


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