Grid Peclet Number

The Peclet number is a non-dimensional term which compares characteristic time for diffusion (dispersion) given a length scale with the characteristic time for advection.

The wiggles start at mesh Peclet number above 2 (Unger A.J.A, Forsyth ,P.A. 1995) and the problem becomes more severe when the Peclet number increase.

Courant Number

Courant-Friedrichs-Lewy number, this parameter gives the fractional distance relative to the grid spacing traveled due to advection in a single time step



With Fourier error analysis it can be shown no matter a scheme (except fully implicit methods) is, it cannot advect a wave more than one grid in each step

Diffusion number

A similar expression may be derived for systems characterized by purely diffusion transport , giving rise to diffusion number:



ND<1

Amplitude and Phase error

**High resolution spatial schemes**

Because of the great interest in numerically simulating high Peclet number transport system (Advection dominant) large numbers of methods have been proposed. These include the method of characteristics or modified versions of it (Konikow and Bredehoeft, 1978; Arbogast et al., 1992; Chilakapati, 1993; Zheng and Bennett 1995; Roache ???) and adjoint Eulerian-Lagrangian methods (Celia et al. 1990). Both of these approaches are based on the treatment of the advection part of the transport equation using a Lagrangian scheme (a reference frame in which one follows the advective displacement of the fluid packet). An Eulerian (fixed) reference frame is then used to simulate dispersive/diffusive transport. The approach reduces numerical dispersion by reducing the effective grid Peclet number for the fixed Eulerian grid. Although there are some implementing restrictions the method of characteristics and its related approaches are still widely used when it is critical that numerical dispersion be avoided.

Another class of high resolution Eulerian methods uses higher-order approximations for the first derivatives, but hybridizes these with low order schemes in an attempt to obtain monotone solutions. The solutions have the higher-order approximations in smooth regions and the low-order accuracy near discontinuities (e.g. near plume fronts). The price to be payed for these schemes is that they are non-linear, even when applied to initially linear problem such as ADR equation. In this class are the flux –corrected transport (FCT) methods (Boris and Book, 1973; Oran and Boris 1987; Zalesak 1987; Hills et al., 1994) which usually gives excellent results when applied to non-reactive solute transport (Hills et al., 1994; Yabusaki et al.,) however, as in some of the other methods discussed here, very low level oscillation still coupled into solution.

TVD or total variation diminishing scheme, gives more nearly oscillation-free behavior (Bobey 1984; Yee 1987; Gupta et al. 1991). The TVD is one of a class of methods which use limiters to ensure monotonicity of solution (Van Leer 1977a,b; Leonard ,1984). TVD methods with flux limiter sometimes performs better than same order FCT counterpart on the reactive transport in case of oscillations (Steefel, C.I., MacQuarrie K.T., 1996)

# Methods for Coupling Reaction and transport

In recent decays much of the discussion about numerical approaches to reactive transport has centered on the question how to couple the reaction and transport terms. The reaction term affected local concentrations which in turn determine the fluxes of aqueous species. In the same way, the magnitude of the fluxes can affect the reaction rates. An accurate solution of the overall problem therefore requires that the terms be coupled at some level. Several methods have been proposed to solve the coupled set of equations. The straightest forward way conceptually, but the most demanding form as computational efficiency point of view, is to solve the governing equations, including both reaction and transport terms, simultaneously . This approach is referred to as a one\_step or global implicit method( Kee et al., 1987; Oran and Boris 1987; Steefel and Lasaga, 1994; Steefel and Yabusaki 1996). Alternatively, it is possible to use operator splitting techniques to decoupled set of equations (SNIA: sequential non-iterative approach by T.Xu) consist of solving the reaction and transport equations within a single timestep in sequence, with no iteration between the two. A method championed by Yeh and Tripathi (1989; 1991) is the sequential iteration approach or SIA where the reaction and transport are solved separately but iteration between the two calculations is carried out until a coverage solution is attained. There are variants on these approaches, including a predictor-corrector approach (Raffensperger and Garven, 1995) and Strang splitting approach (Zysset and Stauffer, 1992).

One –step or Global Method

Since the publication of the influential paper by Yeh and Tripathi (1989) which rejected the use of one-step or global implicit approach as being too CPU time and memory intensive, relatively little discussion of one step method for reaction-transport problem has appeared in the hyrochemical literature. This is despite the fact that the global implicit approach has been used successfully for some time in chemical and mechanical engineering fields (Kee et al. 1987) although even these fields are relatively merits of the decoupled or operator splitting approaches versus the one step approach still rages (Oran and Boris. 1987, Kee et al. 1987)

In one component system there is no difficulty in simply solving the entire system using standard iterative or direct linear algebra method. The problem is only slightly more difficult in case of two or three dimensional transport.

Using a global implicit approach become considerably more difficult in the case of a multi component, multi species system both because the coupling of species via reaction enlarges the size of the coefficient matrix and because it typically results in sets of nonlinear equations which , must be solved. Just as in the case of the time dependent reaction systems, the nonlinearities resulting from the reaction terms require the use of iterative methods. The size of the Jacobian matrix which must be constructed and solved becomes considerably larger since each function will include contributions from the concentrations both at that nodal point itself and from neighboring nodal points which are used in finite volume (or other methods) discretization. The major obstacle to the use of global implicit methods for multi-component reactive transport systems is the need for large amounts of computer memory.

Sequential non-iterative approach (SNIA)

At the other extreme from one step or global implicit method is the SNIA, also called the operator splitting or time splitting approach. In this approach, a single timestep consists of a transport step followed by a reaction step using the transport results. Physically, one can think of the method as equivalent to taking part of contents of one beaker (i.e. one node) and adding it to a second beaker downstream. After this physical process is completed, reactions occur which modify the chemical composition of each of breakers in the sequence. Mathematically, the method can be represented as a two step sequential process consisting of a transport step:



Followed by a reaction step:



where L is the spatial operator . The problem can also be formulated using the total concentration, thus reducing the number of equations which must be solved

Clearly the potential problem with the method is that it views the addition of fluid from one cell to another as being sufficiently rapid that the reactions only begin after the physical transport is complete. The greatest difficulties arise in kinetic systems for the entire timestep (Valocchi and Malmstead, 1992). For decay reaction where the concentration are continuously reduced therefore , the SNIA or operator splitting method would tend to overestimate the amount of reaction.

Strang Splitting

It is possible to reduce some of the errors associated with the SNIA method by using a time centered method referred to Strang splitting (Strang 1968; Zysset and Stauffer 1992). This method involves centering reaction step between two transport steps. The scheme can also be used with multiple reaction and transport steps, but in each case the reaction step will be centered. Where only a single reaction step is used, the method takes the form:



Followed by reaction step:



which is in turn followed by another ½ transport step:



Sequential iteration approach (SIA)

The Sequential iteration approach (SIA) has been suggested as a method which avoids the construction and manipulation of the large matrices characteristic of the global implicit approach and which corrects at the same time the errors which may occur in the use of the sequential non-iterative or classic operator splitting approach (Yeh and Tripathi, 1989; Yeh and Tripathi 1991; Zysset and Stauffer, 1992; Zysset et al., 1994 Walter et al., 1994). The presentation of the method, however, has been less than clear in the literature in fact, several different implementations of the method are possible. The basic idea is to arrive at a fully coupled solution at the n+1time level for both the transport and reaction terms. But rather than solving for the entire system of equations as in the global implicit method, the SIA approach accomplishes the coupling by iterating between the reaction and transport terms. Conceptually the most straightforward method involves solving the reactive transport equations in its full form at every step of the iterative process, alternating which term (reaction or transport) is included on the right hand side as asource term from the previous iteration (Zysset and Stauffer, 1992)





In this case, the iteration continues until the concentration computed in equation (1) agrees with the concentration computed in equation (2) to within some tolerance.

A more commonly used approach is to react the concentration coming out of the transport (plus reaction) step given by equation (1). The SIA method can also be formulated in terms of total concentration include both aqueous and solid phases.

Although the SIA method appears attractive because of its modular structure and its reduction of operator splitting error, it may occasionally show numerically unstable behavior depending on the problem considered. For problems involving decay type reaction, the method appears to reasonably well. But when solving other systems of reaction, however, they may be difficulties in getting the iterative procedure to converge (Engesgaard and Kipp 1992, Steefel and MacQuarrie 1996)