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ABSTRACT

INERTIAL EFFECTS IN TRANSPORT OF RADIOACTIVE WASTE THROUGH ENGINEERED BARRIERS.
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Addition of an inertial term to the constitutive relation for mass flux leads to a mass transport equation which is hyperbolic and describes propagation of a distorted wave with a finite velocity. This approach eliminates the "instantaneous propagation paradox" inherent in parabolic transport equations based on Fick's law. Analytical solutions of the wave transport equation have been derived and have the properties that the leading edge of a solute front propagates at a finite, predictable velocity and is truncated by a step function which decreases in magnitude exponentially with time. The inertial effects on computed solute fronts are most evident near the leading edge, and have potential significance in the prediction of engineered barrier performance.

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Mathematical models used to predict the performance of proposed engineered barrier materials traditionally have been constructed by combining the mass conservation equation with a constitutive relation describing the dependence of mass flux on forces acting on the system. Constitutive relations have taken a variety of forms; the usual practice in mass transport is to ignore thermodynamic couplings to other transport processes, to approximate chemical potential gradients by concentration gradients, and to write the constitutive relation for a single diffusing species in the form of Fick's law. In this form, the diffusive mass flux is stated to be proportional to the (negative) gradient of concentration through a transport coefficient which in a fluid-saturated porous matrix is the coefficient of hydrodynamic dispersion. This procedure results in a parabolic partial differential equation of transport, the "diffusion equation", and is subject to criticism on two grounds.

First, the simple phenomenological relation embodied in Fick's law was deduced from consideration of systems in steady states, and does not account for transient, inertial effects. Its application to systems showing explicit temporal dependence is questionable.

Second, solutions of the diffusion equation have the property that a material or thermal anomaly must be propagated with infinite velocity, i.e., the velocity of a concentration isopleth becomes large without bound as either time or concentration approaches zero. This non-physical result (the "instantaneous propagation paradox") has received increased attention in recent years in the literature of heat transport [e.g., Cattaneo (1958), Vernotte (1958), Swenson (1975), Liu (1979)].

The paradox can be resolved by careful consideration of inertial processes (i.e., temporal changes of forces and fluxes) in a transporting system. Thus, Bearman and Kirkwood (1958) and Bearman (1958, 1959) used a statistical mechanical analysis of momentum balance, and Machlup and Onsager (1953), Luikov (1966), Gyarmati (1977) and others used the thermodynamics of irreversible processes to derive constitutive relations including inertial terms explicitly. The simplest form of an inertial term is the (negative) time derivative of a flux, multiplied by a characteristic relaxation time; this term is added to the diffusive term in Fick's law to give the complete constitutive relation for a given flux. The result of combining such a relation with the mass conservation equation is a hyperbolic partial differential equation of transport describing a propagated wave with distortion caused by dissipative processes.

We have derived solutions to the wave equation of transport in one dimension for initial and boundary conditions appropriate to nuclear waste repositories, and have computed numerical results for a variety of values of transport properties (including the inertial relaxation time) of a hypothetical engineered barrier. Several properties of the solutions obtained are interesting in the context of the nuclear waste disposal problem:

- (1) The leading edge of a solute front propagates at a finite velocity dependent on the relaxation time, the dispersion coefficient, and the mean advective velocity of fluid flow (if any). In the limit as the relaxation time goes to zero, the velocity of propagation increases without bound and the wave solution approaches the diffusion solution. Conversely, as the relaxation time increases in an advective system, the velocity of propagation approaches the advective velocity, and the wave solution approaches a distortionless translation of the initial material anomaly.
- (2) The leading edge of a solute front is truncated by a step function which decreases in magnitude exponentially with time.
- (3) Inertial effects are most evident near the leading edge of the solute front, but as time becomes large relative to the time of arrival of the leading edge at a given location the wave solution approaches the diffusion solution; i.e., the mass flux becomes "Fickian".

It is evident that model calculations of breakthrough curves of radio-nuclides transported through engineered barriers could be erroneous near the leading edge if the inertial effect were sufficiently large. Conversely, theoretical interpretation of the results of laboratory measurements or of field monitoring experiments would be adversely affected by an incorrect choice of transport model. Although the statistical mechanical analysis of Bearman (1959) indicates that the inertial effect would be small relative to other transport processes in entirely fluid systems, the significance of the effect in partially or fully saturated porous media is not clear at this time, and we are currently investigating this point. However, it is clear that inclusion of inertial effects in mass transport provides, in principle, an improved physical basis for the evaluation of barrier performance.

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