

## Solute Extraction in Variable Density Flow: Shock Wave Driven Transport Compared to Pumping

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### ABSTRACT

We present simulations of a one dimensional model addressing solute migration subsequent to an abrupt pressure change applied to a variable density Newtonian fluid saturating a deformable porous medium (Sorek 1996). Mass and momentum balance equations for the fluid and an elastic matrix together with the solute mass balance equation, are solved by the Total Variation Diminishing (TVD) scheme.

The efficiency of extracting solute mass is assessed on a ratio between pumping using an approximate analytical solution following Darcy's equation, and TVD numerical simulations addressing the emitting of an expansion wave. This ratio can be calibrated in reference to four groups of parameters associated with: expansion waves sequence, matrix geometrical properties, fluid characterization and pumping depth. It was found that solute mass extracted by shock wave can be an order of magnitude greater in comparison to that by pumping.

### THE THEORETICAL MODEL

The conceptual model (Sorek 1996) may be summarized by the following set of assumptions: [A.1] The fluid is Newtonian. [A.2] The solid phase preserves its volume and the matrix is assumed to be elastic undergoing small vertical deformations. [A.3] Fluid dispersive and diffusive fluxes of the total mass and momentum are much smaller than the advective one and may, therefore, be neglected. [A.4] Isentropic conditions prevail. [A.5] Adsorption is governed by a linear equilibrium isotherm. [A.6] Porosity is mainly a function of pressure. [A.7] No fluid and solute sources are present. [A.8] Vertical pressure gradients are dominant and gravity body force is negligible. [A.9] Macroscopic stress-strain relationship for the solid matrix has the same form as that of the microscopic counterpart. [A.10] The solute component can be adsorbed on the matrix. Adsorption is governed by a linear isotherm. [A.11] The microscopic solid-fluid interfaces are material surfaces with respect to both phases mass. [A.12] Solid velocity is small in comparison to that of the fluid.

On the basis of assumptions [A.1] to [A.12] and in view of Bear et al. (1992), Krylov et al. (1996) and Sorek et al. (1996), following an abrupt pressure change (Sorek 1996), and accounting for Forchheimer tensor addressing the exchange of inertia at the microscopic solid-fluid interface ((Levy et al. 1995, 1999), during the wave propagation period we write the fluid ( )<sub>f</sub> mass and momentum balance equations respectively

$$\frac{\partial}{\partial t}(\phi \rho_f) + \nabla \cdot (\phi \rho_f \mathbf{v}_f) = 0, \quad (5)$$

$$\frac{\partial}{\partial t}(\phi \rho_f \mathbf{v}_f) + \nabla \cdot (\phi \rho_f \mathbf{v}_f \mathbf{v}_f) + \phi \nabla P \cdot \mathbf{T}_f^* + \phi \rho_f |\mathbf{v}_r| \mathbf{v}_r \cdot \tilde{\mathbf{F}} = 0, \quad \mathbf{v}_r \equiv \mathbf{v}_f - \mathbf{v}_s. \quad (6)$$

The solid ( )<sub>s</sub> mass and momentum balance equations read respectively

$$\frac{\partial}{\partial t}[(1-\phi)\rho_s] + \nabla \cdot [(1-\phi)\rho_s \mathbf{v}_s] = 0, \quad (7)$$

$$\begin{aligned} \frac{\partial}{\partial t}[(1-\phi)\rho_s \mathbf{v}_s] + \nabla \cdot [(1-\phi)\rho_s \mathbf{v}_s \mathbf{v}_s] + (1-\phi)\nabla P \cdot \mathbf{T}_s^* \\ - \nabla \cdot \boldsymbol{\sigma}'_s - \phi \rho_f |\mathbf{v}_r| \mathbf{v}_r \cdot \tilde{\mathbf{F}} = 0, \quad \boldsymbol{\sigma}'_s = (1-\phi)(\boldsymbol{\sigma}_s - \boldsymbol{\sigma}_f), \end{aligned} \quad (8)$$

where  $\rho$  denotes the phase density,  $\mathbf{v}$  denotes its velocity vector,  $\boldsymbol{\sigma}$  denotes its stress tensor with  $\boldsymbol{\sigma}'_s$  as the matrix effective stress,  $\mathbf{T}^*$  denotes its tortuosity tensor,  $P$  denotes pressure,  $\phi$  denotes porosity and  $\tilde{\mathbf{F}}$  denotes the Forchheimer tensor.

Following Sorek (1996), fluid density is pressure dominant at the period when its momentum balance equation conforms to a wave form. Neglecting the exchange of inertia at the microscopic solid-fluid interface and neglecting adsorption, solute mass balance equation reads (Sorek, 1996),

$$\frac{1}{C} \left( \frac{\partial C}{\partial t} + \mathbf{v}_f \cdot \nabla C \right) = -\frac{1-\phi}{\phi} \beta_\phi \rho_s k_d \mathbf{v}_f \cdot \nabla P - \frac{\phi \beta_p + \rho_s k_d S_0}{S_0} \nabla \cdot \mathbf{v}_f, \quad (9)$$

where  $C$  denotes solute concentration,  $\beta_\phi$  denotes the constant matrix compressibility,  $k_d$  denotes the partitioning coefficient associated with the linear equilibrium isotherm,  $\beta_p$  denotes fluid compressibility and  $S_0$  denotes specific storativity of the porous medium. Note that the right hand side of (9) represents source-like terms as (9) is decoupled from (5) and (6). These two latter equations can be combined into one for the case of a traveling wave (Landau and Lifshitz, 1987) when fluid's density, its pressure and velocity are mutually dependent (Sorek 1996). The state function when considering a liquid with constant compressibility  $\beta_p$  reads

$$P = P|_0 + \beta_p^{-1} \ln(\rho_f / \rho_f|_0), \quad (10)$$

where ( )|<sub>0</sub> denotes a reference value. For a perfect, compressible, gas we consider,

$$\frac{P}{\rho_f} = \text{Const.}, \quad \beta_p = (\gamma P)^{-1}, \quad (11)$$

where  $\gamma$  denotes the ratio of the fluid specific heat. Assuming a high Struhal number associated with porosity, small Mach number for the slightly deformable solid matrix, we follow Krylov et al. (1966) and account for

$$\phi = \phi|_0 + \frac{(1-\phi|_0)^2}{\lambda_s''} T_f^* (P - P|_0), \quad (12)$$

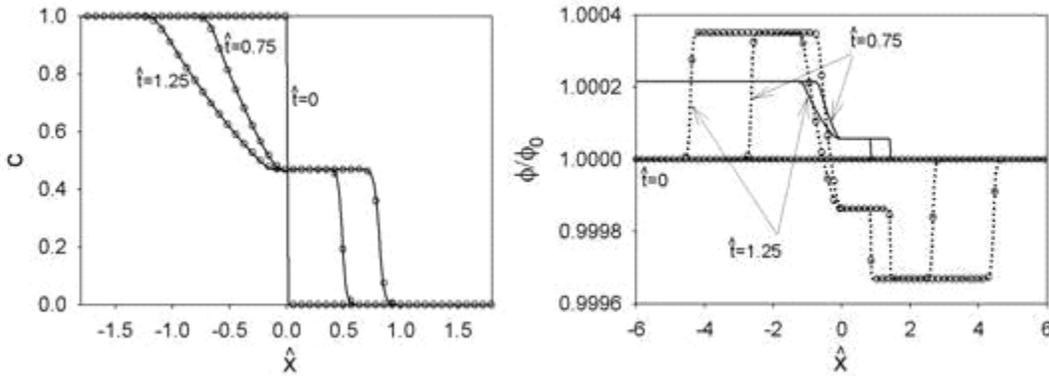
where  $\lambda_s''$  denotes the macroscopic Lamé constant for an elastic matrix, associated with vertical strain. When considering an elastic matrix undergoing small deformations, we refer to a constitutive relation for  $\boldsymbol{\sigma}'_s$  equivalent to the microscopic Hooks law and a strain tensor  $\mathbf{e}_s$  that read,

$$\boldsymbol{\sigma}'_s = \lambda_s'' \nabla \cdot \mathbf{w}_s \mathbf{I} + 2\mu'_s \mathbf{e}_s, \quad \mathbf{e}_s = \frac{1}{2} \left[ \nabla \mathbf{w}_s + (\nabla \mathbf{w}_s)^T \right], \quad (13)$$

where  $\mu'_s$  denotes the macroscopic Lamé constant associated with the shear strain,  $\mathbf{I}$  denotes the unit tensor and  $\mathbf{w}_s$  denotes the matrix displacement vector.

**SIMULATIONS OF SOLUTE MASS EXTRACTION**

Following Sorek (1996), we consider a one dimensional model for fluid pressure and velocity based on (5), (6) and solute migration (9), for an apparent new fluid (without Forchheimer term) concerning a traveling wave, a perfect gas, a slightly deformable matrix with (12) as its state function or for a deformable matrix accounting for (7) and (8). Emitting an expansion wave generates a pressure gradient governing the fluid flow that carries the solute towards the surface domain (Fig. 1).



**Figure 1. TVD numerical solution for Riemann's problem considering gas, high matrix stiffness ( $\lambda''_s \gg 1$ ) and neglecting inertia transfer expressed with Forchheimer term. The case of a deformable (ooooo) and of a slightly deformable (—) matrix.**

Solute extraction by shock waves is simulated by imposing pulses of abrupt pressure rise at the boundary ( $x = 0$ ), each of which emits an expansion wave into the domain. During the time interval between pulses, pressure at the boundary reverts to its former value during which it has no affect on the solute and the fluid (assuming a large reservoir). Hence, during each wave time period  $t_{pulse}$  when a pressure pulse is implemented, solute transport is advection dominant (Sorek, 1996) and associated with a specific mass flux  $Q_{solute} = \phi v_f C$ . During the time span  $[0, t_{final}]$  of

several pressure pulses,  $Q_{solute-w} (\equiv \frac{1}{t_{final}} \int_0^{t_{final}} Q_{solute} dt \Rightarrow Q_{solute-pulse} \frac{t_{pulse}}{t_{cycle}}$ , iff  $t_{final} \gg t_{pulse}$ ) will

be the average specific solute mass flux,  $t_{cycle}$  denotes the pulses time cycle and  $Q_{solute-pulse}$  denotes the extraction of solute specific mass flux during the time of one pulse.

Simulation of solute extraction towards the domain surface by pumping will refer to Darcy's law neglecting gravitational body force, using (10) or (11) as the fluid's state functions. As for pumping simulation drag is assumed dominant at the solid-fluid interface, the matrix momentum balance equation (8) is assumed static and (13) accounts for its stress constitutive law. We considered a practically rigid matrix and an incompressible fluid so that the solution for solute extraction by pumping passes rapidly the transient period and reaches a steady state at which stage, for constant pumping intensity at the surface, a comparison is done with results of solute extraction by the expansion wave. Hence, we developed an approximate analytical solution for the specific solute extraction mass flux  $Q_{solute-p}$  based on the aforementioned pumping conditions,

during the steady state period and for a compressible liquid following (10). The obtained expression reads.

$$\frac{Q_{solute-p}}{Q_{solute-w}} \cong \left( \frac{t_{cycle}}{t_{pulse}} \right) \frac{\kappa}{\mu_f} \frac{1}{\phi|_0} L \sqrt{\frac{\rho_f|_0}{T_f^* \beta_p}}, \quad (14)$$

where 1) Initial domain properties for extraction by an expansion wave are identical to the properties at  $x = L$  (i.e. the undisturbed boundary considering the expansion wave) for the extraction by continuous pumping, namely,  $( )_0 = ( )_L$  and 2) The pressure impulse at the surface ( $x = 0$ ) considering an expansion wave is identical to the pumping pressure for the continuous pumping. Table 1 is thus obtained in view of (14).

	Depth [m]	Pervious	Semi-Pervious	Impervious
		Sand & Gravel; Fractured Rocks	Silt; Loess; layered clay; Oil Reservoir Rocks	Unweathered Clay; Limestone; Dolomite
Water	30	0.06	5.0*E-05 to 5.0*E-07	5.0*E-09
Air	10	0.002	2.0*E-06 to 2.0*E-08	2.0*E-10

**Table 1. Values of  $Q_{solute-p} / Q_{solute-w}$  for typical matrix properties.**

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