SIMULTANEOUS HEAT AND SOLUTE TRANSPORT MODELING OF GROUND WATER WITH LATTICE BOLTZMANN METHODS

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ABSTRACT

Recent advances in Lattice Boltzmann modeling permit simulation of large-scale density-dependent ground water flow and heat/solute transport systems while retaining the advantages of ‘regular’ Lattice Boltzmann methods, such as solute/heat transport at higher Reynolds numbers that can characterize flows in conduits. We model the simultaneous heat/solute problem described by Henry and Hilleke in 1972 as an extension of Henry’s classic 1964 seawater intrusion problem. We also demonstrate the method’s ‘dual domain’ modeling potential.

1. INTRODUCTION

Natural convection driven by density variations can be a significant mode of fluid transfer in porous media. Changes in density can result from changes in solute concentration and temperature, or any combination thereof. Interest in the thermal aspects of convection in ground water systems has grown due to the maturation of modelling techniques and the ever-expanding need for groundwater resources, especially in costal areas (Thorne et al, 2006). As computing power increases, temperature-induced density-dependent modeling has also become more reasonable.

Almost all previous attempts to model convection have been preformed using finite difference or finite element methods (Guo and Zhao, 2005). The Lattice Boltzmann (LB) method can also be used to simulate density dependent flows. In simplistic terms, the LB equation governs the free streaming and collision of groups of particles that can also be subjected to various forces, including buoyant forces. In addition to representing fluid particles, additional particles that represent solutes and heat can be incorporated. In earlier work, buoyant solute transport in a ground water system (the Elder problem) has been accurately modeled with LB models (Thorne and Sukop, 2005), but temperature variations were not considered.

This paper discusses enhancements to a standard LB fluid flow model that allow simulation of density-dependent simultaneous solute and heat transport in a heterogeneous porous medium at any scale using a Darcy formulation and anisotropic dispersion. To include the temperature aspect, the density equation of state was modified to vary with changes in temperature, as well as changes in concentration. Specifically, the equation of state is

$$\rho(C,T) = \rho_f + \frac{\partial \rho}{\partial C}(C - C_0) + \frac{\partial \rho}{\partial T}(T - T_0), \tag{1}$$

where ρ_f is the density of the main fluid, C is the concentration, C_0 is a reference concentration, T is the temperature, and T_0 is a reference temperature (Hughes and Sanford, 2004).

2. METHODS

Simulation of thermohaline convection problems such as the Henry-Hilleke problem at any necessary scale with LB methods requires the extension of the basic fluid flow model to include the transport of 'passive scalars' that represent solutes and heat as well as the incorporation of a mechanism that converts the LB method from a complete Navier-Stokes solver to a Darcy's Law solver in desired portions of the model domain. Anisotropic dispersion (Zhang et al 2002a,b; Ginzburg, 2005) can also be incorporated when necessary. Introductions to LB methods for basic fluid flow can be found in many places (Sukop and Thorne, 2006; Thorne and Sukop, 2004; Succi, 2001; Wolf-Gladrow, 2000). We focus on the implementation of the less well known model extensions here.

2.1 LBM for solute and heat transport.

Yoshino and Inamuro (2003) present a method for simulating solute and heat transport using new LB 'components' – in addition to the main fluid component – that have their own distribution functions f_σ and f_η. We refer to these as the σ- and η-components for solute and heat respectively. These distribution functions are updated in the streaming and collision steps in the same way as the fluid distribution function *f*, except that they have their own relaxation times τ_σ and τ_η and a simpler equilibrium distribution function:

$$f^{eq}_{\sigma,\eta,a} = E_a \rho_\sigma (1 + 3 e_a \cdot u) \tag{2}$$

where

$$E_a = \begin{cases} \frac{4}{9} & a = 0 \\ \frac{1}{9} & a \in \{1,2,3,4\} \\ \frac{1}{36} & a \in \{5,6,7,8\} \end{cases} \tag{3}$$

The density (concentration) $\rho_{\sigma,\eta}$ of the solute or heat component is computed the same way as the density of the fluid:

$$\rho_{\sigma,\eta} = \sum_{a=0}^{8} f_{\sigma,\eta,\alpha} \; . \tag{4}$$

The mass or thermal diffusivity $D_{\sigma,\eta}$ of the solute or heat component is related to $\tau_{\sigma,\eta}$ by

$$D_{\sigma,n} = \frac{1}{3}(\tau_{\sigma,\eta} - \frac{1}{2}), \tag{5}$$

which is analogous to the kinematic viscosity ν for the fluid component. For the implementation of concentration/temperature boundary conditions needed by the Henry-Hilleke problem see Yoshino and Inamuro (2003).

The buoyancy effect is included as an adjustment to the velocity whose magnitude is determined by the relaxation time τ, the gravity $\boldsymbol{g}$, $\partial\rho/\partial C$, $\partial\rho/\partial T$, and the departure from the reference concentration and temperature:

$$\mathrm{u} = 1/\rho\sum_{a=0}^{8}\mathrm{f_a e_a} + \tau g\frac{\rho + \frac{\partial\rho}{\partial \mathrm{C}}\left(\mathrm{C} - \mathrm{C_0}\right) + \frac{\partial\rho}{\partial \mathrm{T}}\left(\mathrm{T} - \mathrm{T_0}\right)}{\rho} \tag{6}$$

where $\boldsymbol{u}$ is the velocity of the fluid and f_a is the distribution function.

2.2 LBM for Darcy's Law.

In accordance with Darcy's Law, the flow of fluid in porous media is proportion to its permeability. Dardis and McCloskey (1998a,b) introduce a volumetric solids fraction parameter n_s, $0 < n_s < 1$, along with a new step in the LB procedure to damp the evolution of momentum in proportion to n_s. This simulates a porous medium with porosity $1 - n_s$ in which permeability is inversely proportional to the solids fraction (see equation (12)). In simplistic terms, this method can be viewed as a probabilistic microscopic bounce-back in response to the fractional solid density.

The new porous media step takes place after the traditional collision step. Considering the traditional collision step as a second intermediate step after streaming, let f^{**} denote the result of the collision step:

$$f_a^{**}(x,t+\Delta t) = f_a^{*}(x,t) + \frac{1}{\tau}[f_a^{eq}(x,t) - f_a^{*}(x,t)], 0 \le a \le 8. \tag{7}$$

Then the porous media step has the form

$$f_a(x,t+\Delta t) = f_a^{**}(x,t+\Delta t) + n_s[f_{a'}^{**}(x+e_a\Delta t,t+\Delta t) - f_a^{**}(x,t+\Delta t)], 1 \le a \le 8 \tag{8}$$

where a' is the index of the direction opposite $\boldsymbol{e}_a$. Note that n_s can be a function of x, $n_s = n_s(x)$, which allows great flexibility in porous medium simulations; fractured porous media can be readily simulated for example.

If $n_s = 0$, the porous media step clearly has no effect, and the process reduces to the usual free-fluid LB method. If $n_s = 1$ on the other hand, then

$$f_a(x,t+\Delta t) = f_a^{**}(x,t+\Delta t) + f_{a'}^{**}(x+e_a\Delta t,t+\Delta t) - f_a^{**}(x,t+\Delta t) \tag{9}$$

$$f_a(x,t+\Delta t) = f_{a'}^{**}(x+e_a\Delta t,t+\Delta t) \tag{10}$$

$$f_a(x,t+\Delta t) = \frac{1}{\tau}[f_{a'}^{*}(x+e_a\Delta t,t) - f_{a'}^{eq}(x+e_a\Delta t,t)] = 0 \tag{11}$$

since $f \leftarrow f^{eq}$ in the beginning. This completely eliminates flow as expected.

Dardis and McCloskey (1998a,b) show that the permeability k of a medium with solid density n_s can be computed as

$$k = \frac{\nu}{2n_s} \tag{12}$$

where ν is the kinematic viscosity. We apply the porous media step only to the fluid component, not the solute or heat components.

2.3 Anisotropic dispersion in Darcy's Law LBM.

The combination of the solute transport and Darcy's Law make many new types of simulations – including for example the Henry-Hilleke problem considered below – possible. One important characteristic of solute and heat transport in porous media is not addressed by these modifications however; unlike diffusion, dispersion under flow conditions in a porous medium is anisotropic. Zhang et al (2002a,b) and Ginzburg (2005) have introduced LB models with multiple relaxation times (MRT) to simulate anisotropic dispersion.

The dispersion tensor is given by (Zhang et al, 2002a,b)

$$D_{\alpha\beta} = \Gamma_T \sqrt{u_x^2 + u_y^2}\,\delta_{\alpha\beta} + \frac{(\Gamma_L - \Gamma_T)u_\alpha u_\beta}{\sqrt{u_x^2 + u_y^2}} \tag{13}$$

where $\delta_{\alpha\beta}$ is the Kronecker Delta and Γ_L and Γ_T are the longitudinal and transverse dispersivities respectively ($\delta_{\alpha\beta} = 1$ for $\alpha = \beta$). This equation is solved at each node.

The dispersion tensor in terms of directional relaxation parameters τ_a is expressed as (Zhang et al, 2002a,b):

$$\begin{aligned} D_{xx} &= \frac{\delta x^2}{18\delta t}\left[4\tau_1 + \tau_5 + \tau_6 - 3\right] \\ D_{yy} &= \frac{\delta y^2}{18\delta t}\left[4\tau_2 + \tau_5 + \tau_6 - 3\right] \\ D_{xy} = D_{yx} &= \frac{\delta x \delta y}{18\delta t}\left[\tau_5 - \tau_6\right] \end{aligned} \tag{14}$$

Given the dispersion tensor, these equations are inverted to solve for relaxation times at each node that are subsequently used in the model.

To insure mass conservation, Zhang et al (2002a,b) used a weighted summation of the particle distribution function as shown in following equation to compute the density (concentration) of species subjected to the anisotropic dispersion:

$$\rho_{\sigma,\eta} = \sum_a \frac{f_a}{\tau_a}\left(\sum_i \frac{w_a}{\tau_a}\right)^{-1}. \tag{15}$$

With all of these modifications in place, we have essentially constructed a LB method density-dependent ground water flow simulator and a tightly coupled anisotropic dispersion CDE solver comparable to a number of available finite difference/finite element models. The new LBM ground water/transport model inherits at least one exceptional capability from its foundation however: it can accurately simulate flow and transport in large conduits or fractures that may involve higher Reynolds number flows and associated eddy mixing.

3. RESULTS

3.1 Dual domain solute transport example.

We present one example that illustrates the power of the combination of process that can be simulated. In Figure 1, a heterogeneous porous medium is cut by a conduit. A solute pulse is applied at the left boundary; it quickly fills the conduit and begins invading the porous medium – particularly in zones of higher hydraulic conductivity like the light colored areas above and to the left of center and at the lower right. Then flushing of the domain with solute-free water begins. Clear 'mushroom cap' plumes of solute-free water develop in the conduit illustrating the eddy mixing phenomenon. Flushing of the conduit will be complete long before the adjacent porous medium is flushed.

FIGURE 1. Model domain (left) showing conduit (white) in porous medium of variable hydraulic conductivity K (K inversely proportional to greyness) and solute invasion into porous medium and eddy mixing in conduit (right). See text for further explanation.

3.2 Henry-Hilleke thermohaline problem.

The Henry-Hilleke problem is an extension of Henry's classic 1964 work on seawater intrusion. Henry studied the Floridian plateau and the interactions between freshwater and seawater due to density differences. Eight years later Henry and Jeffery Hilleke expanded that work to include the temperature variation between geothermally-heated hot freshwater and cold seawater (Henry and Hilleke, 1972).

Several finite element and finite difference modeling programs have successfully simulated this problem: HST3D (Kipp, 1987), SUTRA-MS (Hughes and Sanford, 2004), and SEAWAT (Thorne et al, 2006). The LBM results will be compared to the more recent SEAWAT results.

The Henry-Hilleke problem consists of a rectangular domain representing a confined aquifer with a constant cool temperature boundary condition on the east and fixed linearly-varying temperatures along the top, bottom, and west boundaries (Figure 2).

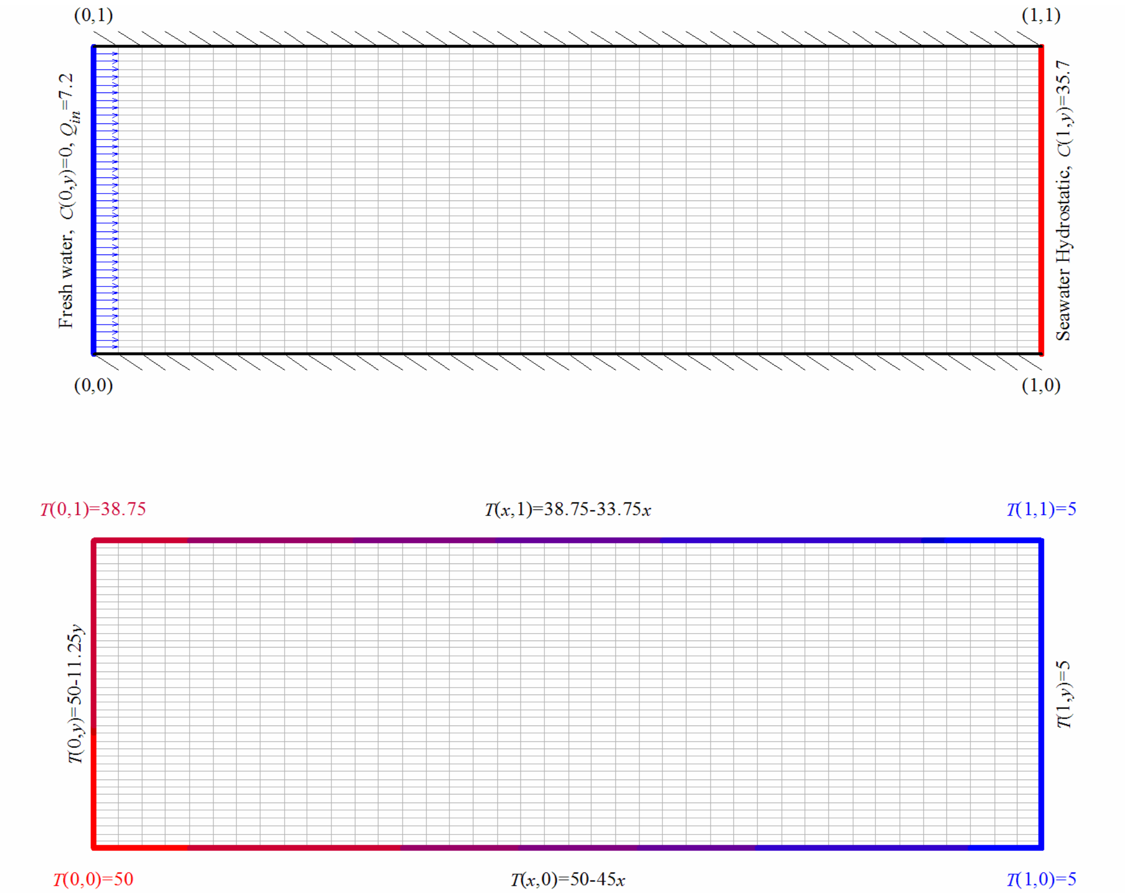

FIGURE 2. Hydrologic, salinity (top) and temperature (bottom) boundary conditions for Henry-Hilleke (1972) problem.

The ground water boundaries include no flow boundaries top and bottom, a specified flux on the west, and a seawater density hydrostatic head on the east. The parameters of the problem have been stated by Hughes and Sanford (2004) and are presented in Table 1.

TABLE 1. Parameters of the Henry-Helleke Problem and their values (Hughes and Sanford, 2004)

Parameter	Variable	Value
Freshwater Hydraulic Conductivity	K	864 m d^{-1} (=.01 m s^{-1})
Porosity	θ	0.35
Molecular Diffusion	D_m	2.0571 m^2 d^{-1} (=2.381×10^{-5} m^2 s^{-1})
Thermal Diffusivity	D^*	20.571 m^2 d^{-1} (=2.381×10^{-4} m^2 s^{-1})
Longitudinal and Transverse Dispersivity	α_l , α_t	0 m
Inflow	Q_{in}	7.2 $m^3 d^{-1}$
Salinity Concentration in Freshwater	C_f	0 kg m^{-3}
Salinity Concentration in Sea Water	C_s	35.7 kg m^{-3}

Density of Freshwater	ρ_f	1000 kg m^{-3}
Density of Sea Water	ρ_s	1025 kg m^{-3}
Density Change with Concentration	$\frac{d\rho}{dC}$	0.7
Density Change with Temperature	$\frac{d\rho}{dT}$	-0.375 kg m^{-3} °C^{-1}

The results of the SEAWAT simulation are shown in Figure 3.

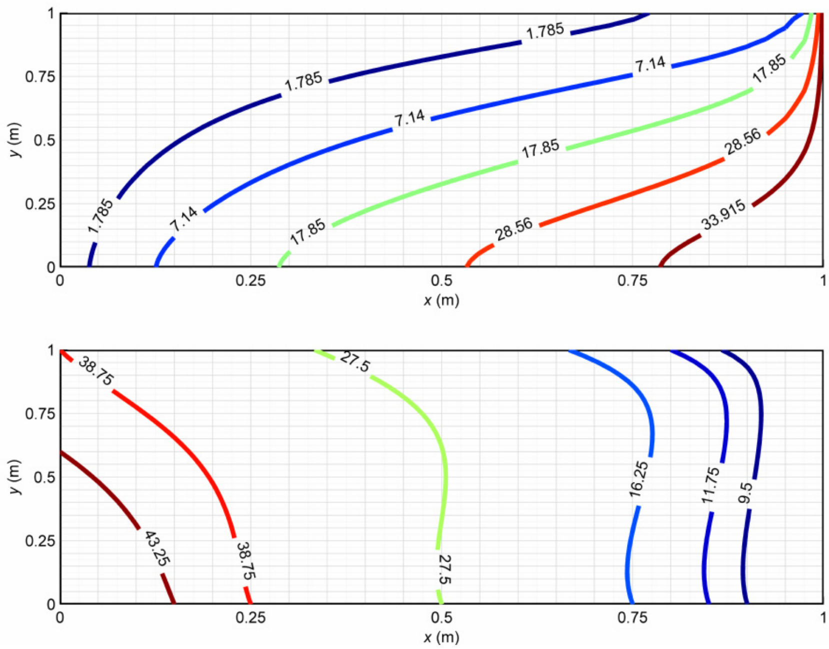

FIGURE 3. New SEAWAT finite difference results (Thorne et al, 2006) for Henry-Hilleke (1972) problem. Top: Salinity (kg m^{-3}). Bottom: Temperature (°C). Comparison with the enhanced LB model discussed here is pending.

4. CONCLUSIONS

Lattice Boltzmann methods can be enhanced to simulate density-dependent flow and anisotropic dispersion of heat and solutes in heterogeneous media at the Darcy scale while retaining their ability to simulate flow and transport at higher Reynolds numbers as occurs in subsurface conduits. The ability to simulate 'dual domain' systems with a complete Navier-Stokes solver that is tightly coupled to the Darcy/anisotropic CDE solver is exceptionally powerful. The addition of a second 'passive scalar' to represent heat transport and variable temperature to the fluid equation of state enables temperature-induced density-dependent flow. Comparison of simulation results for the Henry-Hilleke problem based on the newly expanded SEAWAT finite difference code (Thorne at al, 2006) and those based on the new LBM model is pending.

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