Eulerian-Lagrangian formulation of the equations for groundwater denitrification using bacterial activity

S. Sorek

Present Address: Biomedical Engineering, Technion, Haifa 32000, Israel
Affiliation: Ben-Gurion University of the Negev, J. Blaustein Institute for Desert Research, The Water Resources Research Center, Sede Boqer Campus 84993, Israel

C. Braester

Civil Engineering, Technion, Haifa 32000, Israel

A mathematical model for groundwater denitrification using bacterial activity is presented. The model includes the momentum and mass balance equations for water and nitrogen, substrate and bacteria, and chemical reactions between them. The resulting multiphase, multicomponent, flow and transport governing equations, are coupled and nonlinear. A Eulerian-Lagrangian formulation of the equations is developed. The water and gas flow and transport equations are split into forward advection along characteristics, and a residual at a fixed frame of reference. Discontinuities, sharp fronts and steep gradients of the dependent variables are imposed on the advection mode and solved exactly. It is believed that this novel method will avoid numerical artifacts for the solution of the multiphase flow equations (e.g., upstream permeability) and numerical dispersion for the transport equation.

Key Words: multiphase, multicomponent, flow and transport modelling, groundwater denitrification, nitrogen, substrate and bacterial chemical reactions, mass and momentum balance, Eulerian-Lagrangian decomposition to advection and residual terms.

1. THE MATHEMATICAL MODEL

The denitrification process considered in this study is transformation of nitrate (NO_3^-) to nitrite (NO_2^-) and nitrogen (N_2) in aquifers, using the bacterial activity in which glucose represents the carbon source.

In principle the treatment plant comprises a number of injection wells through which water with glucose, and possibly with nitrate, is injected into the aquifer, and production wells through which water free of nitrate is pumped out.

The main phenomena associated with the treatment are flow of water and nitrogen (gas), transport of substrates (glucose and nitrate) in the water phase, growth and decay of bacteria, adsorbtion of the different components on the solid matrix and chemical reactions between the bacteria and substrates. A quantitative solution to the denitrification problem requires that different processes be expressed mathematically and the resultant equations be solved simultaneously.

1.1 Flow phenomena

The fluids to be considered are water and nitrogen as the gas phase. Depending on the pressure of water in the aquifer, the nitrogen may be dissolved or not in water. With dissolved nitrogen the only fluid to be considered, is water with properties affected by the dissolved gas. With free nitrogen as the gas phase, flow of water and nitrogen is a two-phase flow described by the equations of conservation of momentum and mass as follows[9]:

Darcy's law for each phase ($i=1$ Water and $i=2$ Gas).

$$\mathbf{u}_i = -\frac{\mathbf{k}_i}{\mu_i}(\nabla p_i + \rho_i g \nabla z) \qquad (i \equiv W, G) \tag{1}$$

where $\mathbf{u}_i$ is Darcy's flux vector, $\boldsymbol{k}_i(S_i)$ is the permeability tensor function of fluid saturation S_i, p_i is pressure, $\mu_i(p_i)$ is dynamic viscosity, $\rho_i(p_i)$ is density, g is acceleration of gravity, and z denotes elevation above datum.

Equation (1) may also be expressed in terms of Hubbert's potential defined as:

$$\Phi_i = \int_{P_{o_i}}^{P_i} \frac{dP}{\rho_i g} + z \qquad (i \equiv W, G) \tag{2}$$

where P_{o_i} denotes a reference pressure.

The spatial and the time derivatives of Hubbert's potential are thus

$$\nabla \Phi_i = \frac{1}{\rho_i g} \nabla P_i + \nabla z \tag{3}$$

$$\frac{\partial \Phi_i}{\partial t} = \frac{1}{\rho_i g} \frac{\partial P_i}{\partial t} \tag{4}$$

In view of (1) and (3) we write Darcy's flux vector in terms of Hubbert's potential

$$\mathbf{u}_i=\frac{-\boldsymbol{k}_i}{\mu_i}\rho_i g\nabla\Phi_i \tag{5}$$

With only water and gas present, the sum of fluid saturation equals *one*, i.e.,

$$S_W+S_G=1 \tag{6}$$

The pressure in the water phase (wetting fluid) and in the gas phase (nonwetting fluid) are related through the capillary pressure (p_c) function of saturation

$$p_G-p_W=p_c(S_W) \tag{7}$$

Relationship (7) and the permeability saturation relationships

$$k_i=k_i(S_1) \qquad (i=W,G) \tag{8}$$

have to be determined experimentally for the considered couple of fluids and the considered aquifer.

Conservation of mass for each phase, water and gas, is expressed by

$$\frac{\partial(\phi S_i\rho_i)}{\partial t}+\nabla\cdot(\rho\mathbf{u}_i)=m_i^* \qquad (i\equiv W,G) \tag{9}$$

where ϕ is porosity, t denotes time and m_i^* mass flux per unit bulk volume injected/pumped into/from the aquifer.

By virtue of (6)–(8) we expand the first term of (9) as follows

$$\frac{\partial}{\partial t}(\phi S_i\rho_i)=\phi\rho_i\left[S_i(c_{r_i}+c_i)\frac{\partial P_i}{\partial t}+\frac{dS_i}{dP_c}\left(\frac{\partial P_G}{\partial t}-\frac{\partial P_W}{\partial t}\right)\right] \tag{10}$$

where c_{r_i} is the compressibility of the rock expressed as

$$c_{r_i}=\frac{1}{\phi}\frac{d\phi}{dp_i} \tag{11}$$

and fluid compressibility c_i is defined as

$$c_i=\frac{1}{\rho_i}\frac{d\rho_i}{dP_i} \tag{12}$$

The equations of state relating between density and pressure are:

For water, with c_W considered constant, integration of (12) yields

$$\rho_W=\rho_{oW}\exp[c_W(P-P_o)_W]\cong\rho_{oW}[1+c_W(P-P_o)_W] \tag{13}$$

where ρ_{o_W} is a reference value for water density. For gas

$$\rho_G=\frac{P_G}{Z}\cdot\frac{M}{RT} \tag{14}$$

where M is gas molecular weight, R is the universal constant of gases, T is absolute temperature and Z denotes the deviation factor of a real gas from the ideal behaviour, function of pressure and temperature.

For constant Z and T values, one may write (14) in the form

$$\left(\frac{\rho}{P}\right)_G=\left(\frac{\rho_o}{P_o}\right)_G=\frac{M}{ZRT} \tag{15}$$

Combining (13) and (15), we obtain

$$\Phi_W=z+\frac{1}{g\rho_W c_W}\ln[1+c_W(P-P_o)_W] \tag{16}$$

$$\Phi_G=z+\frac{1}{g\left(\frac{\rho_o}{P_o}\right)_G}\ln\left(\frac{P}{P_o}\right)_G \tag{17}$$

where the reference potential Φ at datum (z_o) equals zero, the pressure equals p_{o_i} and the density equals ρ_{o_i}, i.e.

$$z=z_o:\ \Phi=0;\quad p_i=p_{o_i};\quad \rho_i=\rho_{o_i} \tag{18}$$

In view of equations (4), (5), (6), (9) and (10), one may write the flow equation for water and gas in the following form

$$\rho_i R_i\frac{\partial\Phi_i}{\partial t}+\rho_i Y\rho_j\frac{\partial\Phi_j}{\partial t}=\nabla[\kappa_i\rho_i\nabla\Phi_i]+\frac{m_i^*}{g} \tag{19}$$

$$i\neq j, \qquad i\equiv W,G \qquad j\equiv G,W$$

where

$$R_W=\phi\rho_W\left[S_W(c_{R_W}+c_W)-\frac{dS_W}{dP_c}\right] \tag{20}$$

$$R_G=\phi\rho_G\left[S_G(c_{R_G}+c_G)-\frac{dS_W}{dP_c}\right] \tag{21}$$

$$Y=\phi\frac{dS_W}{dP_C} \tag{22}$$

$$\kappa_W=\frac{\mathbf{k}_W(S_W)}{\mu_W}\rho_W \tag{23}$$

$$\kappa_G=\frac{\mathbf{k}_G(S_G)}{\mu_G}\rho_G \tag{24}$$

Equation (19) has to be solved for Φ_i subject to initial and boundary conditions expressed symbolically as:

initial condition

$$\Phi_i=\Phi_{o_i} \tag{25}$$

boundary condition

$$(\rho\mathbf{u})_i n+\alpha_{\Gamma_i}(\Phi-\Phi_\Gamma)_i=m_{\Gamma_i} \tag{26}$$

where $\mathbf{n}$ is a unit rector normal to the boundary (Γ) and pointing outward for positive direction. The potentials Φ_{o_i}, Φ_{Γ_i} and m_{Γ_i}, the mass flux per unit bulk volume through the boundary are prescribed functions, and α_{Γ_i} controls the type of boundary condition prevailing along Γ.

For Dirichlet condition

$$\left.\begin{aligned}\alpha_{\Gamma_i} &\to \infty \\ \Phi_i &= \Phi_{\Gamma_i}\end{aligned}\right\} \tag{27}$$

For Neumann condition

$$\left.\begin{aligned}\alpha_{\Gamma_i} &= 0 \\ (\rho \mathbf{u})_i \cdot \mathbf{n} &= m_{\Gamma_i}\end{aligned}\right\} \tag{28}$$

and for mixed condition

$$0 \leqslant \alpha_{\Gamma_i} \leqslant \infty \tag{29}$$

Hence upon solving equations (19)–(29) and (5), we obtain the potentials (from which we can derive the pressures) and the velocities of the phases. As will be explained, the velocities are used for solving the transport equations.

1.2 Transport phenomena

The substrates, glucose and nitrate are transported in the water phase. The substrate is assumed to be consumed by the microbes at a rate R_{F_I} and adsorbed by an amount a per unit mass of solid matrix. A numerical model of the microbial transport in soils and groundwater was presented by Corapcioglu and Haridas[2]. This denitrification model is extended here for the two-phase flow of water and nitrogen and the correspondent microbial and chemical process.

The conservation of mass for the substrate I is expressed by

$$\frac{\partial}{\partial t}(S_W \phi C_I + \rho_s a) = R_{F_I} - \nabla[-\mathbf{D}_I S_W \phi \nabla C_I + \mathbf{u}_W C_I] + \left(\frac{m^*}{\rho}\right)_W C_I^* \qquad (I \equiv Gl., N_i) \tag{30}$$

where subscript $I \equiv Gl$ denotes the glucose component and subscript $I \equiv N_i$ denotes the nitrate (NO_3). In equation (30), (S_W, ϕ) denotes the volume occupied by the substrate per unit bulk volume of aquifer, ρ_s is bulk soil density, $\boldsymbol{D}_I$ is the dispersion coefficient tensor of the substrate, $\mathbf{u}_W$ is Darcy's specific flux vector and $[(m^*/\rho)_W C_I^*]$ represents sources/sinks within the water phase.

The chemical reaction is described by the stoichiometric equation

$$5C_6H_{12}O_6 + 24H^+ + 24NO_3^- \rightarrow 12N_2\uparrow + 30CO_2\uparrow + 42H_20 \tag{31}$$

We denote that $m_{Gl} = 5$ and $m_{mi} = 24$ are the mole numbers of the glucose and nitrate respectively.

Also we assume that the resulting product is not an inhibitor so it is not competitive with the substrates on the active site of the reaction in the bacterial medium.

The reactions rate R_{F_I} are described by

$$R_{F_I} = \lambda_I \frac{R_m C_{Gl} C_{Ni}}{\alpha_{Gl} C_{Ni} + \alpha_{Ni} C_{Gl} + C_{Gl} C_{Ni}} \tag{32}$$

$$\lambda_{Gl} = 1; \qquad \lambda_{Ni} = \frac{m_{Ni}}{m_{Gl}} \tag{33}$$

where R_m is the reaction rate which is a function of the enzyme concentration C_E (e.g. in mole/litre) in the bacterial medium.

$$R_m = E C_E \tag{34}$$

Here E denotes an analytic coefficient in [1/time] units. α_{Gl} and α_{Ni} are the Michael-Menton constants of substrate I which are determined by experiments.

Equations (32) and (33) expresses that the rate of production of a toxin can be dependent on its concentration. Thus the detoxification process has to be as fast as possible. This can be achieved by inserting an excess amount of glucose which will lead R_{F_I} to be close to the maximum rate R_m.

If bacteria have the possibility to move then conservation of mass of bacteria is expressed by

$$\frac{\partial (S_W \phi C)}{\partial t} = -\nabla[-\boldsymbol{D} S_W \phi \nabla C + \mathbf{u}_W C] - R_a + R_{d_f} + R_{g_f} + \left(\frac{m^*}{\rho}\right)_W C^* \tag{35}$$

where C is the concentration of bacteria in the water phase, ϕ is the pore space occupied by bacteria, $\boldsymbol{D}$ is the tensor bacteria dispersion coefficient R_a is the rate of bacteria deposition on grains, R_{d_f} is the rate of bacteria decay, R_{g_f} is the rate of bacteria growth and $[(m^*/\rho)_W C^*]$ is the source/sink term. In general, the first term at the right hand side of equation (35) is negligible in comparison to the other terms.

Conservation of deposited material is expressed by

$$\frac{\partial (\rho \beta)}{\partial t} = R_a + R_{ds} + R_{gs} \tag{36}$$

where ρ is the density of bacteria captured in the soil, β is the volume of the deposited bacteria per unit soil bulk volume, R_{ds} and R_{gs} denote respectively the rates of decay and growth of deposited bacteria.

The rate of deposition of bacteria R_a may be expressed in the form

$$R_a = \alpha_{cl}(S_W \phi - \beta) C - \alpha_{dcl} \rho \beta^{-\tau} \tag{37}$$

where α_{cl} and α_{dcl} are the rates of clogging and declogging respectively, τ is a constant and β is the value of the deposited material per unit solid bulk volume.

Death of bacteria may be expressed in the form

$$R_{df} = -\alpha_d S_W \phi C \tag{38}$$

and

$$R_{ds} = -\alpha_d \rho \beta \tag{39}$$

where R_{ds} is the rate of decay of deposited bacteria, α_d is the decay specific rate.

The growth of bacteria is assumed to obey Monod's law

$$R_{gf} = \psi S_W \phi C \tag{40}$$

and

$$R_{gs}=\psi\rho\beta \tag{41}$$

where ψ is the specific growth rate which is a function of substrate concentration C_l (Ref. 6).

$$\psi=\prod_{i=1}^{n}\frac{\psi_{m_l}C_l}{\alpha_{sl}+C_l} \tag{42}$$

where $\prod$ denotes the product of the $n=2$ substrates under consideration, ψ_{m_l} is the maximum growth rate achieved for $C_l \gg \alpha_{sl}$ and α_{sl} is the concentration of the substrate corresponding to hlaf growth rate at maximum value.

To these equations, one must add the chemical stoichiometric reaction equations relating between the amount of substrate, biomass and generated nitrogen.

In order to eliminate the $\nabla\cdot\mathbf{u}_W$ and $\partial(\phi S_W)/\partial t$ terms in (30), we multiply (9) for the water phase by C_l/ρ_W and subtact it from (30). Together with (32) and (33) we thus obtain

$$\phi S_W\frac{\partial C_l}{\partial t}=\nabla[\boldsymbol{D}_l\phi S_W\nabla C_l]-\mathbf{u}_W\cdot\nabla C_l + C_l\left\{\lambda_l\frac{R_m C_J}{\alpha_{Gl}C_{Ni}+\alpha_{Ni}C_{Gl}+C_{Gl}C_{Ni}} + gc_W\rho_W\left[\mathbf{u}_W\cdot\nabla(\Phi_W-z)+\phi S_W\frac{\partial\Phi_W}{\partial t}\right]\right\} + \left(\frac{m^*}{\rho}\right)_W(C_l^*-C_l)+\rho_s\dot{a} \tag{43}$$

where $\dot{a}\equiv da/dt$. $I\equiv Gl,\ Ni$, $J\equiv Ni,\ Gl$ and $J\neq I$.

Similarly, in view of (9), (35), (37), (38), (40) and (42) we write the transport equation for bacteria (B).

$$\phi S_W\frac{\partial C}{\partial t}=\nabla[\boldsymbol{D}\phi S_W\nabla C]-\mathbf{u}_W\cdot\nabla C + C\left\{\phi S_W\left[\left(\frac{\psi_{m_{Gl}}C_{Gl}}{\alpha_{s_{Gl}}+C_{Gl}}\right)\left(\frac{\psi_{m_{Ni}}C_{Ni}}{\alpha_{s_{Ni}}+C_{Ni}}\right)-(\alpha_{Cl}+\alpha_d)\right] + \alpha_{cl}\beta+gc_W\rho_W\left[\mathbf{u}_W\cdot\nabla(\Phi_W-z)+\phi S_W\frac{\partial\Phi_W}{\partial t}\right]\right\} + \left(\frac{m^*}{\rho}\right)_W(C^*-C)+\alpha_{dcl}\rho\beta^{-\tau} \tag{44}$$

Also in view of (36), (37), (39), (41) and (42) we write the conservation of bacteria (B) in the solid part of the soil

$$\beta\frac{\partial\rho}{\partial t}=\rho\left\{\beta\left[\left(\frac{\psi_{m_{Gl}}C_{Gl}}{\alpha_{s_{Gl}}+C_{Gl}}\right)\left(\frac{\psi_{m_{Ni}}C_{Ni}}{\alpha_{s_{Ni}}+C_{Ni}}\right)-\alpha_d\right]-\alpha_{dcl}\beta^{-\tau}-\dot{\beta}\right\} + \alpha_{cl}(\phi S_W-\beta)C \tag{45}$$

where $\dot{\beta}\equiv d\beta/dt$.

By virtue of (43) and (44), we may write a general nonlinear transport equation of the form

$$\phi S_W\frac{\partial C_l}{\partial t}=\nabla[\boldsymbol{D}_l\phi S_W\nabla C_l]-\mathbf{u}_W\nabla C_l+F_{1_l}C_l + \left(\frac{m^*}{\rho}\right)_W(C^*-C)_l+F_{2_l} \tag{46}$$

$l\equiv Gl,\ Ni,\ B$

where F_{1_l} and F_{2_l} are obtained when comparing (46) to (44) for $l=B$ and to (43) when $l\equiv Gl,\ Ni$.

In the case of the bacteria ($l\equiv B$) we write

$$F_{1_B}=\phi S_W\left[\left(\frac{\psi_{m_{Gl}}C_{Gl}}{\alpha_{s_{Gl}}+C_{Gl}}\right)\left(\frac{\psi_{m_{Ni}}C_{Ni}}{\alpha_{s_{Ni}}+C_{Ni}}\right)-(\alpha_{Cl}+\alpha_d)\right]+\alpha_{cl}\beta + gc_W\rho_W\left[\mathbf{u}_W\cdot\nabla(\Phi_W-z)+\phi S_W\frac{\partial\Phi_W}{\partial t}\right] \tag{47}$$

$$F_{2_B}=\alpha_{dcl}\rho\beta^{-\tau} \tag{48}$$

When dealing with the glucose (Gl) and the nitrate (Ni) components, we write for $l=Gl,\ Ni$ the expressions

$$F_{1_l}=\lambda_l\frac{R_m C_J}{\alpha_{Gl}C_{Ni}+\alpha_{Ni}C_{Gl}+C_{Gl}C_{Ni}} + gc_W\rho_W\left[\mathbf{u}_W\cdot\nabla(\Phi_W-z)+\phi S_W\frac{\partial\Phi_W}{\partial t}\right] \tag{49}$$

$$F_{2_l}=\rho_s\dot{a} \tag{50}$$

where $I\equiv Gl,\ Ni$, $J\equiv Ni,\ Gl$ and $J\neq I$.

Equation (46) is solved for C_l subject to

$$C_l(\mathbf{x},0)=C_{o_l}(\mathbf{x}) \tag{51}$$

and a general form concerning boundary conditions

$$(-\boldsymbol{D}_l\phi S_W\nabla C_l+\mathbf{u}_W C_l)\cdot\mathbf{n}+[\alpha_\Gamma(C-C_\Gamma)]_l=m_\Gamma^* C_l^* \tag{52}$$

The ρ value for the bacteria is obtained by solving the nonlinear equation

$$\beta\frac{\partial\rho}{\partial t}=G_1\rho+G_2 \tag{53}$$

subject to

$$\rho(\mathbf{x},0)=\rho_0(\mathbf{x}) \tag{54}$$

G_1 and G_2 are obtained by comparing (53) with (45).

$$G_1=\beta\left[\left(\frac{\psi_{m_{Gl}}C_{Gl}}{\alpha_{s_{Gl}}+C_{Gl}}\right)\left(\frac{\psi_{m_{Ni}}C_{Ni}}{\alpha_{s_{Ni}}+C_{Ni}}\right)-\alpha_d\right]-\alpha_{dcl}\beta^{-\tau}-\dot{\beta} \tag{55}$$

$$G_2=\alpha_{cl}(\phi S_W-\beta)C \tag{56}$$

Finally note the explicit coupling between the flow and transport problems. This coupling is pronounced through the coefficients F_{1_l}, F_{2_l}, G_1 and G_2.

2. EULERIAN-LAGRANGIAN FORMULATION FOR MULTIPHASE FLOW AND TRANSPORT

2.1 Introduction

The Eulerian-Lagrangian method combines the simplicitly of the fixed Eulerian grid with the Lagrangian approach especially effective in regions with advection dominated regimes (high Peclet numbers).

The solution technique consists of the following steps[4,5,7-11]:

(i) Formal decomposition of the dependent variable into two parts, one controlled by pure Lagrangian advection and a residual governed by a combination of Euler-Lagrange approaches.
(ii) Solution of the resulting advection problem, by the method of characteristics for forward particle tracking. The remaining problem is solved by an implicit finite element scheme on a fixed grid.

Information is projected back and forth between the Eulerian-Lagrangian and the Lagrangian schemes.

To understand the concept of such a decomposition, let us consider a governing equation of the form

$$Lu=f \tag{57}$$

where L is the partial differential operator; u is the dependent variable, and f is a source/sink term. u is decomposed into a translative term u_T and a residual term u_R

$$u=u_T+u_R \tag{58}$$

We also decouple the differential operator to

$$L=L_T+L_R \tag{59}$$

where L_T and L_R are the translation and residual differential operators respectively.

In view of equations (57)–(59), one may write

$$(L_T+L_R)(u_T+u_R)=f \tag{60}$$

One way to perform the decomposition is to allow

$$L_T u_T=0 \tag{61}$$

The term u_T is then solved along characteristic lines defined by

$$L_T\mathbf{X}=\mathbf{V} \tag{62}$$

where $\mathbf{X}$ is the vector of spatial position, and $\mathbf{V}$ is the velocity vector along the characteristic path. The exact solution of (61) is that u_T is constant along its path, yet the location $\mathbf{X}$ is known only if $\mathbf{V}$ is known. Otherwise iterations are required.

By virtue of (61), the next step is to solve the equation

$$Lu_R=f-L_R u_T \tag{63}$$

However, we may expect the condition

$$Lu_R \gg L_R u_T \tag{64}$$

In view of (63) and (64), we hence obtain

$$Lu_R \cong f \tag{65}$$

Since (65) is similar to a Poisson equation it is not expected to be subject to stability difficulties typical to advection dominant regimes. In cases with dominant source terms one may perform the decomposition, expressed in (60), by allowing u_T to obey

$$L_T u_T=f \tag{66}$$

By virtue of (63) and (64), we obtain the Laplacian form

$$Lu_R \cong 0 \tag{67}$$

which is more stable than equation (65).

The major problem of the decomposition strategy is the interpolation between the residual and translation solutions (as these two solutions are obtained at different spatial locations).

The interpolation (coupling between the solutions) should be performed in a mass conservation fashion to allow a conservative solution.

The following paragraphs will describe the theory of adopting the above mentioned method to the mass transport and flow problems for an aquifer environment.

2.2 The flow problem

Let us consider for convenience a typical 1-D flow equation of the form

$$R\frac{\partial \Phi}{\partial t}=\frac{\partial}{\partial X}\left[K\frac{\partial \Phi}{\partial X}\right]+M \tag{68}$$

Equation (68) written in a dimensionless form (subscript d) will be

$$\sigma_1\frac{\partial \Phi_d}{\partial t_d}=\frac{\partial^2 \Phi_d}{\partial X_d^2}+S_o\frac{\partial \Phi_d}{\partial X_d}+\sigma_2 M_d \tag{69}$$

Where the dimensionless parameters are defined by

$$X_d=\frac{X}{l} \qquad K_e=\frac{1}{l}\int_l K\,dx$$

$$\Phi_d=\frac{K}{K_e} \qquad \Phi_l=\frac{1}{l}\int_l \Phi\,dx$$

$$K_d=\frac{K}{K_e} \qquad R_e=\frac{1}{l}\int_l R\,dx$$

$$R_d=\frac{R}{R_e} \qquad t_e=\frac{R_e}{K_e}l^2$$

$$t_d=\frac{t}{t_e} \qquad M_e=\frac{K_e\Phi_e}{l^2}$$

$$M_d=\frac{M}{M_e} \tag{70}$$

Here l is a characteristic length which in a 1-D case denotes also the solution spatial domain.

The dimensionless numbers σ_1, σ_2 and the Sorek number S_o (Ref. 9) are

$$\sigma_1=\frac{R}{R_e}\frac{K_e}{K} \tag{71}$$

$$\sigma_2=\frac{K_e}{K} \tag{72}$$

$$S_o=\frac{l|\partial K/\partial X|}{K} \tag{73}$$

The governing equation (69) may become hyperbolic ($S_o\to\infty$) or parabolic ($S_o\to 0$) depending on relative importance of the Sorek number S_o.

Let us now define a material time derivative for the 1-D nondimensional problem.

$$\frac{D_1}{D_1 t}=\frac{\partial}{\partial t_d}+v\frac{\partial}{\partial X_d} \tag{74}$$

where v is the velocity along a characteristic path described by

$$\frac{D_1 X}{D_1 t}=v \tag{75}$$

We may rewrite (69) in the form

$$\left[\sigma_1\left(\frac{\partial}{\partial t_d}-\frac{S_o}{\sigma_1}\frac{\partial}{\partial X_d}\right)-\frac{\partial^2}{\partial X_d^2}\right]\Phi_d=\sigma_2 M_d \tag{76}$$

Comparison of equations (57), (74) and (76) yields

$$v=-\frac{S_o}{\sigma_1} \tag{77}$$

$$L=\sigma_1\frac{D_1}{D_1 t}-\frac{\partial^2}{\partial X_d^2} \tag{78}$$

$$u\equiv\Phi_d \tag{79}$$

$$f\equiv\sigma_2 M_d \tag{80}$$

By comparing equations (58), (59), (78) and (79) we write

$$L_T\equiv\sigma_1\frac{D_1}{D_1 t} \tag{81}$$

$$L_R\equiv-\frac{\partial^2}{\partial X_d^2} \tag{82}$$

$$\Phi_d=\Phi_{d_T}+\Phi_{d_R} \tag{83}$$

Thus, we can decompose (76) in one of the following two schemes:

Scheme A:

$$\sigma_1\frac{D_1\Phi_{d_T}}{D_1 t_d}=0 \tag{84}$$

to which the exact solution during time difference $D_1 t_d$ is

$$\Phi_{d_T}=\text{Const.} \tag{85}$$

The residual problem express by Φ_{d_R} is solved via the residual governing equation

$$\sigma_1\frac{D_1\Phi_{d_R}}{D_1 t_d}=\frac{\partial^2\Phi_d}{\partial X_d}+\sigma_2 M_d \tag{86}$$

Scheme B:

$$\sigma_1\frac{D_1\Phi_{d_T}}{D_1 t_d}=\sigma_2 M_d \tag{87}$$

to which the exact solution in increments of $D_1 t_d$, is

$$\Phi_{d_{T(t_d+D_1(t_D))}}=\left(\frac{\sigma_2}{\sigma_1}M_d\right)\cdot D_1 t_d+\Phi_{d_T}(t_d) \tag{88}$$

Φ_{d_R} is then solved through the residual equation

$$\sigma_1\frac{D_1\Phi_{d_R}}{D_1 t_d}=\frac{\partial^2\Phi_d}{\partial X_d^2} \tag{89}$$

An example of decoupling the multiphase flow equations into hyperbolic and parabolic parts was developed for a 1-D model by Bell *et al.*[1]. The model disregards gravitational effects and ignores capillarly pressure. Their spliting method uses the hyperbolic mass balance equation for transferring mass and a parablic equation for solving pressure distribution.

The method developed herein differs entirely from the one developed by Bell *et al.*. The Eulerian-Lagrangian method is applied to the combined mass balance and Darcy's equations in order to decompose the differential operator and the dependent variable.

We now proceed in reformulating the multiphase flow equations (equation (19)) using the Eulerian-Lagrangian concept.

We define an hydrodynamic time derivative for phases i

$$\frac{D_i}{Dt}=\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla\right)_i \qquad i\equiv W,G \tag{90}$$

where $\mathbf{v}_i$ is the velocity vector for phase i.

By virtue of equations (19) and (90) we rewrite (19) to the form

$$R_i\frac{D_i\Phi_i}{Dt}+Y\rho_j\frac{\partial\Phi_j}{\partial t}=\kappa_i\nabla^2\Phi_i+\frac{m_i^*}{\gamma_i} \tag{91}$$

where $\gamma_i=\rho_i g$. From (19), (90) and (91) it follows:

$$\mathbf{v}_i=-\left[\frac{1}{\rho R}\nabla(\rho\kappa)\right]_i \tag{92}$$

Expanding (92) and combining with equations (3), (7), (8), 12), (23) and (24), we obtain after some mathematical manipulations

$$\mathbf{v}_i=-\left(\frac{\rho}{\mu R}\right)_i\left\{\left(\frac{dk}{dS}\right)_i\frac{dS_i}{dP_c}\left[\gamma_G\nabla(\Phi_G-z)-\gamma_W\nabla(\Phi_W-z)\right]\right.$$
$$\left.+k_i\gamma_i(2c-\eta)_i\nabla(\Phi_i-z)\right\} \tag{93}$$

where

$$\eta_i=\left(\frac{1}{\mu}\frac{d\mu}{dP}\right)_i \tag{94}$$

The physical meaning v_i will be explained through the correlation between $\mathbf{v}$ and Darcy's specific flux $\mathbf{u}$.

In view of (5) and (23,24) we may rewrite Darcy's equation in the form

$$\mathbf{u}_i = -\left\{\left(\frac{k\rho}{\mu}\right)\left[\frac{\partial\Phi}{\partial\left(\frac{k\rho^2}{\mu}\right)}\right]\nabla\left(\frac{k\rho^2}{\mu}\right)\right\}_i \tag{95}$$

In view of (23,24), (92) and (95) we obtain

$$\mathbf{u}_i = \left\{R\left[(\kappa\rho)\frac{\partial\Phi}{\partial(\kappa\rho)}\right]\mathbf{v}\right\}_i \tag{96}$$

Note that in (19) Φ_i is evaluated at a fixed point of reference (Eulerian formulation) while in (91) Φ_i is evaluated in motion along its characteristic path line (Lagrangian formulation) described by

$$\frac{D_i\mathbf{X}_i}{Dt} = \mathbf{v}_i \tag{97}$$

where $\mathbf{X}_i$ denotes the spatial position vector for phase i.

Let us now decompose Φ_i into a translation term $\bar{\Phi}_i$ and a residual $\mathring{\Phi}_i$ term, i.e.

$$\Phi_i = (\bar{\Phi} + \mathring{\Phi})_i \tag{98}$$

One way to perform this decomposition is to let $\bar{\Phi}$ satisfy

$$\frac{D_i\bar{\Phi}_i}{Dt} = 0 \tag{99}$$

subject to the conditions

$$\bar{\Phi}_i(\mathbf{X}_i, 0) = \Phi_{o_i}(\mathbf{X}_i) \tag{100}$$

and

$$[\alpha_\Gamma(\bar{\Phi} - \Phi_\Gamma)]_i = m_{\Gamma_i} \tag{101}$$

By virtue of equations (25), (26), (91) and (99)–(101), the residual term $\mathring{\Phi}$ must satisfy

$$R_i\frac{D_i\mathring{\Phi}_i}{Dt} + Y\rho_j\frac{\partial\Phi_j}{\partial t} = \kappa_i\nabla^2\Phi_i + \frac{m_i^*}{\gamma_i} \tag{102}$$

subject to

$$\mathring{\Phi}_i\Phi\mathbf{X}_i, 0) = 0 \tag{103}$$

and

$$[\alpha_\Gamma\Phi_\rho - \kappa\rho\nabla\mathring{\Phi}\cdot\mathbf{n}]_i = 0 \tag{104}$$

We thus rigorously decomposed the multiphase flow problem (equations (19), (25) and (26)) into formal translation and residual problems described by (99)–(101) and (102)–(104) respectively.

The approach is to solve first the translation problem for $\bar{\Phi}_i$ and then to solve the residual problem, for $\mathring{\Phi}_i$ using the source terms generated by $\bar{\Phi}_i$.

2.3 The transport problem

Let us rewrite (46)–(50) the transport formulation for C_l ($l = Gl, N_i, B$) in the following general form

$$L_lC_l = f_l \tag{105}$$

Where L_l, the differential operator is expressed by

$$L_l = \phi S_w\left\{\frac{\partial}{\partial t} + \frac{1}{\phi S_w}[\mathbf{u}_w - \nabla(\boldsymbol{D}_l\phi S_w)]\cdot\nabla - (\boldsymbol{D}_l\phi S_w)\nabla^2 + \left[\left(\frac{m^*}{\rho}\right)_w - F_{1_l}\right]\right\} \tag{106}$$

and f_l the source term is given by

$$f_l = \left(\frac{m^*}{\rho}\right)_w C_l^* + F_{2_l} \tag{107}$$

We now define a material time derivative (D_l/Dt) for each l tracer

$$\frac{D_l}{Dt} = \frac{\partial}{\partial t} + \mathbf{v}_l\cdot\nabla \tag{108}$$

By comparing (108) to (106) we conclude that $\mathbf{v}_l$ may be comprised from a velocity $\mathbf{v}'$ associated with Darcy's specific flux ($\mathbf{u}_w$) *and a secondary term* $\mathbf{v}_l''$ in a direction from higher to lower values of the product ($\boldsymbol{D}_l\phi S_w$).

We thus write

$$\mathbf{v}_l = \mathbf{v}' + \mathbf{v}_l'' = \left[\frac{\mathbf{u}_w}{\phi S_w}\right] + \left[-\frac{\nabla(D_l\phi S_w)}{\phi S_w}\right] \tag{109}$$

By virtue of (108) and (109) we rewrite (106) to

$$L_l = \phi S_w\frac{D_l}{Dt} - (\boldsymbol{D}_l\phi S_w)\nabla^2 + \left[\left(\frac{m^*}{\rho}\right)_w - F_{1_l}\right] \tag{110}$$

Let us now decouple the differential operator L_l into an advective $\bar{L}_l$ and a dispersive (residual) $\mathring{L}_l$ differential operator

$$L_l = \bar{L}_l + \mathring{L}_l \tag{111}$$

where

$$\bar{L}_l = \phi S_w\frac{D_l}{Dt} \tag{112}$$

$$\mathring{L}_l = \phi S_w\left[\nabla^2 + \left(\frac{m^*}{\rho}\right)_w - F_{1_l}\right] \tag{113}$$

Note that the advective operator is associated with the Lagrangian formulation. The characteristic path lines for the Lagrangian formulation are defined by

$$\frac{D_l\mathbf{X}}{Dt} = \mathbf{v}_l \tag{114}$$

The concentration C_l is decomposed into an advective term $\bar{C}_l$ and a dispersive (residual) one $\mathring{C}_l$.

$$C_l = \bar{C}_l + \mathring{C}_l \tag{115}$$

Next we follow the scheme of (84) to obtain the governing equation for $\bar{C}_l$.

$$\bar{L}_l\bar{C}_l=\phi S_w\frac{D_l\bar{C}_l}{Dt}=0 \tag{116}$$

We solve (116) for $\bar{C}_l$ along its path line defined by (114) and subject to its initial and boundary conditions which in view of (51) and (52) are chosen as

$$\bar{C}_l(\mathbf{X},o)=C_o(\mathbf{X}) \tag{117}$$

and

$$\mathbf{u}_w\bar{C}_l\cdot\mathbf{n}+[\alpha_\Gamma(\bar{C}-C_\Gamma)]_l=m_l^*C_l^* \tag{118}$$

The solution of the advection problem for $\bar{C}_l$ (equations (114) and (116) to (118)) generates source terms for solving $\mathring{C}_l$.

By virtue of (105), (110), (115) and (116) the dispersion (residue) problem is then solved for C_l governed by a Eulerian-Lagrangian equation of the form

$$\frac{D_l\mathring{C}_l}{Dt}=\mathbf{D}_l\nabla^2C_l+\frac{F_{1_l}}{\phi S_w}C_l+\frac{1}{\phi S_w}\left(\frac{m^*}{\rho}\right)_w(C^*-C)_l+\frac{F_{1_l}}{\phi S_w} \tag{119}$$

subject to (in view of (51), (52), (117) and (118))

$$\mathring{C}_l(\mathbf{X},0)=0 \tag{120}$$

and

$$(-\mathbf{D}_l\phi S_w\nabla C_l+\mathbf{u}_w\mathring{C}_l)\cdot\mathbf{n}+(\alpha_\Gamma\mathring{C}_l)=0 \tag{121}$$

Note that the C_l value appearing in (119) holds $\bar{C}_l$ values which are solved separately along the pathline (114) and by the set (116) to (118).

Finally note that the two sets (116)–(118) and (119)–(121) describe a formal decomposition of the transport problem (46)–(50). Each set is solved separately, the advection problem by an exact solution for $\bar{C}_l$. We then reflect $\bar{C}_l$ onto prescribed spatial points where we solve the dispersion problem for $\mathring{C}_l$ using a numerical scheme such as the Finite Element method.

3. CONCLUSIONS

Most of the governing equations are nonlinear partial differential equations with functions determined experimentally. The only method of solution in this case is by a numerical technique.

At this stage of the investigation we focused our attention to develop a novel formulation for multiphase multicomponent flow and transport equations. The reason for this is that existent solutions for simultaneous two-phase flow include the artifiact of considering the upstream permeability proved to be unaccurate for large permeability values or/and low velocity values[12].

Numerical solutions of the transport type equation are associated with numerical dispersion and lack of accuracy in some range of the Peclet numbers.

To overcome the above mentioned difficulties encountered in the numerical flow and transport problem, a Eulerian-Lagrangian formulation of the equations was developed. The flow and transport equations are coupled and nonlinear. The developed method decomposes rigorously the flow equation of each phase into translative and residual modes. The same decomposition is also applied to the transport of each phase. The translative governing equation solves for the translative term of the dependent variable along characteristic lines. The residual governing equation solves for the residual term, of the dependent variable, at a fixed frame of reference. The translative mode enables an exact solution incorporating the advection of discontinuities, sharp fronts and steep gradients of the dependent variable. Tailoring between the translative and residual modes (for each phase within the flow and transport equations) is mass conservative. It is believed that because of the above mentioned reasons, the developed method will be found superior in numerical implementations.

ACKNOWLEDGEMENT

The present research was sponsored by a grant from the National Council for Research and Development – Israel, and the Commission of European Communities.

REFERENCES

1 Bell, J. A., Shublin, G. R. and Trangenstein, J. A. A method for Reducing Numerical Dispersion in Two-Phase Black-Oil Reservoir Simulation, *J. of Computational Physics*, 1986, **65**, 71–106

2 Corapcioglu Yavuz, M. and Haridas, A. Microbial Transport in Soils and Groundwater: A Numerical Model, *Adv. W. Resour.*, 1985, **8**, 188–200

3 Hoopes, J. A. and Harleman, D. R. F. Waste Water Recharge and Dispersion in Porous Media, *J. Hydraulics Div. Am. Soc. Civ. Eng.*, 1967, **93**, 51–71

4 Neuman, S. P. Adaptive Eulerian-Lagranian finite element method for advection-dispersion, *Int. J. Num. Meth. in Eng.*, 1984, **20**, 321–337

5 Neuman, S. P. and Sorek, S. Eulerian-Lagrangian Methods for Advection-Dispersion, Proc. 4th Inter. Conf. F.E.W.R., FGR, 1982, 14.41–14.68

6 Segel, I. Enzyme Kinetics, John Wiley, NY, 1975

7 Sorek, S. Eulerian-Lagrangian Formulation for Flow in Soils, *Adv. W. Res.*, 1985a, **8**, 118–120

8 Sorek, S. Adaptive Eulerian-Lagrangian Method for Transport Problems in Soils, Scientific basis for water resources management, *IAHS Pub.*, 1985b, **153**, 393–403

9 Sorek, S. and Braester, C. An Adaptive Eulerian-Lagrangian Approach for the Numerical Simulation of Unsaturated Flow, Proc. 6th Inter. Conf. F.E.W.R., Portugal, 1986, 87–100

10 Sorek, S. 2-D Adaptive Eulerian-Lagrangian Method for Mass Transport with Spatial Velocity Distribution, *Transport in Porous Media*, 1988a, **3**, 473–489

11 Sorek, S. Eulerian-Lagrangian Method for Solving Transport in Aquifers, *Adv. W. Res.*, 1988b, **11**(2), 67–73

12 Yorotos, Y. C. and Fokas, A. S. An analytical solution for linear waterflood including the effects of capillary pressure, *SPE*, 1983, 115–124