

# Theory and Application of Numerical Simulation of Chemical Flooding in High Temperature and High Salt Reservoirs

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# Abstract

Applications, theoretical analysis and numerical methods are introduced for the simulation of mechanical models and principles of the porous flow in high temperature, high salt, complicated geology and large-scale reservoirs in this paper. Considering petroleum geology, geochemistry, computational permeation fluid mechanics and computer technology, we state the models of permeation fluid mechanics and put forward a sequence of implicit upwind difference iteration schemes based on refined fractional steps of the upstream, which can compute the pressures, the saturation and the concentrations of different chemistry components. A type of software applicable in major industries has been completed and carried out in numerical analysis and simulations of oil extraction in Shengli Oil-field, which brings huge economic benefits and social benefits. This software gives many characters: spatial steps are taken as ten meters, the number of nodes is up to hundreds of thousands and simulation time period can be tens of years and the high-order accuracy can be promised in numerical data. Precise analysis is present for simplified models of this type and that provides a tool to solve the international famous problem.

# Keywords

High Temperature and High Salt Complicated Chemical Flooding, Computational Permeation Fluid Mechanics, Numerical Method and Engineering Software, Actual Application of Oil-Fields, Theoretical Analysis

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## 1. Introduction

At present an effective method, water-flooding, to keep the pressure of reservoirs is popular in the world, and the recovery efficiency is more outstanding than any other natural exploring forms. It gives more benefits and helps Chinese oil fields keep high quantity production. It continues to be more important and a strategic job to develop the exploiting efficiency of crude oil in the way water-flooding driving.

Much crude oil remains in the reservoir after water-flooding exploiting, which stays underground due to the constraint of capillary force, or doesn't move due to slight influenced region and the fluidity ratio between displacement phase and driven phase. How to develop the displacement efficiency? A popular method considered is that the injected mixture includes chemical addition agents such as polymer, surface active agent and alkali. Polymer can optimize the fluidity of displacement phase, modify the ratio with respect to driven phases, balance the leading edges well, weaken the inner porous layer, and increase the efficiency of displacement and the pressure gradient. Surface active agent and alkali can decrease interfacial tensions of different phases, then make the bounded oil move and gather. Some hypotheses should be made for the mathematical models. Local thermodynamic equilibrium holds in the reservoir, solid phase has no motion, and the rock and mixture fluid are slight-compressible, of Fick dispersion, ideal and suitable for Darcy Law.

The equilibrium equation of multi-phase, multi-components and slight compressible mixture is formulated by a nonlinear coupled system of partial differential equations. It is hard to solve this system because many modern numerical methods such as mixed element, finite element, finite difference and numerical algebra, will be involved in the simulation. In general speaking, based on physical means the pressure function is solved by an implicit scheme and the concentration values are obtained by an explicit solver or an implicit solver. The scholars try to find good ways analyzing the data and numerical results and doing some research work in simulation, which describe the whole process of chemistry displacements very well and help the engineers control the rules and process of displacement and forecast the recovery efficiency of natural oil and compute the oil percentage of output liquid and the percent of polymer and surface active agent. By numerical research the curves describing different components motion are shown, and some plans are made about the beginning and end of injected liquid and some related parameters of natural oil efficiency are derived. These conclusions, important techniques in chemistry displacements, can be used in forecasting the characters of fields, choosing different optimization plans, establishing the models of chemical displacements of reservoir, completing computational software and carrying out the numerical simulation. Petroleum engineers and mathematicians pay more attention to modern new techniques of exploiting natural oil.

Yuan visited United States and accomplished some work cooperate with Prof. R. E. Ewing during 1985 to 1988, and kept a series of research in theoretical analysis and applications of numerical simulation. With the leading of Yuan several research groups undertook some important projects from 1991 to 1995 such as "Eighth-Five" national key science and technology program (the Program for Tackling Key Programs) (85-203-01-087) entitled "research and application of the polymer displacement software" [1]-[6]. The software was applied in designing plan and research work of polymer displacements in industrial production region of Daqing Oilfield. Many conclusions from actual numerical results are illustrated such as effects of fragments, fragments setting of rinsing protection, quantity of polymer, and used in actual simulations which give rise to outstanding economic and social benefits [7]-[9]. Later the authors undertook a key tackling program of oil administration of Daqing Oilfield (DQYJ-1201002-2006-JS-9565)—solving development of mathematical models and completing explain of reservoir [10]. This software system is also applied in three compound combination flooding of Gudong Little Well experimental region of Shengli Oilfield, polymer flooding of Gudong West region and feasibility of active water flooding of Gudong eighth region, and many interesting results are obtained [11].

Theory, method and application of numerical simulation are studied for high temperature, high salt, complicated geology and large-scale reservoirs and the principle of chemical flooding in this paper. Based on the former research, the conclusions and more discussion of the national major special project on science and technology (2008ZX05011-004) "Study on key technology of chemical flooding numerical simulation in high temperature and high salt reservoirs (on numerical simulation)" are given, which consists of permeation fluid mechanical models of numerical simulation of high temperature and high salt polymer flooding and compound combination flooding, numerical methods, applicable software, theoretical analysis and applications in oilfields.

# 2. Mathematical Model of Polymer Flooding and Compound Combination Flooding

This section includes five subsections: Section 2.1, basic hypothesis, Section 2.2, conservation equation of matter, Section 2.3, the pressure equation, Section 2.4, the concentration equation, Section 2.5, the concentration equation of chemical components.

## 2.1. Basic Hypothesis

Mathematical model of polymer flooding and compound combination flooding is derived under the following hypothesis. Local thermodynamic equilibrium holds in the reservoir, solid phase doesn't motion, rock and mixture fluid are slight-compressible, of Fick dispersion, ideal and suitable for Darcy Law [1]-[3] [7]-[10].

#### 2.2. Conservation Equation of Matter

Under the primary hypothesis, a conservation equation of the *i*-th component is stated as follows dependent of the *i*-th concentration  $\tilde{C}_i$ :

$$\frac{\partial}{\partial t} \left( \phi \tilde{C}_i \rho_i \right) + \operatorname{div} \left[ \sum_{l=1}^{n_p} \rho_i \left( C_{il} \boldsymbol{u}_l - \tilde{\boldsymbol{D}}_{il} \right) \right] = Q_i, \qquad (1)$$

where  $C_{il}$  represents the concentration the concentration of the *i*-th component in the *l*-phase,  $Q_i$  means source sink term,  $n_p$  means the number of phases, and subscripts *l* denotes the order of phases. The symbol  $\tilde{C}_i$  represents the total concentration of the *i*-th component, *i.e.* the summation of concentrations of the *i*-th component in different phases (including adsorbed phase):

$$\tilde{C}_{i} = \left(1 - \sum_{k=1}^{n_{cv}} \hat{C}_{k}\right) \sum_{l=1}^{n_{p}} S_{l} C_{il} + \hat{C}_{i}, \qquad i = 1, \cdots, n_{cv},$$
(2)

where  $n_{cv}$ , the number of component whose volume couldn't be ignored, and  $\hat{C}_k$  denotes the adsorption concentration of the component k.

The density of the *i*-th component is dependent of the pressure  $\rho_i$  under slight compressible case:

$$\rho_i = \rho_i^o \Big[ 1 + C_i^o \left( p - p_r \right) \Big], \tag{3}$$

where  $\rho_i^o$  is the density of the *i*-th component under considering reference pressure  $p_r$ , and *p* means the pressure and  $C_i^o$  is the coefficient of compressibility of the *i*-th component.

Suppose that the rock is compressible, then the function of the porosity  $\phi$  and the pressure is

$$\phi = \phi_o \left[ 1 + C_r \left( p - p_r \right) \right], \tag{4}$$

where  $C_r$  means the coefficient of compressibility of the rock.

Darcy velocity,  $u_i$ , is described by Darcy Law,

$$\boldsymbol{u}_{l} = \frac{KK_{rl}}{\mu_{l}} \big( \nabla p_{l} - \gamma_{l} \nabla D \big), \tag{5}$$

where  $p_l$  means the pressure of phases, K is the permeability tensor, D is the depth,  $K_{rl}$  is the relative permeability,  $\mu_l$  is the viscosity and  $\gamma_l$  is the proportion.

The dispersion flux is expressed in the following Fick formation:

$$\tilde{\boldsymbol{D}}_{il} = \phi S_l \begin{pmatrix} F_{xx,il} & F_{xy,il} & F_{xz,il} \\ F_{yx,il} & F_{yy,il} & F_{yz,il} \\ F_{zx,il} & F_{zy,il} & F_{zz,il} \end{pmatrix} \begin{pmatrix} \partial C_{il} / \partial x \\ \partial C_{il} / \partial y \\ \partial C_{il} / \partial z \end{pmatrix}.$$
(6)

The dispersion tensor  $F_{il}$ , including molecular diffusion  $(D_{kl})$ , can be formulated as

$$F_{mn,il} = \frac{D_{il}}{\tau} \delta_{mn} + \frac{\alpha T_l}{\phi S_l} |\boldsymbol{u}_l| \delta_{mn} + \frac{(\alpha L_l - \alpha T_l)}{\phi S_l} \frac{u_{lm} u_{ln}}{\boldsymbol{u}_l},$$
(7)

where  $\alpha L_l$  and  $\alpha T_l$  denote the longitudinal and the lateral dispersion parameters of the *l*-th phase,  $\tau$  is the tortuosity,  $u_{lm}$  and  $u_{ln}$  are the components, and  $\delta_{mn}$  means Kronecher Delta. The net flow of each phase is:

$$|\boldsymbol{u}_{l}| = \sqrt{u_{xl}^{2} + u_{yl}^{2} + u_{zl}^{2}}.$$
(8)

## 2.3. The Pressure Equation

Considering all the conservative equations of each matter with positive volume together, using Darcy Law and capillary pressure to express the flux and the pressure relations of different phases respectively, and combining with the following constraints

$$\sum_{i=1}^{n_{ev}} C_{il} = 1,$$
(9)

We can get the pressure equation of referenced phase:

$$\phi C_t \frac{\partial p_w}{\partial t} + \operatorname{div} \cdot \left( K \lambda_T \nabla p_w \right) = -\operatorname{div} \cdot \left( \sum_{l=1}^{n_p} K \lambda_l \nabla h \right) + \operatorname{div} \cdot \left( \sum_{l=1}^{n_p} K \lambda_l \nabla p_{clw} \right) + \sum_{l=1}^{n_{cv}} Q_l,$$
(10)

where

$$\lambda_l = \frac{K_{rl}}{\mu_l} \sum_{i=1}^{n_{ev}} \rho_i C_{il}, \qquad (11)$$

and the total relative fluidity  $\lambda_T$  is

$$\lambda_T = \sum_{i=1}^{n_{cv}} \lambda_i.$$
(12)

The total coefficient of compressibility  $C_t$ , is a function dependent of the compressibility of rocks  $C_r$  and components of the mixture  $C_i^o$ :

$$C_t = C_r + \sum_{i=1}^{n_{cv}} C_i^o \tilde{C}_i.$$

## 2.4. The Concentration Equation

Let  $S_w$  and  $S_o$  be concentrations of water phase and oil phase denoted by subscripts w and o denote and the relation  $S_w + S_o = 1$  holds obviously. The equations on concentrations of water and oil phases are expressed as follows by conservation of the mass (1)

$$\frac{\partial}{\partial t} (\phi S_o \rho_o) + \operatorname{div} \cdot (\rho_o \boldsymbol{u}_o) = Q_o, \qquad (13)$$

$$\frac{\partial}{\partial t} (\phi S_w \rho_w) + \operatorname{div} \cdot (\rho_w u_w) = Q_w.$$
<sup>(14)</sup>

By Darcy Law the velocities of different phases are derived by

$$\boldsymbol{u}_{w} = -K\lambda_{rw} \left(\nabla P_{1} - \gamma_{1}\nabla D\right), \tag{15}$$

$$\boldsymbol{u}_{o} = -K\lambda_{ro}\left(\nabla P_{2} - \gamma_{2}\nabla D\right) = -K\lambda_{ro}\left(\nabla P_{1} + \nabla P_{c} - \gamma_{2}\nabla D\right),\tag{16}$$

where  $\lambda_{rw} = K_{rw}(S_w)/\mu_w(S_w, C_{1w}, \dots, C_{Lw})$ ,  $\lambda_{ro} = K_{ro}(S_w)/\mu_o(S_w)$  are the fluidities of two phases, and K,  $K_{rw}$  and  $K_{ro}$  are the absolute permeability tensor, relative permeabilities. K is the absolute permeability of medium, and  $\mu_w$ ,  $\mu_o$  are the viscosities of water-oil phases dependent on their concentrations and the saturations of polymer and the two opposing principles in nature.  $P_1$ ,  $P_2$  and  $\gamma_1$ ,  $\gamma_2$  respectively denote the pres-

sures and the densities of water phase and oil phase and D is the depth function,

$$D = D(x, y, z) = z.$$

#### 2.5. The Concentrations of Chemical Substance Components

Note that all the components (polymer and different principles) are mixed in the water phase and no transmission takes place, then

$$C_{il} = \begin{cases} C_{iw}, & l = w \\ 0, & l \neq w. \end{cases}$$
(17)

Substitute (17) into (1),

$$\frac{\partial}{\partial t} \left( \phi \rho_i \lambda_i C_{iw} \right) + \operatorname{div} \left[ \rho_i \left( C_{iw} \boldsymbol{u}_w - \tilde{\boldsymbol{D}}_{iw} \right) \right] = Q_i, \qquad (18)$$

where  $\lambda_i = S_w + A(C_{iw})$  and  $A(C_{iw})$  is dependent of the absorptions.

# **3. Numerical Methods**

This section consists of three subsections: Section 3.1 solving the pressure equation, Section 3.2 solving the concentration equation, and Section 3.3 structuring a numerical algorithm of components.

#### 3.1. Solving the Pressure

Let the parameters with subscripts w, o be related with the water and the oil respectively, such as  $S_w$ ,  $S_o$  and  $P_w$ ,  $P_o$  denote the saturations and the pressures of water and oil phases. Note that the mixture fluid is only made by oil and water two phases in the model of polymer flooding and compound combination flooding and we can describe the pressure in a simple formula

$$\phi c_t \frac{\partial P}{\partial t} + \operatorname{div} \cdot \left( \boldsymbol{u}_w + \boldsymbol{u}_o \right) = Q_w + Q_o.$$
<sup>(19)</sup>

Using Darcy Law and the formula of capillary force, we rewrite the above equation as follows with respect to an unknown variable  $P(P_w)$ ,

$$\phi c_t \frac{\partial P}{\partial t} - \operatorname{div} \cdot \left[ \left( \lambda_{rw} + \lambda_{ro} \right) \nabla P \right] = Q_w + Q_o + \operatorname{div} \cdot \left[ \lambda_{ro} \nabla P_c - \left( \gamma_w + \gamma_o \right) \nabla D \right].$$
(20)

The initial values of the saturations are known at the beginning of simulations while the pressure values should be initialized in the following process. When the pressure  $P^n$  at the *n*-th time step are known, then the flow velocities are obtained and the values of the saturation and components at the next step  $(t = t^{n+1})$  are computed. The pressure, denoted by a parabolic equation, is obtained by a seven-point central difference method. Considering the physical features of two-phase we assign  $\lambda_{rw}$  and  $\lambda_{ro}$ , the values of the left-side term, in accordance with upstream principles. At the injected wells and produced wells with fixed quantities, the right source term can be assigned directly and the values of quantity are determined by the difference between the pressure of local regions and the pressure of bottom holes at injected wells and produced wells with fixed pressures. The production quantities of different phases are distributed by the relative fluidity of oil-water phases. In addition, the pressure equation is degraded into an equation of elliptic type, and the matrix is not strictly diagonal-dominated under an impressible assumption (the coefficients of compressibility are assumed to be zero). In the way of taking the diagonal unit be 1 and non-diagonal units be zero, the equation of feature edges is consistent with the equation of normal oil deposits. The data in feature edges don't need to be replaced by the values of solutions, which makes the quantity of physical data as a constant in the computation. If the program (necessary for the design) runs at feature edges virtual data will be used in the whole computation.

Given  $P^n$ , using upstream seven-point central difference algorithm to compute  $P^{n+1}$ ,

$$\begin{split} \phi_{ijk} c_{i,ijk} \frac{P_{ijk}^{n+1} - P_{ijk}^{n}}{\Delta t} &- \frac{\left(\lambda_{rw,i_{j}jk} + \lambda_{ro,i_{j}jk}\right) \left(P_{i+1,jk}^{n+1} - P_{ijk}^{n+1}\right) - \left(\lambda_{rw,i_{j}jk} + \lambda_{ro,i_{j}jk}\right) \left(P_{ijk}^{n+1} - P_{i-1,jk}^{n+1}\right)}{(\Delta x)^{2}} \\ &- \frac{\left(\lambda_{rw,ijk} + \lambda_{ro,ijk}\right) \left(P_{ij,k+1}^{n+1} - P_{ijk}^{n+1}\right) - \left(\lambda_{rw,ijk} + \lambda_{ro,ijk}\right) \left(P_{ijk}^{n+1} - P_{i,j-1,k}^{n+1}\right)}{(\Delta y)^{2}} \\ &- \frac{\left(\lambda_{rw,ijk_{+}} + \lambda_{ro,ijk_{+}}\right) \left(P_{ij,k+1}^{n+1} - P_{ijk}^{n+1}\right) - \left(\lambda_{rw,ijk_{-}} + \lambda_{ro,ijk_{-}}\right) \left(P_{ijk}^{n+1} - P_{i,j-1,k}^{n+1}\right)}{(\Delta z)^{2}} \\ &= Q_{w,ijk}^{n+1} + Q_{o,ijk}^{n+1} - \frac{\lambda_{ro,ij,k}}{(P_{c,ijk}^{n+1} - P_{c,ijk}^{n+1}\right) - \lambda_{ro,i,jk}}{(\Delta x)^{2}} \left(\frac{\lambda_{rw,ijk_{+}} + P_{o,ijk_{-}}^{n+1}}{(\Delta y)^{2}} - \frac{\lambda_{ro,ij,k}}{(P_{c,ij,k+1}^{n+1} - P_{c,ijk}^{n+1}\right) - \lambda_{ro,ij,k}}{(P_{c,ijk}^{n+1} - P_{c,ij,k-1}^{n+1}\right)} \\ &+ \frac{\left(\frac{\gamma_{w,ij,k+1} + \gamma_{w,ijk}}\right) \left(D_{ij,k+1}^{n+1} - D_{ijk}^{n+1}\right) - \left(\gamma_{w,ijk} + \gamma_{w,ij,k-1}\right) \left(D_{ijk}^{n+1} - D_{ij,k-1}^{n+1}\right)}{2(\Delta z)^{2}}}. \end{split}$$

The subscript denotes the upstream position in the first direction between the *i*-th point and the (i+1)-th point. An assumption is given that there is no flow moving through the boundary. That is to say that its boundary condition is homogeneous of Neumann type. The quantities at the injected wells  $Q_o^{n+1} = 0$ ,  $Q_w^{n+1}$  are known and those at the produced wells  $Q_o^{n+1} = Q_o^{n+1}(P_f, P_o, S_o)$ ,  $Q_w^{n+1} = Q_w^{n+1}(P_f, P_w, S_w)$  are given implicitly by the flowing bottom hole pressure  $P_f$ , the pressures of phases and the relative mobility ratio. Distributed quantities are computed by an allocation program after the pressure values are obtained. It is easy to solve the saturation equation when the values of source and sink terms.

#### 3.2. Solving the Saturation

Using upstream order, implicit upwind Newton iteration to solve the saturation of water phase, then the values of oil saturation  $S_a = 1 - S_w$  are computed. The saturation of water phase is described by

$$\phi \frac{\partial S_w}{\partial t} + \operatorname{div} \cdot \boldsymbol{u}_w = Q_w,$$

or expressed in another form combined with Darcy Law

$$\phi \frac{\partial S_{w}}{\partial t} + \operatorname{div} \left( \lambda_{w} \left( S_{w} \right) \left( \nabla P_{w} - \gamma_{w} \nabla D \right) \right) = Q_{w}.$$
(22)

The pressure of water phase  $P_w$  at  $t^{n+1}$  and the quantity  $Q_w$  are known, then the saturation of water  $S_w$  at  $t^{n+1}$  are computed by the following discrete algorithm,

$$\phi_{ijk} \frac{S_{w,ijk}^{n+1} - S_{w,ijk}^{n}}{\Delta t} - \frac{\lambda_{w} \left(S_{w,i_{+}}\right) \left(P_{i+1,jk}^{n+1} - P_{ijk}^{n+1}\right) - \lambda_{w} \left(S_{w,i_{-}}\right) \left(P_{ijk}^{n+1} - P_{i-1,jk}^{n+1}\right)}{\left(\Delta x\right)^{2}} - \frac{\lambda_{w} \left(S_{w,j_{+}}\right) \left(P_{i,j+1,k}^{n+1} - P_{ijk}^{n+1}\right) - \lambda_{w} \left(S_{w,j_{-}}\right) \left(P_{ijk}^{n+1} - P_{i,j-1,k}^{n+1}\right)}{\left(\Delta y\right)^{2}} - \frac{\lambda_{w} \left(S_{w,k_{+}}\right) \left(P_{ij,k+1}^{n+1} - P_{ijk}^{n+1}\right) - \lambda_{w} \left(S_{w,k_{-}}\right) \left(P_{ijk}^{n+1} - P_{ij,k-1}^{n+1}\right)}{\left(\Delta z\right)^{2}} - \frac{2Q_{w,ijk}^{n+1}}{P_{w,ijk}} + \frac{\lambda_{w} \left(S_{w,k_{+}}\right) \left(D_{ij,k+1}^{n+1} - D_{ijk}^{n+1}\right) - \lambda_{w} \left(S_{w,k_{-}}\right) \left(D_{ijk}^{n+1} - D_{ij,k-1}^{n+1}\right)}{\left(\Delta z\right)^{2}} ,$$

$$(23)$$

where the subscript  $i_{+}$  denotes the upstream position according to the moving trend between  $x_{i}$  and  $x_{i+1}$ , *i.e.* 

it is either *i* or *i*+1. It is hard to solve the nonlinear equations directly.  $S_w^{n+1,l+1}$  at the (l+1) iteration step is obtained by Newton iteration under taking the value at the previous step as the initial condition  $S_w^{n+1,0} = S_w^n$ . Note the following Taylor expansion,

$$\begin{split} & \lambda_{w}\left(S_{w,i,jk}^{n+1,l+1}\right) = \lambda_{w}\left(S_{w,i,jk}^{n+1,l}\right) + \lambda_{w}'\left(S_{w,i,jk}^{n+1,l}\right) \left(S_{w,i,jk}^{n+1,l+1} - S_{w,i,jk}^{n+1,l}\right) + O\left(\left(S_{w,i,jk}^{n+1,l+1} - S_{w,i,jk}^{n+1,l}\right)^{2}\right), \\ & \lambda_{w}\left(S_{w,i,jk}^{n+1,l+1}\right) = \lambda_{w}\left(S_{w,i,jk}^{n+1,l}\right) + \lambda_{w}'\left(S_{w,i,jk}^{n+1,l}\right) \left(S_{w,i,jk}^{n+1,l+1} - S_{w,i,jk}^{n+1,l}\right) + O\left(\left(S_{w,i,jk}^{n+1,l+1} - S_{w,i,jk}^{n+1,l}\right)^{2}\right), \\ & \lambda_{w}\left(S_{w,i,jk}^{n+1,l+1}\right) = \lambda_{w}\left(S_{w,i,jk}^{n+1,l}\right) + \lambda_{w}'\left(S_{w,i,jk}^{n+1,l}\right) \left(S_{w,i,jk}^{n+1,l+1} - S_{w,i,jk}^{n+1,l}\right) + O\left(\left(S_{w,i,jk}^{n+1,l+1} - S_{w,i,jk}^{n+1,l}\right)^{2}\right), \\ & \lambda_{w}\left(S_{w,i,jk}^{n+1,l+1}\right) = \lambda_{w}\left(S_{w,i,jk}^{n+1,l}\right) + \lambda_{w}'\left(S_{w,i,jk}^{n+1,l}\right) \left(S_{w,i,jk}^{n+1,l+1} - S_{w,i,jk}^{n+1,l}\right) + O\left(\left(S_{w,i,jk}^{n+1,l+1} - S_{w,i,jk}^{n+1,l}\right)^{2}\right), \\ & \lambda_{w}\left(S_{w,i,jk}^{n+1,l+1}\right) = \lambda_{w}\left(S_{w,i,jk}^{n+1,l}\right) + \lambda_{w}'\left(S_{w,i,jk}^{n+1,l}\right) \left(S_{w,i,jk}^{n+1,l+1} - S_{w,i,jk}^{n+1,l}\right) + O\left(\left(S_{w,i,jk}^{n+1,l+1} - S_{w,i,jk}^{n+1,l}\right)^{2}\right), \\ & \lambda_{w}\left(S_{w,i,jk}^{n+1,l+1}\right) = \lambda_{w}\left(S_{w,i,jk}^{n+1,l}\right) + \lambda_{w}'\left(S_{w,i,jk}^{n+1,l}\right) \left(S_{w,i,jk}^{n+1,l+1} - S_{w,i,jk}^{n+1,l}\right) + O\left(\left(S_{w,i,jk}^{n+1,l+1} - S_{w,i,jk}^{n+1,l}\right)^{2}\right), \\ & \lambda_{w}\left(S_{w,i,jk}^{n+1,l+1}\right) = \lambda_{w}\left(S_{w,i,jk}^{n+1,l}\right) + \lambda_{w}'\left(S_{w,i,jk}^{n+1,l}\right) \left(S_{w,i,jk}^{n+1,l+1} - S_{w,i,jk}^{n+1,l}\right) + O\left(\left(S_{w,i,jk}^{n+1,l+1} - S_{w,i,jk}^{n+1,l}\right)^{2}\right). \end{split}$$

Delete the remainder truncation, substitute the approximation expressions into the difference algorithm, take  $S_{w,ijk}^{n+1,0} = S_{w,ijk}^{n}$  as iteration initial conditions and obtain the iteration values  $S_{w,ijk}^{n+1,l+1}$  at the (l+1)-th step by solving the following linear equations

$$\begin{split} \phi_{jk} \frac{S_{w,ijk}^{n+1} - S_{w,ijk}^{n}}{\Delta t} \\ - \left\{ \left[ \lambda_{w} \left( S_{w,i,jk}^{n+1,l} \right) + \lambda_{w}' \left( S_{w,i,jk}^{n+1,l} \right) \left( S_{w,i,jk}^{n+1,l+1} - S_{w,i,jk}^{n+1,l} \right) \right] \left( P_{i+1,jk}^{n+1} - P_{ijk}^{n+1} \right) - \left[ \lambda_{w} \left( S_{w,i,jk}^{n+1,l} \right) \left( S_{w,i,jk}^{n+1,l} \right) \left( S_{w,i,jk}^{n+1,l+1} - S_{w,i,jk}^{n+1,l} \right) \right] \left( P_{ijk}^{n+1} - P_{i-1,jk}^{n+1} \right) \right\} / (\Delta x)^{2} \\ - \left\{ \left[ \lambda_{w} \left( S_{w,ij,k}^{n+1,l} \right) + \lambda_{w}' \left( S_{w,ij,k}^{n+1,l} \right) \left( S_{w,ij,k}^{n+1,l+1} - S_{w,ij,k}^{n+1,l} \right) \right] \left( P_{i,j+1,k}^{n+1} - P_{ijk}^{n+1} \right) - \left[ \lambda_{w} \left( S_{w,ij,k}^{n+1,l} \right) + \lambda_{w}' \left( S_{w,ij,k}^{n+1,l} - S_{w,ij,k}^{n+1,l} \right) \right] \left( P_{ijk}^{n+1} - P_{i,j-1,k}^{n+1,l} \right) \right\} / (\Delta y)^{2} \\ - \left\{ \left[ \lambda_{w} \left( S_{w,ij,k}^{n+1,l} \right) + \lambda_{w}' \left( S_{w,ij,k}^{n+1,l} \right) \left( S_{w,ij,k}^{n+1,l+1} - S_{w,ij,k}^{n+1,l} \right) \right] \left( P_{ij,k+1}^{n+1} - P_{ijk}^{n+1} \right) - \left[ \lambda_{w} \left( S_{w,ij,k}^{n+1,l} \right) \left( S_{w,ij,k}^{n+1,l+1} - S_{w,ij,k}^{n+1,l} \right) \right] \left( P_{ij,k}^{n+1} - P_{ij,k}^{n+1,l} \right) - \left[ \lambda_{w} \left( S_{w,ij,k}^{n+1,l} \right) \left( S_{w,ij,k}^{n+1,l+1} - S_{w,ij,k}^{n+1,l} \right) \right] \left( P_{ij,k}^{n+1} - P_{ij,k}^{n+1,l} \right) - \left[ \lambda_{w} \left( S_{w,ij,k}^{n+1,l} \right) \left( S_{w,ij,k}^{n+1,l+1} - S_{w,ij,k}^{n+1,l} \right) \right] \left( P_{ij,k}^{n+1} - P_{ij,k-1}^{n+1,l} \right) \right] \left( \Delta z \right)^{2} \\ = Q_{w,ij,k}^{n+1,l} \\ + \left\{ \left[ \lambda_{w} \left( S_{w,ij,k}^{n+1,l} \right) + \lambda_{w}' \left( S_{w,ij,k}^{n+1,l} \right) \left( S_{w,ij,k}^{n+1,l+1} - S_{w,ij,k}^{n+1,l} \right) \right] \left( D_{ij,k+1}^{n+1} - D_{ij,k}^{n+1,l} \right) - \left[ \lambda_{w} \left( S_{w,ij,k}^{n+1,l} \right) \left( S_{w,ij,k}^{n+1,l+1} - S_{w,ij,k}^{n+1,l} \right) \right] \left( D_{ij,k}^{n+1,l} - D_{ij,k-1}^{n+1,l} \right) \right] \left( \Delta z \right)^{2} \\ = Q_{w,ij,k}^{n+1,l} \\ + \left\{ \left[ \lambda_{w} \left( S_{w,ij,k}^{n+1,l} \right) + \lambda_{w}' \left( S_{w,ij,k}^{n+1,l+1} - S_{w,ij,k}^{n+1,l} \right) \right] \left( D_{ij,k+1}^{n+1} - D_{ij,k}^{n+1,l} \right) - \left[ \lambda_{w} \left( S_{w,ij,k}^{n+1,l} \right) \left( S_{w,ij,k}^{n+1,l+1} - S_{w,ij,k}^{n+1,l} \right) \right] \left( D_{ij,k-1}^{n+1} - D_{ij,k-1}^{n+1,l} \right) \right\} \right\} / \left( \Delta z \right)^{2} \\ = Q_{w,ij,k}^{n+1,l} \\ + \left\{ \left[ \lambda_{w} \left( S_{w,ij,k}^{n+1,l} \right) + \left\{ \left\{ N_{w} \left( S_{w,ij,k}^{n+1,l} \right\} \right\} \right] \left( S_{w,ij,k}^{$$

The program runs based on upstream sequence rule, and the iteration value at the (l+1)-th step is computed until the relative error meets a designed requirement or the iteration reaches the steps when the values at upstream points are known. The final iterative value is denoted by  $S_w^{n+1}$ .

#### 3.3. Numerical Algorithm of Concentration Components

The components of water phase keep conservation of the mass of anions, cations and molecules and other particles, whose equation is of diffusion-convection and convection dominated. It has more strengths such as high order of accuracy and high efficiency of simulation applying decomposition of operators into the non-linear system and solving two subproblems: a hyperbolic equation of convection type and a diffusion equation. The former is solved implicitly by an upwind method, which can be carried out explicitly by an upstream technique. The latter is solved by alternating directions finite difference method, which can improve the computational speed. The concentration equation of k-component, a typical convection-diffusion equation, is simplified as follows

$$\phi \frac{\partial}{\partial t} (S_w C_k) + \operatorname{div} \cdot (C_k u_w - \phi S_w K \nabla C_k) = Q_k, \qquad (25)$$

where the dispersion tensor is a diagonal form. Given the saturation  $S_w$  and the flow field  $u_w$ , the concentration  $C_k$  is to be computed by using an implicit upwind method to solve a convection problem, where the subscript k is ignored and C denotes a component concentration.

$$\phi_{ijk} \frac{S_{w}^{n+1}C_{ijk}^{n+1,0} - S_{w}^{n}C_{ijk}^{n+1}}{\Delta t} + \left[C_{i_{+}jk}^{n+1,0}u_{w,ijk}^{n+1} - C_{i_{-}jk}^{n+1,0}u_{w,i-1,jk}^{n+1}\right] / \Delta x + \left[C_{ij_{+}k}^{n+1,0}u_{w,ijk}^{n+1} - C_{ij_{-}k}^{n+1,0}u_{w,i,j-1,k}^{n+1}\right] / \Delta y + \left[C_{ij_{+}k}^{n+1,0}u_{w,ijk}^{n+1} - C_{ij_{-}k}^{n+1,0}u_{w,ij,k-1}^{n+1}\right] / \Delta z = Q_{ijk}^{n+1},$$

$$(26)$$

The values  $C^{n+1,0}$  is obtained, then the diffusion equation is discretized alternatively in three directions. In *x*-direction,

$$\phi_{ijk} \frac{S_{w}^{n+1}C_{ijk}^{n+1,1} - S_{w}^{n}C_{ijk}^{n+1,0}}{\Delta t} - \left[\phi_{i+1/2, jk}S_{w,i_{+},jk}^{n+1}K_{xx,i+1/2, jk}\left(C_{i+1, jk}^{n+1,1} - C_{ijk}^{n+1,1}\right)\right] - \phi_{i-1/2, jk}S_{w,i_{-},jk}^{n+1}K_{xx,i-1/2, jk}\left(C_{ijk}^{n+1,1} - C_{i-1, jk}^{n+1,1}\right) / (\Delta x)^{2} = 0,$$
(27a)

Then in y-direction,

$$\phi_{ijk} \frac{S_{w}^{n+1}C_{ijk}^{n+1,2} - S_{w}^{n}C_{ijk}^{n+1,1}}{\Delta t}$$

$$- \left[\phi_{i,j+1/2,k}S_{w,ij_{+}k}^{n+1}K_{yy,i,j+1/2,k}\left(C_{i,j+1,k}^{n+1,2} - C_{ijk}^{n+1,2}\right)\right] - \phi_{i,j-1/2,k}S_{w,ij_{-}k}^{n+1}K_{yy,i,j-1/2,k}\left(C_{ijk}^{n+1,2} - C_{i,j-1,k}^{n+1,2}\right) / (\Delta y)^{2} = 0,$$
(27b)

At last in z -direction,  $C_{n+1}$  is obtained,

$$\phi_{ijk} \frac{S_{w}^{n+1}C_{ijk}^{n+1} - S_{w}^{n}C_{ijk}^{n+1,2}}{\Delta t} - \left[\phi_{ij,k+1/2}S_{w,ijk_{+}}^{n+1}K_{zz,ij,k+1/2}\left(C_{ij,k+1}^{n+1} - C_{ijk}^{n+1}\right)\right] - \phi_{ij,k-1/2}S_{w,ijk_{-}}^{n+1}K_{zz,ij,k-1/2}\left(C_{ijk}^{n+1} - C_{ij,k-1}^{n+1}\right) / (\Delta z)^{2} = 0,$$
(27c)

Then the discrete solutions  $P_w^{n+1}$ ,  $P_o^{n+1}$ ,  $S_w^{n+1}$ ,  $S_o^{n+1}$ ,  $C_k^{n+1}$  are obtained and the computation runs in the next step.

#### 3.4. Viscosity Computation of High Temperature and High Salt Reservoir

The polymer hydrolysis can decrease the viscosity in the high temperature and high salt reservoirs, and the viscosity is different under different polymers. The viscosity is computed by

$$\mu_{ap} = \mu_{w} + \left(\mu_{o} - \mu_{w}\right) \left[1 + \left(\gamma/\gamma_{1/2}\right)^{n(p)-1}\right]^{-1}, \qquad (28)$$

where the values of parameters are defined as follows,

$$\gamma_{1/2} = 375.3\mu_o^{-1.378} + 0.0356 , \quad n(p) = 1.163\mu_o^{0.0311} , \quad \mu_o = \mu_w + 0.634C_p \left[\mu\right] + 0.193\left(C_p \left[\mu\right]\right)^2 + 0.921\left(C_p \left[\mu\right]\right)^3 , \\ \left[\mu\right] = 4.665 \times 10^{-3} \,\overline{M}^{0.7969} + 4.219 \times 10^{-2} \left(1 - h_p^{1/2}\right) h_p \overline{M}^{0.76} / \sqrt{C_s} . \quad \overline{M} \quad \text{denotes the average molecular weight of}$$

polymer, and  $h_p$  denotes the degree of hydrolysis of the polymer with decimal unit.  $C_s$  means the degree of mineralization and  $C_p$  means the concentration of polymer, whose units are mol/L and mg/L, respectively.

#### 4. Computation Program Illustration

This section illustrates the computation program by Figure 1.

## **5. Actual Experimental Tests of Oil Fields**

The adaptation efficiency of the software SLCHEM is tested in view of three aspects: dependability, universality and special applicability for large-scale oilfields. The numerical results are dependable by comparing with the actual results and popular business software computations. The software is applied successfully in different fields of Shengli Oilfield and the universality is tested. The software is used in large-scale oilfields and the special applicability is tested.

#### 1) Experiments of the polymer flooding in small-scale oilfields

The rectangle computational domain (Tuo Block 28) is partitioned into  $22 \times 24 \times 6$  subdomains with uni-

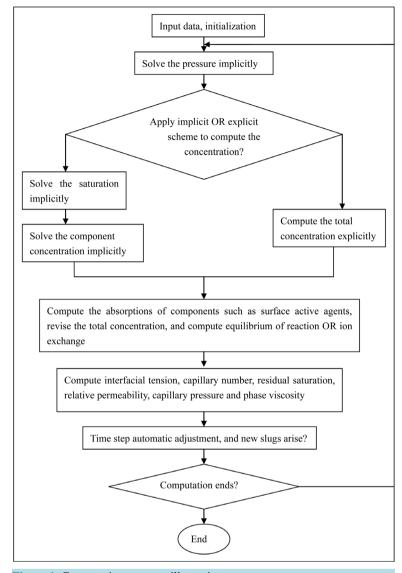


Figure 1. Computation program illustration.

form steps and the spacial steps in x-direction and y-direction are taken as 45.61 m and 47.35 m, respectively. The irreducible water saturation is 0.175, residual oil saturation is 0.25, and formation reserve is  $9.9843 \times 10^7$  m<sup>3</sup>. There are fifty four wells in this block. The simulation works about 22,402 days and is considered in three periods. It works in November, 1966 and water is injected in March, 1967. The polymer, whose concentration is 1500 ppm, is injected from June, 2008 to April, 2015. Water is injected again from April, 2015 to January, 2030. The simulation results are illustrated in Table 1.

The comparison of moisture content of produced oil of SLCHEM, VIP, and actual results are shown in Figure 2.

The time cost of SLCHEM is about 0.44 hour, and the material balance error is satisfactory. The relative total error comparison with actual moisture content is about 7.8% before the polymer flooding is injected. All the results show that the computation of SLCHEM runs fast, the numerical results are reliable and this scheme can be applied into present oilfields production.

#### 2) Experiments of surfactant-polymer flooding agents in middle-scale oilfields

The rectangle computational domain (Sheng Block 2) is partitioned into  $82 \times 74 \times 7$  subdomains with uniform steps and the spacial steps in x-direction and y-direction are taken as 33.60 m and 29.29 m, respectively. Formation reserve is  $3.4938 \times 10^8$  m<sup>3</sup>. There are sixty three wells in this block. The simulation works about

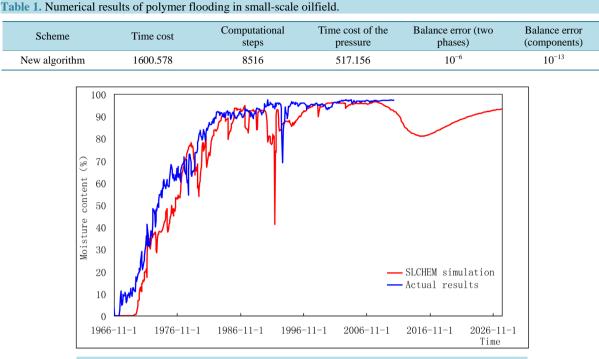


Figure 2. Curve of moisture content simulation of produced oil of polymer flooding in smallscale oilfields.

\$2362 days and is considered in three periods. It works on April 1, 1966 and water is injected on January 1, 1974. The polymer, whose concentration is 1600 ppm, is injected from August, 2010 to September, 2016. Surfactant, whose concentration is 0.4%, is injected from August, 2011 to October, 2011. The largest time step is less than five days and the simulation results are illustrated in Table 2.

The comparison of moisture content of produced oil of SLCHEM, ECLIPSE, and actual results are shown in **Figure 3**. The time cost of SLCHEM is about 4.2 hours, and the material balance error is satisfactory. The relative total error comparison with actual moisture content is about 7.10%. All the results show that the computation of SLCHEM runs fast, the numerical results are reliable and this scheme can be applied into present oilfields production.

#### 3) Experiments of large-scale oilfields

The rectangle computational domain (Gudaoguan Block 3) is partitioned into  $72 \times 62 \times 26$  subdomains with uniform steps and the spacial steps in *x*-direction and *y*-direction are taken as 25 m. Formation reserve is 22,708,200.0 m<sup>3</sup>. There are one hundred and ninety one wells in this block. The simulation works about 12,965 days and is considered in three periods. It works on September 1, 1971 and water is injected on September 1, 1974. The polymer, whose concentration is 1000 ppm, is injected from March 1, 1994 to November 30, 2003. Water is injected again from December 1, 2003 to March 1, 2007. The largest time step is less than ten days and the simulation results are illustrated in Table 3.

The comparison of moisture content of produced oil of SLCHEM and actual results are shown in Figure 4.

The time cost of SLCHEM is about 8.45 hours, and the material balance error is  $10^{-6}$ . The relative total error comparison with actual moisture content is about 7.0%. All the results show that the computation of SLCHEM runs fast, the numerical results are reliable and this scheme can be applied into present oilfields production.

#### 4) Numerical simulation of surfactant polymer flooding

The polymer, whose concentration is 1000 ppm, is injected from March 1, 1994 to November 30, 2003. Surfactant, whose concentration is 0.5%, is injected from May 1, 1996 to December 1, 2003. Then water is injected again from December 1, 2003 to March 1, 2007. The largest time step is less than ten days and the simulation results are illustrated in Table 4.

Numerical results of SLCHEM of water flooding, polymer flooding and surfactant-polymer flooding are compared in Figure 5. The time cost of SLCHEM is about 13.5 hours, and the material balance error is satis-

Table 2. Numerical results of surfactant-polymer combination flooding in middle-scale oilfields.							
Scheme	Time cost	Computational steps	Time cost of the pressure	Balance error (two phases)	Balance error (components)		
New algorithm	15213.343	5520	12929.656	10 <sup>-6</sup>	10 <sup>-12</sup>		
Cable 3. Numerical results of polymer flooding in large-scale oilfields.							

Scheme	Time cost	Computational steps	Time cost of the pressure	Balance error (two phases)	Balance error (components)
New algorithm	30426.28	6106	20214.90	$10^{-6}$	$10^{-14}$

## Table 4. Numerical results of surfactant-polymer flooding.

Scheme	Time cost	Computational steps	Time cost of the pressure	Balance error (two phases)	Balance error (components)
New algorithm	48877.72	6894	33276.23	$10^{-6}$	$10^{-14}$

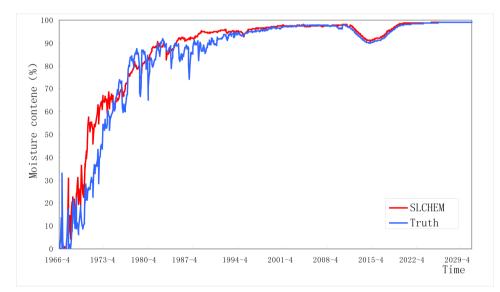


Figure 3. Curve of moisture content simulation of produced oil of two components combination flooding in middle-scale oilfields.

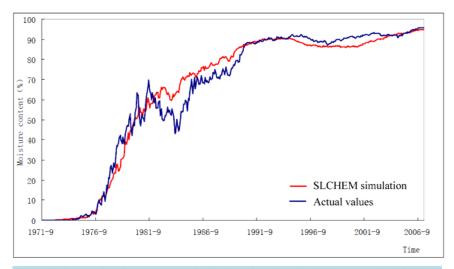


Figure 4. Curve of moisture content simulation of produced oil in large-scale oilfields.

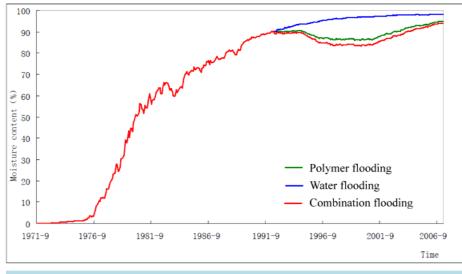


Figure 5. Curve of moisture content simulation of produced oil of surface active agent and combination flooding.

factory. The software has three flooding functions and physical-chemical parameters can be processed effectively. The software simulates reliably and generally based on the above experiments of different scales oilfields and the simulation scale is up to hundreds of thousands nodes.

## 6. Numerical Analysis of the Model Problem

In this section theoretical analysis is discussed for the numerical simulation of the polymer of porous media. For simplification and without loss of generality, a simple model is analyzed here, a three-dimensional multi-components compressible displacement [1] [2] [12]-[16]. It is a nonlinear system coupled with partial differential equations with initial values and boundary values described as follows

$$d(c)\frac{\partial p}{\partial t} + \nabla \cdot \boldsymbol{u} = q(x,t), \ x = (x_1, x_2, x_3)^{\mathrm{T}} \in \Omega, \ t \in J = (0,T],$$
(29a)

$$\boldsymbol{u} = -a(c)\nabla p, \ x \in \Omega, \ t \in J,$$
(29b)

$$\Phi\left(x\right)\frac{\partial c_{\alpha}}{\partial t} + b_{\alpha}\left(c\right)\frac{\partial p}{\partial t} + \boldsymbol{u}\cdot\nabla c_{\alpha} - \nabla\cdot\left(D\nabla c_{\alpha}\right) = g\left(x,t,c_{\alpha}\right), \ x \in \Omega, \ t \in J, \alpha = 1, 2, \cdots, n_{c} - 1,$$
(30)

where p(x,t) is the pressure of the mixture,  $c_{\alpha}(x,t)$  is the concentration of the  $\alpha$  -th component  $(\alpha = 1, 2, \dots, n_c - 1)$  and  $n_c$  is the number of components. Because of  $\sum_{\alpha=1}^{n_c} c_{\alpha}(x,t) = 1$ , the only  $n_c - 1$  components are independent. Let  $c(x,t) = (c_1(x,t), \dots, c_{n_c-1}(x,t))^T$  be a vector function of component saturation,  $d(c) = \Phi(x) \sum_{\alpha=1}^{n_c} z_{\alpha} c_{\alpha}, \Phi(x)$  be the porosity,  $z_{\alpha}$  represent a compressible constant of  $\alpha$  -th component, u be the Darcy velocity.  $a(c) = \kappa(x)\mu(c)^{-1}$ , where  $\kappa(x)$  is the permeability,  $\mu(c)$  is the fluid viscosity, and  $b_{\alpha}(c) = \Phi c_{\alpha} \left\{ z_{\alpha} - \sum_{j=1}^{n_c} z_j c_j \right\}$ , D = D(x) is the convection coefficient. The pressure p(x,t) and the vector function of saturations  $\alpha(x,t)$  are to be computed later.

function of saturations c(x,t) are to be computed later.

Impermeable boundary value conditions:

$$\boldsymbol{u} \cdot \boldsymbol{\gamma} = 0, \ \boldsymbol{x} \in \partial \Omega, \quad \left( D \nabla c_{\alpha} - c_{\alpha} \boldsymbol{u} \right) \cdot \boldsymbol{\gamma} = 0, \ \boldsymbol{x} \in \partial \Omega, \ t \in J, \alpha = 1, 2, \cdots, n_{c} - 1,$$
(31)

where  $\gamma$  is the outer normal vector of the boundary  $\partial \Omega$  of  $\Omega$ . Initial value conditions:

$$p(x,0) = p_0(x), x \in \Omega, \quad c_{\alpha}(x,0) = c_{\alpha,0}(x), x \in \Omega, t \in J, \alpha = 1, 2, \dots, n_c - 1.$$
(32)

For convenience, the computational domain is taken as  $\Omega = \{[0,1]\}^3$  and the problem is supposed to be  $\Omega$ -peri odic, and the impermeable boundary value conditions are dropped. Let h = 1/N,  $X_{ijk} = (ih, jh, kh)^T$ ,  $t^n = n\Delta t$  and  $W_{ijk}^n = W(X_{ijk}, t^n)$ , and take

$$A_{i+1/2,jk}^{n} = \left[ a \left( X_{ijk}, C_{ijk}^{n} \right) + a \left( X_{i+1,jk}, C_{i+1,jk}^{n} \right) \right] / 2,$$
(33a)

$$\delta_{\overline{x}_{1}}\left(A^{n}\delta_{x_{1}}P^{n+1}\right)_{ijk} = h^{-2}\left[A^{n}_{i+1/2,\,jk}\left(P^{n+1}_{i+1,\,jk} - P^{n+1}_{ijk}\right) - A^{n}_{i-1/2,\,jk}\left(P^{n+1}_{ijk} - P^{n+1}_{i-1,\,jk}\right)\right],\tag{33b}$$

Then  $A_{i,j+l/2,k}^n$ ,  $A_{ij,k+l/2}^n$  and other notations can be defined similarly.

An implicit fractional finite difference algorithm for the diffusion Equation (29),

$$d\left(C_{ijk}^{n}\right)\frac{P_{ijk}^{n+1/3} - P_{ijk}^{n}}{\Delta t} = \delta_{\bar{x}_{1}}\left(A^{n}\delta_{x_{1}}P^{n+1/3}\right)_{ijk} + \delta_{\bar{x}_{2}}\left(A^{n}\delta_{x_{2}}P^{n}\right)_{ijk} + \delta_{\bar{x}_{3}}\left(A^{n}\delta_{x_{3}}P^{n}\right)_{ijk} + q\left(X_{ijk}, t^{n+1}\right), \quad 1 \le i \le N, \quad (34a)$$

$$d\left(C_{ijk}^{n}\right)\frac{P_{ijk}^{n+2/3} - P_{ijk}^{n+1/3}}{\Delta t} = \delta_{\bar{x}_{2}}\left(A^{n}\delta_{x_{2}}\left(P^{n+2/3} - P^{n}\right)\right)_{ijk}, \quad 1 \le j \le N,$$
(34b)

$$d\left(C_{ijk}^{n}\right)\frac{P_{ijk}^{n+1} - P_{ijk}^{n+2/3}}{\Delta t} = \delta_{\bar{x}_{3}}\left(A^{n}\delta_{x_{3}}\left(P^{n+1} - P^{n}\right)\right)_{ijk}, \quad 1 \le k \le N.$$
(34c)

Compute the Darcy velocity  $\boldsymbol{U} = (U_1, U_2, U_3)^{\mathrm{T}}$  as follows,

$$U_{1,ijk}^{n+1} = -\frac{1}{2} \left[ A_{i+1/2,jk}^{n} \frac{P_{i+1,jk}^{n+1} - P_{ijk}^{n+1}}{h} + A_{i-1/2,jk}^{n} \frac{P_{ijk}^{n+1} - P_{i-1,jk}^{n+1}}{h} \right],$$
(35)

 $U_{2,ijk}^{n+1}$ ,  $U_{3,ijk}^{n+1}$  can be obtained analogously.

An implicit fractional upwind difference method for the saturation Equation (30)

$$\Phi_{ijk} \frac{C_{\alpha,ijk}^{n+1/3} - C_{\alpha,ijk}^{n}}{\Delta t} = \delta_{\bar{x}_{1}} \left( D\delta_{x_{1}} C_{\alpha}^{n+1/3} \right)_{ijk} + \delta_{\bar{x}_{2}} \left( D\delta_{x_{2}} C_{\alpha}^{n} \right)_{ijk} + \delta_{\bar{x}_{3}} \left( D\delta_{x_{3}} C_{\alpha}^{n} \right)_{ijk} - b_{\alpha} \left( C_{\alpha,ijk}^{n} \right) \frac{P_{ijk}^{n+1} - P_{ijk}^{n}}{\Delta t} + g \left( X_{ijk}, t^{n+1}, C_{\alpha,ijk}^{n} \right) \qquad , 1 \le i \le N, \alpha = 1, 2, \cdots, n_{c} - 1,$$
(36a)

$$\Phi_{ijk} \frac{C_{\alpha,ijk}^{n+2/3} - C_{\alpha,ijk}^{n+1/3}}{\Delta t} = \delta_{\bar{x}_2} \left( D\delta_{x_2} \left( C_{\alpha,ijk}^{n+2/3} - C_{\alpha}^n \right) \right)_{ijk}, \qquad 1 \le j \le N, \alpha = 1, 2, \cdots, n_c - 1,$$
(36b)

$$\Phi_{ijk} \frac{C_{\alpha,ijk}^{n+1} - C_{\alpha,ijk}^{n+2/3}}{\Delta t} = \delta_{\bar{x}_3} \left( D\delta_{x_3} \left( C_{\alpha,ijk}^{n+1} - C_{\alpha}^n \right) \right)_{ijk} - \sum_{\beta=1}^3 \delta_{U_{\beta,x_{\beta}}^{n}} C_{\alpha,ijk}^{n+1}, \qquad 1 \le k \le N, \alpha = 1, 2, \cdots, n_c - 1, \qquad (36c)$$

where  $\delta_{U_{\beta,x_{\beta}}^{n}C_{\alpha,ijk}^{n+1}} = U_{\beta,ijk}^{n} \left\{ H\left(U_{\beta,ijk}^{n}\right)\delta_{\overline{x_{\beta}}} + \left(1 - H\left(U_{\beta,ijk}^{n}\right)\right)\delta_{x_{\beta}} \right\} C_{\alpha,ijk}^{n+1}, \ \alpha = 1, 2, \cdots, n_{c} - 1. \quad H\left(z\right) = \begin{cases} 1, \ z \ge 0 \\ 0, \ z < 0. \end{cases}$ 

Initial value conditions:

$$P_{ijk}^{0} = p_0\left(X_{ijk}\right), \quad C_{\alpha,ijk}^{0} = c_{\alpha 0,ijk}, \quad 1 \le i, j, k \le N, \quad \alpha = 1, 2, \cdots, n_c - 1.$$
(37)

The program of implicit upwind fractional difference method runs as follows. Given  $\{P_{ijk}^n, C_{\alpha,ijk}^n, \alpha = 1, 2, \dots, n_c - 1\}$ , the values  $\{P_{ijk}^{n+1/3}\}$  of transition layer is computed by using speedup method in  $x_1$ -direction by (34a),  $\{P_{ijk}^{n+2/3}\}$  is obtained by (34b), and the solution of pressure  $\{P_{ijk}^{n+1}\}$  is solved by (34c). The values of Darcy velocity  $\{U_{ijk}^{n+1}\}$  are computed by (35). Secondly, the values  $\{C_{\alpha,ijk}^{n+1/3}\}$  of transition layer is computed by using speedup method in  $x_1$ -direction by (36a),  $\{C_{\alpha,ijk}^{n+2/3}\}$  is obtained by (36b), and the solution

of concentration  $\{C_{\alpha,ijk}^{n+1}\}$  is solved by (36c). Note that the problem is positive definite, the solution of (34)-(36) exists and is sole.

For the model (29)-(32), applying variation technique, energy analysis, decomposition of high order difference operators and theory and technique of product communitivity we can get error estimates in  $L^2$  of the implicit fractional upwind difference method stated in the following theorem. The computational algorithms discussed in this paper is based on the mathematical and mechanical considerations.

**Theorem** Suppose that the exact solutions of (29)-(32) are sufficiently smooth, and discrete solutions are computed by an implicit fractional step upwind difference algorithm (34)-(36). It holds

$$\|p - P\|_{\overline{L}^{c}(J;h^{1})} + \sum_{\alpha=1}^{n_{c}-1} \|c_{\alpha} - C_{\alpha}\|_{\overline{L}^{c}(J;h^{1})} + \|d_{t}(p - P)\|_{\overline{L}^{2}(J;l^{2})} + \sum_{\alpha=1}^{n_{c}-1} \|d_{t}(c_{\alpha} - C_{\alpha})\|_{\overline{L}^{2}(J;l^{2})} \le M^{*} \{\Delta t + h\},$$
(38)

where the constant  $M^*$  is dependent on p(x,t),  $c_{\alpha}(x,t)(\alpha = 1, 2, \dots, n_c - 1)$  and their derivatives.

# 7. Conclusion and Discussion

Theory, method and application of numerical simulation of high temperature, high salt, complicated geology and large scale oilfields and complicated chemical flooding of flow mechanics in porous media are discussed in this paper consisting of several sections. Summary is stated about our project in Section 1. Mathematical model of permeation fluid mechanics is presented in view of petroleum geology, geochemistry, and computational permeation fluid mechanics Section 2. An implicit refined fractional step combined with upwind difference numerical algorithm based on upstream sequence, is structured in Section 3. A type of software applicable in major industries has been accomplished, mostly carried out the spacial step of ten meters, ten thousands of nodes and tens of years simulation period in Section 4. Some experimental tests taking place successfully in major oil fields such as Shengli Oilfield, are illustrated in Section 5. Numerical analysis proceeds for the model problem and precise theoretical results are stated on mathematical and mechanical consideration in Section 6.

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