

## **Compositional Reservoir Modelling By An Equation Oriented Chemical Process Simulator - I. Analysis And Development**

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### **Introduction**

A significant portion of our research team effort is to improve our understanding of reservoir production mechanisms, and to explore alternative strategies for improving performance and cost effectiveness. In achieving this goal it is of primary importance for us to have at our disposal a very flexible simulator that, directly, easily and in a very short time, can be corrected, modified or widened to analyze different "constitutive" models or to change the level of their detail. By this way we gain two significant advantages. First, we verify, shortly and explicitly, the implications of the assumptions used in our chemical-physical models; then, all the researchers of our team can use the simulator as a communications tool where all assumptions will be explicit and the results will be consistent with all team assumptions.

For the last twenty years several researchers have been working on the development of reservoir simulators. Nowadays many commercial reservoir simulators are routinely used to predict the performance of a reservoir and to explore methods for increasing the oil and gas recovery. Particular attention is devoted to modelling enhanced oil recovery (EOR), by thermal, chemical or solvent methods. Most of these packages are very efficient and flexible, but they are in general black-box reservoir simulators; just a few of them are open-source.

This work is a detailed description of the upgrading of our equation oriented chemical process simulator CheOpe to model gas and oil production.

Pioneering research being conducted by our system engineering group since 1985 has provided a scientific and engineering basis for modelling chemical process operations. This research has resulted in the development and application of CheOpe (Pagani and d'Arminio Monforte 1985; Pagani et al. 1989, 1996, 2001), an Equation-Oriented (E.O.) simulator based on an interconnected cells approach. CheOpe is a multicomponent, multiphase, simulator which accounts for complex phase behaviour, chemical and physical transformations, TDN equilibrium and mass-transfer models. It solves the main stationary process analysis problems (simulation, design, optimization and so on) by using a lumped sub-unit called "cell": each process unit is described by a suitable cells configuration.

CheOpe generates an equation block for each cell. All the equations blocks are then collected in a large sparse system solved with high numerical accuracy by advanced Newton-Raphson methods.

Thanks to its architecture and its numerical algorithms, CheOpe was a promising starting point for a porous media flow simulator development. The purpose of this work is a description of the assumptions we have introduced and of the main activities we

have performed to build a simulator called “CheOpe\_Oil” starting from CheOpe. We are programming a large test plan at laboratory and near-well scales to analyse both convergence properties and model feasibility; in a next paper we’ll report detailed results of these analysis.

### Model structure

The goal of our work is to develop CheOpe\_Oil, a chemical flooding simulator that can simulate, efficiently and accurately, oil reservoirs at both the laboratory and field scales. CheOpe\_Oil will support isothermal and non-isothermal model, one- two or three dimensional cartesian or radial geometry, multiple phases containing multiple species plus an immobile solid rock phase with adsorbing components. Phase chemical-physical properties (densities, viscosities, fugacity, interface and surface tension, internal energy, etc.) may be arbitrary functions of pressure, temperature and composition. Porosity and permeability may vary with location. An arbitrary number of wells may be completed at arbitrary locations.

The use of any commercial mathematical, chemical, physical library is prohibited.

Mass conservation equation for a component  $i$  can be formulated in a representative elementary volume (REV).  $V$  is a volume that is large with respect to the pore dimensions, but small compared to the dimensions of the permeable medium (Bear 1972, Gray 1975). In  $V$  each fluid phase is considered homogeneous and embedded within the permeable medium.

Generally  $V$  is dealt as an infinitesimal, by supposing that all properties are continuous and derivable functions of  $V$ . Chosen a suitable number of points (“grid”), space derivatives are replaced by difference approximations on this point. The resulting nonlinear difference equations are solved by either fully implicit or semi-implicit techniques. Grid block has to be chosen to satisfy both numerical stability and internal physical detail.

We prefer to use lumped equations directly, without converting them into partial differential equations and choosing the grid on the basis of geometrical and structural details that are effectively known.

This approach offers two main advantages: the model consists of a DAE system with ordinary differential equations in which the independent variable is time; grid block can be chosen on the basis of internal physical detail with a regular or irregular discretizations.

Gear’s method (Gear, 1984) or another predictor-corrector method where predictor is based on Crank-Nicolson’s approach are used to solve the system at each grid block and time step.

### Main simulator changes to deal with oil recovery processes

The main problems for enabling CheOpe to simulate oil recovery processes depend on the following basic conceptual differences between a steady-state chemical process and an oil recovery process :

- a. Chemical process simulation just depends on plant topology; oil recovery process simulation depends on its topography too.
- b. Flow-driven simulation is generally suitable for a steady-state chemical process analysis; on the contrary oil recovery process simulation requires a more rigorous pressure-driven simulation.
- c. Both processes can be represented by a digraph (directed graph) describing information flow structure; but each flow direction is not univocally defined in a reservoir problem.

- d. Steady-state models have an algebraic structure, not suitable for a dynamic process like oil recovery whose models have an algebraic-differential structure.
  - e. Graphical user interfaces for enabling user to deal with the two problems are quite different.
  - f. Graph describing a reservoir structure is very larger and more complex.
- a.** In mass conservation equation superficial velocity, and then mass flow, can be expressed by a finite form of Darcy's law for flow in permeable media, where some terms depend on the graph topography (relative position among grid cells).
- b., c.** A chemical process is generally analyzed in the form of graph. In particular, a flow-driven model can be easily represented by a directed graph where edges direction is the same of known material and/or energy flow direction. A pressure-driven model too can be represented by a directed graph, but information flows don't correspond exactly to physical flows.
- In both cases, for a chemical process model, the original structure matrix is invariant during the solution procedure. On the contrary, a reservoir model is a conditional (Rico-Ramirez and Westerberg, 2002) pressure-driven model; i.e. model equations and variables are not correlated by an invariant structure matrix. In fact, variables occurrence in partial mass and energy balance equations is changing, depending on the local pressure values.
- d.** By our approach, a reservoir model consists of a DAE system with ordinary differential equations where independent variable is time. Predictor-corrector methods can be used to solve the system at each time step. By collecting DAE equations in blocks, corresponding to the chosen space grid blocks, we can exploit CheOpe architecture to efficiently solve resulting sparse block-equations.
- e.** The numbers and the results to be reported in a dynamic reservoir simulation are much larger than the stationary process simulation ones. So it is impossible to report them by tabulation. We use level maps and plots to display results, depending on the time and on the local position in the reservoir.
- f.** Grid block can be chosen on the basis of internal physical detail: it may happen that large reservoir areas can be discretized with a little number of large blocks. Even so, resulting graph dimension and complexity are not low; in particular DAE sparseness is dramatically reduced in comparison with a chemical process problem, especially for 3-D problems.

### Model formulation

An oil recovery process performance depends on both the reservoir and the wells features. To simulate the process we have to suitably link models of both systems and to choose significant initial and boundary conditions. Both systems are described by multicomponent, multiphase flow equations, where fluids move in permeable media for reservoir, and in pipes for wells. The equations are unsteady state mass and energy balances. Compositions in each phase are evaluated assuming TDN equilibrium among fluid phases (oil, gas, water) and, in the reservoir, also between oil, water and adsorbed phase.

Reservoir is described by a pressure driven model, where flux vector of each component in each phase results by the sum of a convective and a dispersive flow. The former are evaluated by the Darcy's law for multiphase flow, the latter are neglected in our model. The oil pressure is evaluated by an overall mass balance on rock free volume; the other phase pressures are computed adding capillary pressure between phases.

Wells model is a flow driven model; the top or the bottom pressure is imposed by fixing the same pressure or the flow rate; pressure and phase saturation along the well are evaluated by some multiphase flow model in pipes.

In alternative, on the boundaries we can assume no-flux through boundaries or we can specify pressure on them.

Two important peculiarities strongly affect the simulator behaviour:

- variables occurrence in partial mass and energy balance equations is changing, depending on the local pressure values
- fluid phases can appear or disappear in a reservoir with time and location.

To solve the first problem we have connected the grid cells each other by a couple of convective fluxes  $i-j$  and  $j-i$ ; during the simulation, one of these is cleared by multiplying it by a suitable function of the difference  $P_i - P_j$ . The function  $\arctan(P_i - P_j)$  gives good results.

The second is a very cumbersome problem (Bausa and Marquardt, 2000). In the next paragraph we shortly describe our approach to detect and handle phase changes.

Main assumptions made in developing our reservoir cell model are:

- One, two or three dimensions;
- Temperature assigned (isothermal cell);
- Multiphase flow of fluids through porous media described by Darcy's law;
- One, two or three fluid phases and an adsorbed phase combined to represent 13 different phase configurations;
- Thermodynamic equilibrium among fluids and between fluids and adsorbed phase, with negligible capillary pressure effect on phase equilibrium;
- Each component distributed among all phases or only in some phase;
- Rock compressibility.

Cells can be combined in a cartesian or radial variable-spacing grid; each cell can have different properties (porosity, permeability and rock compressibility), and the chemical-physical properties (densities, viscosities, fugacity, interface and surface tension, internal energy, etc.) are calculated as functions of pressure, temperature and composition. Relative permeability and capillary pressures are calculated as functions of saturations and rock type. Wells can operate under specified pressure or flow rate.

In a volume  $V_j^*$ , mass conservation equations for species  $i$  and conservation equation are expressed as:

$$-V_j^* \frac{d}{dt} \left[ \varepsilon_j \cdot \sum_{\alpha=1, Nph} \rho_j^\alpha \xi_{i,j}^\alpha S_j^\alpha + (1 - \varepsilon_j) \cdot (\rho_j^S \chi_{i,j}^S) \right] = -F_{j, in} Z_{i, j, in} + \sum_{\alpha=1, Nph} \sum_{h=1, 3} (\Phi_{i, j, h}^\alpha - \Phi_{i, jin, h}^\alpha) \quad (1)$$

$$-V_j^* \frac{d}{dt} \left[ \varepsilon_j \cdot \sum_{\alpha=1, Nph} \rho_j^\alpha S_j^\alpha + (1 - \varepsilon_j) \cdot \rho_j^S \right] = -F_{j, in} + \sum_{\alpha=1, Nph} \sum_{h=1, 3} (\Phi_{j, h}^\alpha - \Phi_{jin, h}^\alpha) \quad (2)$$

being

$$\Phi_{jin, h}^\alpha = \frac{\Re_{jin, h}^\alpha}{\mu_{jin}^\alpha} \left( \frac{(P_{jin}^\alpha - P_j^\alpha)}{\Delta \ell_{jin, h}} \left[ + \rho_{jin}^\alpha g \frac{Z_{jin, h} - Z_{j, h}}{\Delta \ell_{jin, h}} \right] \right) \rho_{jin, h}^\alpha A_{j, h}^\perp \quad (3a)$$

$$\Phi_{i, jin, h}^\alpha = \Phi_{jin, h}^\alpha \cdot \xi_{i, jin}^\alpha \quad (3b)$$

$$\Phi_{j, h}^\alpha = \frac{\Re_{j, h}^\alpha}{\mu_j^\alpha} \left( \frac{(P_j^\alpha - P_{jout, h}^\alpha)}{\Delta \ell_{jout, h}} \left[ + \rho_j^\alpha g \frac{Z_{j, h} - Z_{jout, h}}{\Delta \ell_{jout, h}} \right] \right) \rho_{jout, h}^\alpha A_{jout, h}^\perp \quad (4a)$$

$$\Phi_{i, jout, h}^\alpha = \Phi_{jout, h}^\alpha \cdot \xi_{i, j}^\alpha \quad (4b)$$

where

$$\Re_{jin, h}^\alpha = k_{r, jin}^\alpha \cdot k_{jin, h} \quad \Re_{j, h}^\alpha = k_{r, j}^\alpha \cdot k_{j, h}$$

TDN equilibrium among fluid phases and, in the reservoir, between oil phase and adsorbed phase, are formulated as algebraic equations

$$f_{i,j}^{\alpha} = f_{i,j}^{\beta} \quad (5)$$

stating equality fugacity of each component  $i$   $f_{i,j}$  between each phase couple  $\alpha$ - $\beta$ .

The pressure of each non-wetting phase  $\alpha$  is kept equal to the pressure of the wetting phase  $w$  increased by the capillary pressure

$$P_j^{\alpha} = P_j^w + P_{c_j^{w-\alpha}} \quad (6)$$

Sum equations for molar compositions and saturations complete the reservoir model.

$$\sum_{i=1, Ncp} \xi_i^{\alpha} = 1 \quad (7)$$

$$\sum_{k=1, Nph} S^k = 1 \quad (8)$$

### Phase behavior

In the simulation and design of chemical processes the determination whether or not a given phase will split into multiple phases is a difficult problem, generally called phase stability problem. The more fundamental approach to stability testing is to examine the Gibbs free energy of the system to search its lowest possible value. The problem is generally formulated in term of the "tangent plane criterion" (Baker et al., 1981)

On the other side, as the number of phases changes the corresponding process model becomes a conditional model (Grossmann and Türkay, 1996). So, during process model solution, we have to iteratively solve first a stability test and later a set of non-linear equations depending on the basis of the stability test itself. In particular, in an equation oriented approach, we have to perform two sequential or imbricate loops, introducing a likely instability (Widagdo and Seider, 1996). This transition between different phase configurations is particularly critic in dynamic processes where it is necessary to detect the transition events and to reinitialize the discontinuous variables.

An alternative method, named  $\tau$ -method, has been proposed to handle any phase configuration with the same set of equations and without a stability analysis, for both steady state (Han and Rangaiah, 1998) and unsteady state (Thery and al., 2004) models. However this method, which for steady state models requires an optimization formulation that restricts ulteriorly its applications, doesn't seem to work very well for LL equilibria. To solve the problem we have developed a method similar to  $\tau$ -method, that doesn't require a solution of an optimization problem and it works both for steady and unsteady state models. By this method, we assume that the sum equation of each guessed phase  $\alpha$  can be written as

$$\sum_{i=1, Ncp} \xi_i^{\alpha} + \frac{b \cdot S^{r\alpha}}{S^{\alpha} + \tau \cdot S^{r\alpha}} = 1$$

being  $\tau$  a suitable constant whose value depends on computer numerical round-off.

When phase  $\alpha$  is thermodynamically unstable and disappears ( $S^{\alpha} \rightarrow 0$ ), the second term of equation approaches 1 and sum equation keeps its consistency, while values of compositional variables have no physical meaning.

### Solution procedure

Our reservoir model consists of the DAE system (1), (2), (5), (6), (7), (8), where independent variable is time. In the original DAE system derivatives are approximated by finite-differences; at each time step, solution of the resulting non linear system is

first estimated by an explicit predictor method and then calculated by a corrector method with the desired precision. Time step is reduced and solution procedure restarted if, by a suitable stability test (Mehra et al., 1982; Caoats, 1980, Jensen, 1980), difference equations are not representative of the original DAE system. Solution of the non linear system is achieved by a Newton-Raphson method; linear equations are collected in blocks, corresponding to the chosen space grid blocks, and resulting sparse block-equations are processed using the original CheOpe algorithms (Pagani et al., 1985).

## Test

We tested our simulator Cheope-Oil on a variety of examples regarding both laboratory and literature cases. Here we shall only present one set of results, dealing with the first SPE Comparative Solution Project (Odeh, 1981). Although the SPE report is dealing with a black-oil reservoir problem, we used a compositional fluid description with a two components characterization, with appropriate PVT properties and relative permeabilities. A 10 by 10 by 3 finite difference grid was used as shown in Figure 1. Stratification and reservoir properties are given in Figure 2. An injection well is located at grid block (1,1), and one production well is located at grid block (10,10). The following results are here reported:

- Gas Saturation of Production well Cell: Figure 3.
- Oil rate production: Figure 5.
- Maps of pressure along the reservoir at  $t=10$  years, layer 1: Figure 6.
- Maps of Oil saturation along the reservoir at  $t=10$  years, layer 1: Figure 7.

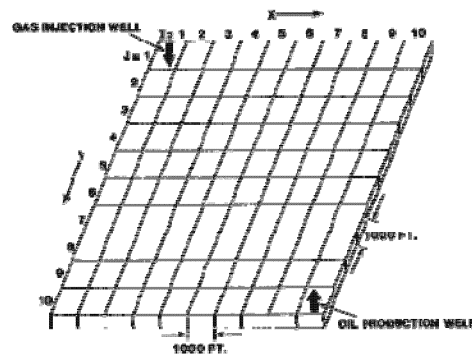


Figure 1: Reservoir grid

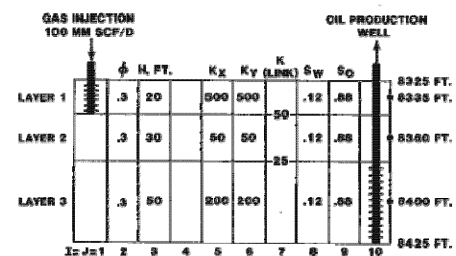


Figure 2: Stratification and reservoir properties

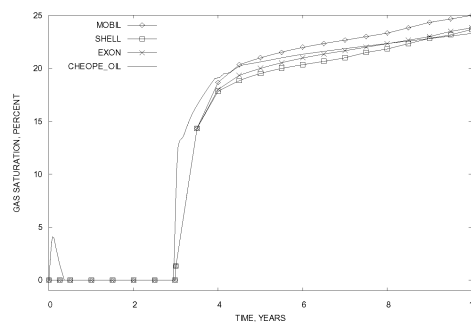


Figure 3: Gas Saturation of Production well Cell

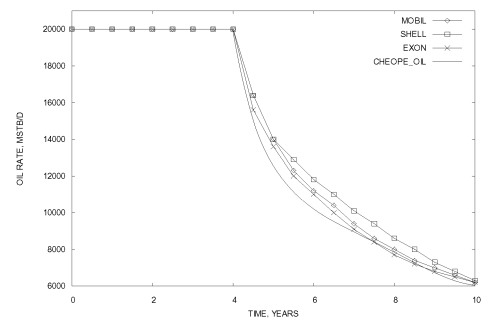


Figure 5: Oil rate production

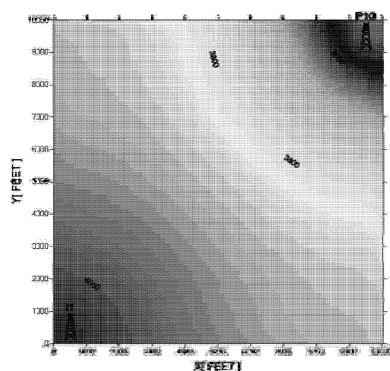


Figure 6: Pressure at t=10 years, layer 1

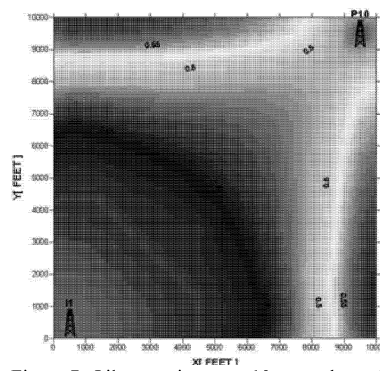


Figure 7: Oil saturation at t=10 years, layer 1

## Conclusions

Our equation oriented chemical process simulator CheOpe has been upgraded to model gas and oil production. By this way we have gained two main goals. First, we have developed a proprietary high performance porous media flow simulator in a very short time. Second, thank to the architecture of our new simulator, we can analyze oil and gas production system consisting of the reservoir and wells, alone or integrated with surface facilities. In a next paper we'll report detailed results of a large test plan we are being carried out at laboratory and near-well scales to analyse both convergence properties and model feasibility of CheOpe\_Oil package.

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### Nomenclature

$A$	surface	$\Re$	phase permeability
$f_{i,j}$	fugacity of component $i$ in the cell $j$	$S$	saturation
		$S^r$	residual saturation
$g$	gravitation acceleration	$t$	time
$k_{j,h}$	effective absolute permeability of the cell $j$ along $x_h$ coordinate	$V_i^*$	cell $j$ volume
		$x_h$	$h^{\text{th}}$ coordinate
$k_r$	relative permeability	$z_{i,jf}$	molar fraction of component $i$ in the $jf$ flow, being $jf$ a feed flow
$N_{cp}$	number of components		
$N_{ph}$	number of phases	$z_{j,h}$	barycentre coordinate of the cell $j$ along vertical coordinate
$P_i$	cell $j$ pressure		
$P$	pressure		

### Greek Letters

$\varepsilon$	rock porosity
$\Delta \ell_{j,h}$	distance between the barycentre of two cells
$\mu$	viscosity
$\rho$	density
$\xi$	molar fraction
$\Phi$	flow rate

### Subscripts and Superscripts

$i$	component $i$
$j_{in}$	index of the cell from which is coming the flux entering the cell $j$
$j$	index of the cell
$j_{out}$	index of the cell into which is coming the flux leaving the cell
$w$	wetting phase
$\alpha, \beta$	phases