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A General Unstructured Grid, Parallel, Thermal Simulator and its Application for Large Scale Thermal Models

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Abstract

We describe the contruction of a general unstructured grid, parallel, fully-implicit simulator for complex physics associated with heavy oil thermal recovery. The primary focus of the simulator is on the physics associated with steam injection and Steam Assisted Gravity Drainage (SAGD) and to simulate such models efficiently using parallel processing. The simulator solves component material balance, energy balance and mass equilibrium equations for component mole fractions, saturation, temperature and pressure using the Newton-Raphson method. External heat sources and sinks are included in source terms to model the energy interaction with over-burden and under-burden rocks. The solution procedure and the treatment of phase transition to achieve stable non-linear iterations are discussed.

The simulator is verified by comparing results from problem No. 3 of the Fourth SPE Comparative Solution Projects and a cyclic steam injection case with other commercial simulators. We also demonstrate the performance and parallel scalability of the simulator via testing a large scale SAGD model with 9 horizontal well-pairs.

Introduction

Numerical simulation of thermal processes, such as steam flooding, steam assisted gravity drainage (SAGD), and cyclic steam stimulation, plays an important role in design of a thermal project. The frequent use of simulation results in the reservoir engineering decision-making process indicates confidence in reservoir simulation techniques. Since thermal simulation started in the early 1970's, many papers have been published for models with structured grids (Coats 1980; Chien 1989; Mifflin 1991; Watts 1996). In recent years, several papers describe general simulators using unstructured grids (Beckner 2001; Debaun 2005; Beckner 2006; Liu 2007). These papers noted that unstructured grids reduced simulation cycle-time significantly via integration with geologic models. On the other hand, unstructured grids can achieve accurate geologic features by using fewer grid blocks and save simulation time dramatically. Liu, *et al.* (2007) described a general unstructured grid thermal simulator based on mass variable formulation with the selection of pressure, energy and component moles as primary variables.

This paper describes a general unstructured grid, fully-implicit thermal simulator based on a nature variable formulation. The first section describes the mathematical formulation used in simulator, solution procedure, primary variable selection, fluid property calculation, and heat loss model. The second section presents comparison of simulation results against other simulators to verify the physical results.

Mathematical Formulation

The thermal model described here is based on the assumption that Darcy's law and instantaneous phase equilibrium are valid. It is also assumed that the aqueous phase contains no components that partition into either of the hydrocarbon phases, and that the water component could not reside in the hydrocarbon liquid phase.

Balance Equations

The governing equations include component material balance equations, an energy balance equation, mass equilibrium equations, and saturation, and composition constraint equations. For thermal models where water component could reside in the gas phase, the total number of variables for grid cells containing three phases is $2N_c+6$, where N_c is the total number of components in the fluid models, excluding water component using natural variable formulation.

The material balance equations for hydrocarbon components can be written as:

$$\frac{V}{\Delta t}\delta\left[\sum_{j=1}^{N_p}\left(\phi\cdot\rho_j\cdot S_j\cdot x_{ij}\right)\right]=-\sum_{j=1}^{N_p}q_{ij}^{n+1}+\Delta\left[\sum_{j=1}^{N_p}T\cdot\left(\rho_j\cdot x_{ij}\frac{k_{rj}}{\mu_j}\right)(\Delta P_g-\Delta P_{cgj}-\gamma_j\cdot\Delta Z)\right]^{n+1}, \quad (1)$$

where i = 1, N_c. P_g is the pressure of gas phase.

The material balance equation for water component is written as:

$$\frac{V}{\Delta t}\delta\left[\phi(\rho_g S_g y_w+\rho_w S_w)\right]=-q_w^{n+1}+\Delta\left[T\rho_g y_w\frac{k_{rg}}{\mu_g}\left(\Delta p_g-\gamma_g\Delta Z\right)\right]^{n+1}+\Delta\left[T\rho_w\frac{k_{rw}}{\mu_w}\left(\Delta P_g-\Delta P_{cgo}-\Delta P_{cwo}-\gamma_w\Delta Z\right)\right]^{n+1}. \quad (2)$$

Finally, the energy equation can be expressed as:

$$\frac{V}{\Delta t}\delta\left[U_{Tot}\right]=-\sum_{j=1}^{N_p+1}\left(H_j\cdot q_j\right)^{n+1}-q_{source}^{n+1}+\Delta\left[\sum_{j=1}^{N_p+1}T\cdot\left(H_j\cdot\rho_j\cdot\frac{k_{rj}}{\mu_j}\right)\cdot(\Delta P_g-\Delta P_{gj}-\gamma_j\cdot\Delta Z)\right]^{n+1}+\Delta\left[T_h\cdot\Delta\theta^{n+1}\right], \quad (3)$$

where the source term, q_{source}, includes external heat sources and sinks due to heaters and enrgy interactions with over-burden and under-burden rocks.

The internal energy of a cell, U_{Tot}, is defined as follows:

$$U_{Tot}=(1-\phi)\left[C_{pr}\left(T-T^o\right)\right]+\sum_{j=1}^{N_p+1}\left(\phi\cdot\rho_j\cdot S_j\cdot U_j\right). \quad (4)$$

Mass Equilibrium Equations

We assume that water component can only reside in the aqueous and gas phases, but not in oil phase. When K-values either provided by K-value table or by correlations are used to calculate phase equilibrium for the hydrocarbon components partition between oil and gas phases, we have:

$$x_{ij}=K_{ij}\cdot x_{io}, \quad (5)$$

where j = 2, N_p, i= 1, N_c.

For the water component phase equilibrium, we have assumed that the water component in the gas phase can be treated as an ideal gas and the steam mole fraction y_w can be calculated using the following equation:

$$y_w=P_s/P, \quad (6)$$

where P_s is the water saturation pressure at the given grid cell temperature.

Constraint Equations

The saturation constrain is:

$$\sum_{j=1}^{N_p+1}S_j=1. \quad (7)$$

The composition constrains, which apply only when a phase is present, are defined as:

$$\sum_{i=1}^{N_c}x_{ij}+\delta_{gj}\cdot y_w=1, \quad (8)$$

where δ_{gj} is Kronecker delta.

The corresponding set of variables in Equations (1)-(8) can be summarized as:

x_{ij} , i = 1, N_c; j = 1, N_p,
y_w,
p_g, (9)
S_j , j = 1, N_p+1,
θ.

The $2N_c$+6 equations are used to solve for $2N_c$+6 variables defined in Equation (9). Thus, the number of unknowns to be solved equals the number of equations.

Numerical Solution Method

A robust numerical method for a thermal simulation involves proper primary variable selection, time step solution procedure and non-linear iteration control.

Primary Variable Selection

The primary variables are those need to be solved after mass equilibrium, saturation, and composition constrains. The primary variables must be independent in order to avoid a singular Jacobian matrix. Proper selection of primary variables is essential for a robust thermal numerical simulation method.

In 1989, Chien, *et al*. (1989) pointed out that special attention should be paid on primary variable selection for the cells where gas and water coexist, especially when they are in a narrow boiling point range. The details on narrow boiling point range and wide boiling point range as well as the criteria to determine if a cell is within one of these ranges are presented in the paper by Chien, *et al* (1989). Narrow boiling point condition exists in geothermal reservoirs, reservoirs with dead oil and regions near steam injectors or regions inside a steam chamber. These cells have a low overall hydrocarbon mole fraction. Pressure and temperature can be inferred from each other. One of these dependent variables has to be dropped from the primary variable list. In this work, temperature is selected as secondary variable for cells in the narrow boiling point range and treated as a primary variable for cells in the wide boiling point range where temperature and pressure are fairly independent. The selection of primary variable and its line-up to the selected mass equilibrium, mass balance and energy balance equations for the cells where gas and water coexist are summarized in Table 1, where ΔM_i and ΔM_w indicate the mass balance equations for component i and w, respectively. ΔU is the total energy balace equation.

Table 1 Primary Variable Selection

	Equation	Wide Boiling Point	Narrow Boiling Point
Secondary	$P_s/P - y_w = 0$	y_w	T
Primary	ΔU	T	S_g
	ΔM_i	S_g	y_w
	ΔM_w	P	P

Another goal of proper primary selection and equation/variable line-up is to obtain a diagonally dominant Jacobian matrix and to avoid small numbers in the main diagonal. Cells where all vaporizable oil components are depleted from the grid block can result in a tiny mole fraction and small numbers on the matrix main diagonal associated with small accumulation terms. One solution for this problem is to have the possible small mole fraction to line-up with corresponding mass balance equation. If this is not possible, a perturbation on the composition is needed during Jacobian generation to avoid tiny number in main diagonal.

Time-Step and Nonlinear Iteration Controls

When Newton iteration is used to solve non-linear finite difference equations, rapid convergence can be expected only if the initial guess is close to the solution and the Jacobian matrix properly captures the linearization of the balance equation. In many instances, oscillating convergence behavior has been observed due to many complex mechanisms including high degree of non-linearity present in a thermal model. Robust nonlinear iteration controls must be coordinated with time step control to achieve stability of the numerical solution procedure.

Time step size is maintained within a range that allows for acceptable time truncation error, while preventing excessively small steps given a user-defined minimum time step size. Upon completion of a time step, a time-step control algorithm is applied to select the next time step size based on the ratio of current solution change and target solution change values.

A damping strategy is used to update variables in order to prevent unnecessary overshoot of the solution. A local modification is applied for any cells with negative saturation or composition using regular damping updates. Special care is needed to eliminate convergence oscillation near relative permeability end-points.

The solution procedure is outlined as follows:

1. Initialize the reservoir at time zero.
2. For a given time-step:
    a. Calculate all the physical properties and its corresponding partial derivatives.
    b. Set up Jacobian matrix for the reservoir cells and the well model.
    c. Solve for changes of primary and secondary variables.
    d. Update solution variables.
    e. Repeat step a through d until global Newton convergence is achieved. If after some number of iterations, convergence is not achieved, reduce the proposed time step (cut the time step size) and start the iterations again.

If convergence is achieved, estimate the next time step size and start going through step 2 again.

Unstructured Parallel Graph

This work is an extension to implement thermal modeling capability based on the architecture described in a paper written by Debaun, *et al* (2005). The unstructured graph topology proposed by Debaun et al. (2005) is used to accommodate

fully unstructured grids. The parallel graph, property data structures including node and edge properties, Jacobian generation are based on connection lists and support arbitrary grid connection. The resulting algorithm is independent of the grid structures and is applicable to both structured and unstructured grids.

Fluid Property Calculation

We used a temperature dependent K-values to model the fluid phase behavior. The hydrocarbon component enthalpy is computed as a function of temperature using coefficients of heat capacity (Chien et al. 1989). Both correlations and tabular input as a function of pressure and temperature are available for computing component K-values, densities and viscosities. The oil- and gas-phase properties are computed using various mixing rules, such as linear mixing rule and so on. Steam and water properties are computed as a combination of the saturated steam table and correlations for under-saturated properties. The saturated steam and water properties are obtained from "IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam".

Given the temperature, pressure, and composition in a grid cell, the fluid phase-state can be determined directly using the method proposed by Michelsen and Mollerup (2004). Once the phase-state is known, the amount and composition of each phase can be obtained by performing flash calculations. A small tolerance at the phase boundary is applied to avoid excessive phase-state oscillation during the Newton iterations of a given time step.

Heat Loss Model

The heat loss model accounts for the energy loss to the surrounding formation by conduction. Rock only cells (no fluid flow in these cells), which contain only energy balance equations, can be introduced to account for heat loss through overburden/underburden rocks. If the heat conduction parallel to reservoir inside overburden/underburden rocks can be ignored, heat loss model can be decoupled from reservoir equations. This assumption results in a contribution to the energy balance equation as a source/sink term without altering the matrix structure. A generic framework has been implemented to account for heat loss to the over-burden/under-burden and side-burden rocks. Two different methods have been implemented to calculate heat loss: A semi-analytical method as proposed by Vinsome and Westerveld (1980) and a 1-dimensional numerical model, where a variable number of cells may be used to numerically model the heat conduction to the surrounding formation.

Linear Solver

With typical simulation run time overwhelmingly dominated by the linear solver, it is critical to select a proper linear solver in order to achieve both serial and scalable parallel performance.

The efficient parallel linear solver presented by Debaun *et al*. (2005) is used in this work. Its preconditioner is an efficient parallel algebraic multigrid (PAMG) with a GMRES iterations together with a constrained pressure residual technique (CPR) approach of Wallis[11]. Non-pressure parts of the linear system are handled by a local preconditioner with an FGMRES outer iteration. Well terms are treated through a Schur complement approach.

Well Model

A conventional well model has been used in this study. Wells can be controlled by Bottom Hole Pressure (BHP), liquid rate, and steam production rate control. Heaters are treated as special wells and are also implemented with the current well model framework.

Comparison of Simulation Results

The simulator has been validated against other commercial and proprietary simulators using Model No. 3 of the Fourth SPE Comparative Solution Project (SPE 4) (Aziz *et al*. 1985), a cyclic steam injection case and a large scale SAGD model case. Very good agreement has been observed for the SPE 4 case compared to other simulator. This section presents some comparison results for these three cases.

SPE 4

The SPE 4 Comparison Solution Model No. 3 was used for this comparison case. This model is an inverted nine-spot pattern by considering one-fourth of the full pattern. The fluid and rock properties are similar to those described in SPE 4. Heat loss is modeled in both simulators using the semi-analytical method as proposed by Vinsome-Westerveld (1980). Comparison of cumulative oil and water production between commercial simulator and this study is shown in Figure 1. Results appear to agree closely between the commervial simulator and this study.

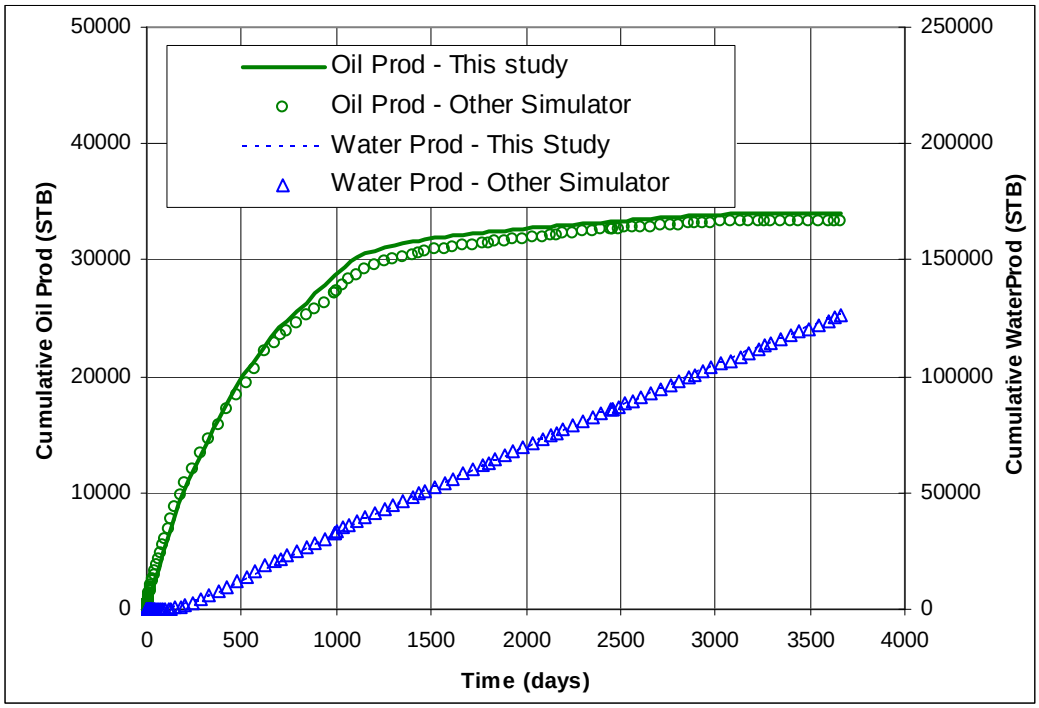

Figure 1 Comparisons of Cumulative Oil and Water Production for SPE 4

Cyclic Steam Injection Case

This model is used to validate the simulator compared to a proprietary "in-house" simulator. The reservoir was discretized into a 52×52×30 grid, and contained oil with 3 hydrocarbon components, with one of them being a non-volatile component. It has 4 injectors 3 producers and one huff-and-puff well. The four injectors are controlled by maximum cold water equivalent (CWE) rates and maximum BHP. The three producers are controlled by maximum liquid rate and minimum BHP. One huff-and-puff well starts on three 3-month cycles, followed by changing to a producer. Figure 2 presents the comparison of field cumulative oil production and cumulative water production between the "in-house" simulator and this study. Due to the different implementation of well model, a minor difference on Cumalative Oil Production around 1000 day has been noticed.

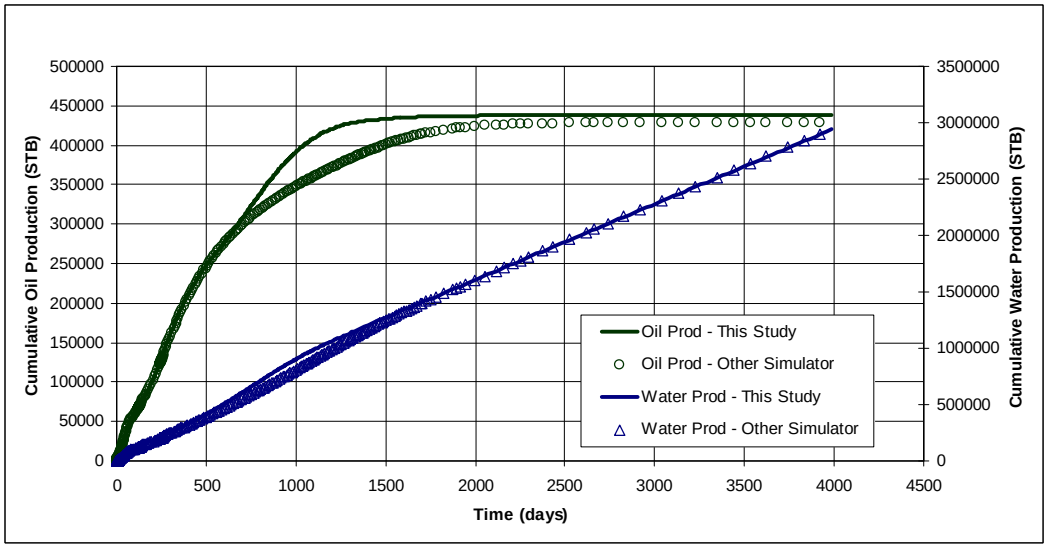

Figure 2 Comparisons of Cumulative Oil and Water Production for cyclic steam injection case

Large-Scale 9-PAIR SAGD Model

This example illustrates the capability of the simulator to model a large-scale SAGD case as well as its parallel scalability. The model is a 1.7 million cells 9-pair SAGD study of a heavy oil reservoir. This is an extremely heavy oil case with oil viscosities over 1.5×10^6 cp (centipoise). The oil is modeled using two pseudo-components (one distillable and one

non-volatile). The model has 18×1126×85 grid blocks, with heterogeneous permeability and porosity properties. The producers are controlled by steam production rate, maximum liquid rate, and minimum BHP. The injectors are controlled by maximum liquid rate and maximum BHP. The injected steam quality is about 90%. Figure 3 shows the well arrangement of SAGD well pairs.

In order to evaluate the efficiency of each part of the simulator, the time spent in the linearizer (discretization of accumulation, flux, and mass equilibrium terms), linear solver, the property computations (density, viscosity, enthalpy, internal energy, mobility, etc.), the flash calculations, and the convergence checks have been monitored during an 8-CPU parallel run. Figure 4 shows the CPU time breakdown among these different components. About 77% of the total CPU time is spent on linear solver, while linearizer takes about 6.8% of total CPU time.

A detail parallel scalability study has been conducted using this large scale model by running the model on 2, 4, 8, 16, 32, 64 CPU. Figure 5 shows the parallel speedup relative to 2 processors run. We did not make a serial run on this model due to hardware memory limitations.

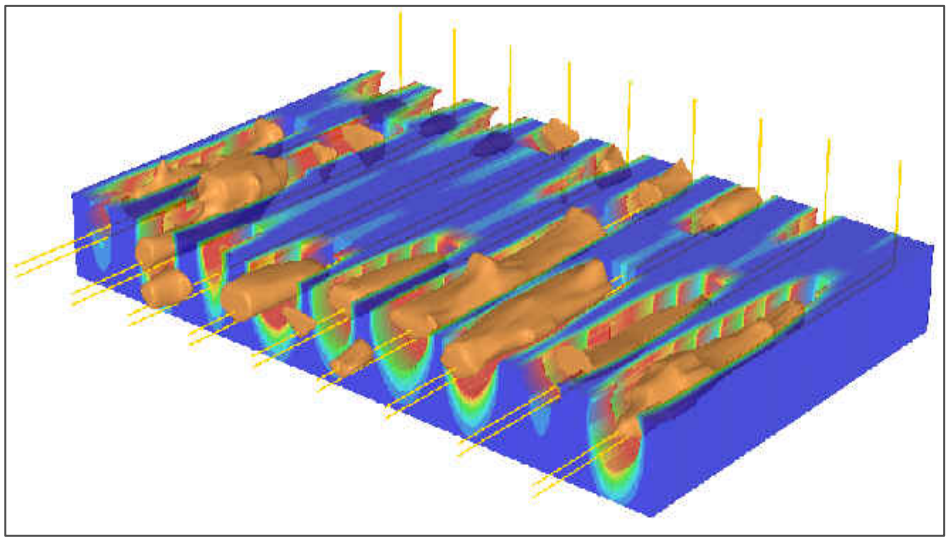

Figure 3 Well arrangement of SAGD well pairs

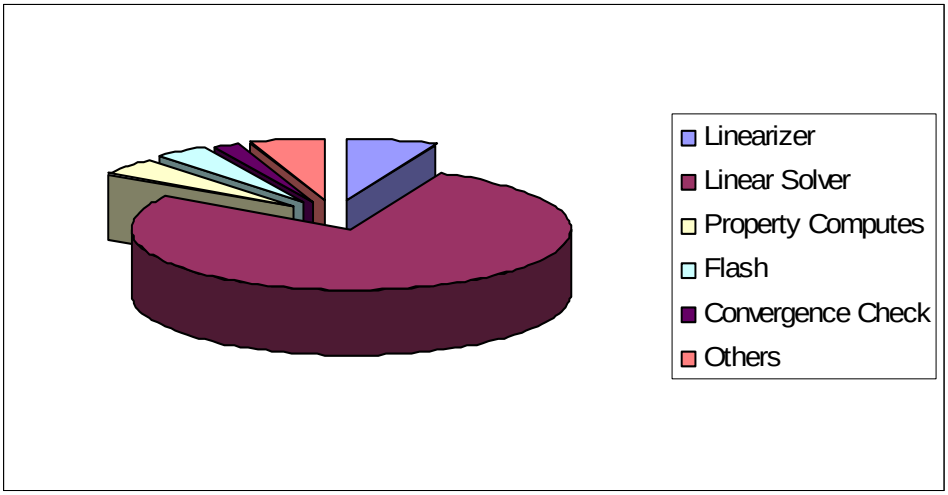

Figure 4 CPU time breakdown among different components

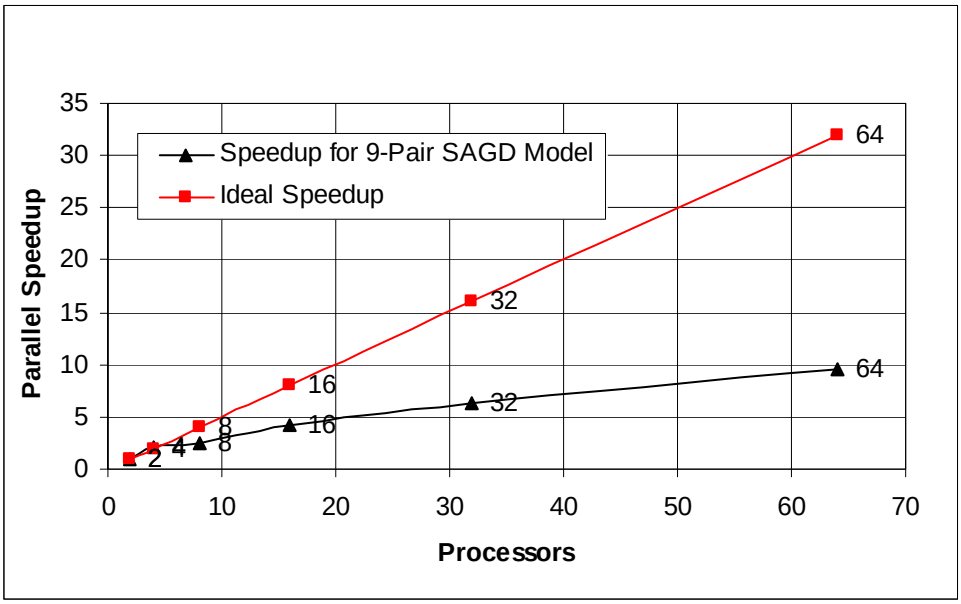

Figure 5 Parallel speedup relative to 2 processors run (9-Pair SAGD model)

Summary

A general unstructured grid, fully implicit thermal simulator has been developed. Proper primary variable selection and its alignment with balance equations have been presented. A robust time step selector as well as efficient nonlinear controls is necessary to achieve stability of numerical solution method.

We verified our simulator with various models of thermal recovery processes, such as the cyclic steam injection and SAGD proxesses. The simulator exhibits high performance and very good scalability for a large scale 1.7 million cell 9-pair SAGD case.

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Nomenclature

C_{pr}	Rock heat capacity
H	Enthalpy
k_r	Relative permeability
K	K-value (phase Equilibrium Ratio)
N_c	Number of hydrocarbon components
N_p	Number of hydrocarbon phases
P	Pressure
P_g	Pressure of gas phase
P_{cjo}	Capillary pressure of phase j referring to oil phase
q	Production and injection rate
q_{source}	External heat sources and sinks
S	Saturation
t	Time
T	Geometric part of fluid flow transmissibility
T^0	Reference temperature
T_h	Heat conduction transmissibility
x	Mole fraction of hydrocarbon components
y_w	Mole fraction of water component in gas phase
U	Internal energy
V	Cell volume
Z	Depth

Greek Letters

Δ	Difference operator in space
δ	Difference operator in time or Kronecker delta
μ	Viscosity
ρ	Density
ϕ	Porosity
θ	Temperature
γ	Phase gradient

Superscripts

n, n+1	Time step levels

Subscript

i	Component i
j	Phase j

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SI Metric Conversion Factors

bbl × 1.589 973	E-01 = m^3
cp × 1.0	E-03 = Pa·s