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A Geothermal Reservoir Simulator with AD-GPRS

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ABSTRACT

The AD-GPRS framework was modified to simulate geothermal reservoirs. AD-GPRS (automatic differentiation – general purpose reservoir simulator) is a computational framework that allows for a fully compositional and thermal reservoir simulation. However, this study looks specifically at the geothermal single component, two phase case. AD-GPRS is based on an automatic differentiation library that allows for a flexible treatment of the variable formulation and the nonlinear terms within the formulation. This allows a geothermal application functionality to be integrated within this framework. To verify the results obtained from geothermal AD-GPRS, comparisons with other models were carried out. The geothermal AD-GPRS results were compared to analytical and semianalytical models to verify the solutions obtained from the simulator. For situations where an analytical solution was unavailable, TOUGH2, a commonly used reservoir simulator was used for comparison.

1. INTRODUCTION

Numerical simulation and modeling for geothermal reservoirs is an important aspect in the forecasting and management of geothermal resources (O'Sullivan *et al.,* 2001). Reservoir models are useful tools for predicting the performance of a particular geothermal field and also to assess the outcomes of various production scenarios (Axelsson *et al.* 2002). With the increase in computing power, there has been an increase in demand for models with increasingly complex geometries, (O'Sullivan *et al.* 2013b, Burnell *et al.* 2012), nonlinear physics (O'Sullivan *et al.* 2013a) and larger models (Yeh *et al.* 2011).

With these added complexities, often a simulator can experience numerical issues when finding a solution to a problem. For instance, Magnúsdóttir (2013) experienced difficulty when using TOUGH2 (Pruess *et al.* 1999), a general purpose simulator to solve a discrete fracture model. This was thought to be due to the complexity of the numerical grid, resulting in a 'domain' error. Another problem observed in geothermal reservoir models, (Noy *et al.* 2012) is where a stalling behavior in the time step is observed. This can occur in various situations but particularly when the simulation is approaching a natural-state solution, where large time steps are taken. Reservoir simulation operates in terms of linear and nonlinear solvers. Usually the nonlinear solver struggles to converge for large time steps that generates badly conditioned or inaccurate Jacobians, hence time step cuts are performed.

With the growth in computational power, not only are more complicated models being run but in some cases ensembles of models are being run. These ensembles of models are needed for uncertainty evaluation and parameter estimation in the geothermal industry (Burnell *et al.* 2012). However, these inverse modelling techniques often need a large number of forward models to be run with perturbations to different model parameters. Due to the large number of forward model runs, these forward models have to be robust and able to run within a reasonable computational time frame. The convergence and time step issues described earlier can greatly hinder the performance of an inverse model run (O'Sullivan *et al.* 2013a).

However due to the complexity of most traditional simulators, the ability to understand or investigate some of these numerical issues can be difficult. Even if the problem is understood and changes are needed to be made, this can often be a difficult task. In particular, one of the most complicated computations in reservoir simulation is in the construction and solution of the Jacobian used by the nonlinear solver. The Jacobian matrix contains the derivatives of all the residual equations with respect to each independent variable in the nonlinear formulation. These residual equations and independent variables can change depending on the type of nonlinear formulation used or the physics that is modeled. Currently, most codes either employ a manual implementation of the derivatives (Schlumberger, 2011) or compute a numerical approximation of these derivatives (Pruess *et al.* 1999). Although a numerical Jacobian would allow greater flexibility in the computation, this is less accurate and could result in instability when solving the nonlinear equations (Vanden and Orkwis, 1996). These hurdles can make it difficult to implement or investigate the effects of different formulations or solution strategies into a general purpose simulator.

One method of overcoming this hurdle is to implement an automatic-differentiation library that forms the analytical Jacobian automatically based on the residual formulation. This library (ADETL) was developed initially by Younis (2009) and further extended by Zhou (2012a). Automatic-Differentiation General Purpose Research Simulator (AD-GPRS) (Voskov and Zhou, 2012b, Zhou 2012b) is a reservoir modeling platform developed and sustained by the SUPRI-B research group in the Energy Resources Engineering Department at Stanford University. AD-GPRS allows the flexible treatment of all nonlinear physics or formulations through the automatic differentiation framework inherent in the simulator (Voskov *et al.* 2009, 2012a). Other AD-GPRS options include flexible Multi-Point Flux Approximation discretization and general Adaptive Implicit Method (Zhou *et al.* 2011), OpenMP and Multi-GPU parallel implementation (Zhou 2012a, Tchelepi and Zhou 2013), advanced thermal-compositional formulation (Iranshahr *et al.* 2010, Zaydullin *et al.* 2013), fully-coupled geomechanics for fractured media (Garipov *et al.* 2013) and adjoint-based optimization (Kourounis *et al.* 2010, Volkov *et al.* 2013). This framework allows the implementation of a geothermal fluid module into the simulator such that it can be applied to geothermal problems. Also, with this flexibility, different variable formulations could be implemented and investigated further to determine the most effective choice of variables for geothermal problems.

The objective of this work was to implement a geothermal fluid module into AD-GPRS such that the various unique capabilities of AD-GPRS could be investigated in a geothermal context. To verify that AD-GPRS is able to represent and solve the correct mass and energy balance equations, test cases were run. These test cases were based on the 1980 Code Comparison study (Stanford Geothermal Program, 1980). Once AD-GPRS is verified to be able to sufficiently solve these test problems, other formulations and numerical issues can be studied further.

2. GOVERNING EQUATIONS

2.1 Conservation Equations

The governing equations for modeling the flow in a reservoir are given by the mass and energy conservation equations:

$$\frac{\partial}{\partial t}\left(\phi \sum_{k}^{p} \rho_k S_k\right) - \nabla . \sum_{k=1}^{p} (\rho_k u_k) - Q_M = 0 \tag{1}$$

and

$$\frac{\partial}{\partial t}\left[(1-\phi)\rho_R U_R + \phi \sum_{k=1}^{p} \rho_k U_k S_k\right] - \sum_{k=1}^{p} (\rho_k H_k u_k + S_k G_k) - Q_E = 0 \tag{2}$$

where ϕ is the porosity, ρ is the mass density, S is the saturation, u_k is the volumetric flow and Q is a source/sink term, U is the internal energy, S is the saturation and G is the heat conduction flux. The subscripts k represent a certain phase, R the rock property, p the number of phases.

Including these two conservation equations, the saturation constraint must be satisfied, that is, the sum of all the phase saturations sums to 1.

$$\sum_{k=1}^{p} S_k = 1 \tag{3}$$

2.2 Darcy's Law

To model the flow rates of each phase, Darcy's Law is used to describe the fluid flow through the porous media.

$$u_p = \frac{k k_{rp}}{\mu_p} \nabla(p_p + \rho_p g z) \tag{4}$$

where u_k the superficial velocity of the phase p, k is the rock permeability, k_{rp} is the relative permeability for phase p, p_p is the pressure for phase p, g is the gravitational constant and z is the coordinate direction of gravity.

2.3 Thermal Heat Conduction

The heat conduction equation used is:

$$G_k = -K \nabla T \tag{5}$$

Where K is the total thermal conductivity of the fluid and rock and T is the temperature and ∇ denotes the gradient of a vector.

2.4 Phase Equilibrium

A fundamental step in the formulation of the numerical solution for these conservation equations is the choice of primary variables that define the thermodynamic state of a phase. Based on the phase composition, these thermodynamic variables may change based on the formulation chosen. For the most basic case, where the only component in the flow is water, in single phase, only the pressure p and temperature T values are needed to describe the thermodynamic state fully. However, for a two-phase system, the pressure and temperature values are now related with the saturated-pressure relationship $p = p_{sat}(T)$. In this case, the pressure and temperature are dependent on each other.

There are two main methods that are used to formulate and solve this phase equilibrium problem: 1) Natural variable formulation (Coats 1980); or 2) a "persistent" variable approach. The "persistent" variable approach involves choosing a set of variables that remain independent through all phase regions. Possible choices of these variables are (pressure, enthalpy) (Faust and Mercer, 1975) or (density, internal energy) (Pritchett, 1975). However one of the disadvantages is that often thermodynamic properties are formulated in terms of pressure and temperature and formulating variables in terms of these "persistent" variables can be difficult, because they require the solution of implicit equations, which can result in a loss of accuracy. An alternative approach is to formulate it in terms of (pressure, temperature) and to switch variable sets if a phase change is encountered (pressure, saturation). From literature it is found that both methods (Pruess *et al.* 1999, Voskov and Tchelepi 2012a) have been proven to work and the efficiency of both methods is model-dependent. In this study, a natural variable formulation was implemented, using (pressure, temperature) for single-phase conditions and (pressure, temperature, saturation) for two-phase regions.

3. AD-GPRS

AD-GPRS is a flexible reservoir simulation research simulator which focuses on an extendable structure. Consequently, a modular object-orientated code structure was implemented. AD-GPRS focuses on providing a flexible, efficient and extendable numerical framework that is designed for reservoir simulation research. AD-GPRS solves the governing mass and energy balance equations with the finite volume method and linearizing the nonlinear equations using Newton-Raphson method. The entire code is written in standard C++. A full description of the entire structure and implementation of the code is available in (Voskov and Zhou 2012b).

The main capabilities of AD-GPRS directly related to geothermal problem are:

1. An extensible treatment of all the nonlinear formulation.
2. Fully thermal-compositional formulation
3. General grid description and range temporal discretization schemes
4. Thermal geomechanical modeling for fracture media
5. A variety of complex well models
6. Integrated adjoint-based optimization capability

3.1 Automatic-Differentiation

AD-GPRS is built based on the Automatic Differentiation Expression Template Library (ADETL) (Younis 2009, Zhou 2012b). The computation of these automatic derivatives consists of: 1) analyzing the expressions and to determine the basic operators (+,-,*, /) that are involved; and 2) performing basic differentiation rules -- linearity, product, quotients, function derivatives and chain rule to evaluate the derivative. The key benefit that this provides is the ability to compute analytical derivatives automatically without any manual implementation of the Jacobian or computing a numerical Jacobian. This manual implementation is often tedious and can be difficult to debug. Another alternative is to compute numerical derivatives by using a truncated Taylor series representation of the derivatives to represent the analytical derivatives. The main downside to this is that numerical derivatives lead to large truncation errors and small intervals would result in considerable round-off errors. A full description of this automatic differentiation library and implementation is available in (Voskov and Zhou 2012b, Zhou 2012b)

3.2 Variable Formulation

To compute these automatic derivatives, a set of independent variables needs to be defined. These independent variables are chosen such that they are able to fully define the thermodynamic state of the status of that block, this is analogous to the choice of primary variables. This choice would vary from block to block dependent on the current status of the block. In a liquid-water/steam system, there are three possible statuses:

Table 1: Status table for liquid water and steam

	Phases		**Nonlinear unknowns**		
Status	**Liquid Water**	**Steam**	p	T	S_g
1	x	-	x	x	-
2	-	x	x	x	-
3	x	x	x	(x)	x

Each of these statuses, corresponds to a certain thermodynamic state, where x represents the existing phases in that status. Based on the status, there is also a different variable formulation, with the single-phase statuses using p the pressure and T the temperature. For two-phase regions, p and S_g are chosen to be the primary independent variables and temperature as a secondary variable. The derivatives for each block will be computed using these variables as the independent variable.

3.3 Building Residual Equations

Utilizing the ADETL library, all the variable sets are stored as an ADscalar. The ADscalar type stores value of the variable and also the derivative with respect to all the independent variables. The residual equations are formed using these same AD variable structures. There are three main steps in the construction and utilization of these residual equations:

1. Specifying independent variables

   As discussed earlier, the choice of the independent variables is dependent on the block status. Based on the thermodynamic state of the block, the independent variables for each individual blocks could be determined. For each independent variable, the gradient will be set to 1 to itself and 0 to all other variables.

2. Constructing residual equations

   The construction of the residual equations can be split into different parts:

   1) Properties calculation – calculates various properties (e.g. fluid viscosity, enthalpy) as a function of the independent variables
   2) Calculate accumulation term and add to residual
   3) For each connection between blocks, compute the associated flux terms and add it to the residual equations
   4) For each well compute the associated source/sink terms and add it to the associated well control equation

4. NUMERICAL TEST CASES

The problem specifications of test Cases 1, 2 and 3 are based on the 1980 Geothermal Model Comparison study (Stanford Geothermal Program 1980).

4.1 Test Case 1 (Injection)

4.1.1 Problem Specification

This test case involves a one-dimensional, radial steady-state flow with unsteady heat transport for single-phase liquid water. The objective of this test case is to verify the heat conduction and convection of single-phase liquid water.

This problem involves the injection of 160°C liquid water at a flow rate of $q = 10\text{kg/s}$ into a reservoir of 170°C water. The boundary condition imposed is a pressure of 50 bars at the outer radius of 1000m. The initial condition is that the entire reservoir has a temperature of 170°C. The model properties are as follows:

Table 2: Model parameters for Test Case 1

Rock Permeability	1000 md
Rock Density	2500 kg/m^3
Rock Specific Heat Capacity	1.0 J/g°C
Reservoir Thickness	100 m
Porosity	0.12
Spatial Grid	Uniform 25m grid spacing

The results from this test case can be compared with the Avdonin analytical solution (Avdonin 1964). This would verify that simulator is solving the mass and energy balance equations sufficiently and also handling the units and treatment of a constant volume injection rate correctly.

4.1.2 Results

Figure 1 shows the spatial temperature distribution at the final time of 10^9 seconds and the temporal temperature distribution at each time step for the block with its block center at 37.5m. As can be seen from the results, AD-GPRS compares well with the analytical solution, within the range of the thermodynamic parameters used. The temperature distribution over time for the block at 37.5m is slightly greater than the analytical Advonin solution. A similar deviation was reported in the results that were obtained in the code comparison study and could be due to the fact that fluid properties were assumed constant in the Advonin solution.

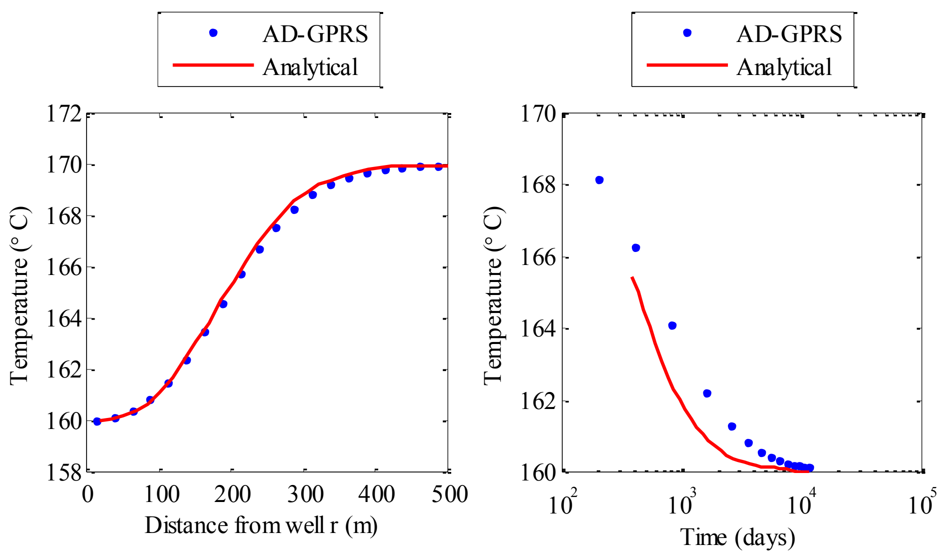

Figure 1: Temperature distribution at time = 10^9 seconds (Left) and the temperature distribution corresponding to the block with a block center of 37.5 over the simulated time

4.2 Test Case 2 (Drainage)

4.2.1 Problem Specification

This test case involves three different production scenarios. Each of these test cases involves the constant rate production of fluid in a one-dimensional radial flow problem. However each of the different test cases results in a different fluid mixture and resultant flow scheme.

a. The reservoir remains liquid water throughout production scheme
b. The reservoir begins a two-phase mixture of liquid water and steam and remains a two-phase mixture throughout
c. Reservoir begins as liquid water and changes to a two-phase mixture as the flash-front propagates throughout the reservoir

The simulation properties for each of the cases are as follows:

Table 3: Model parameters for Test Case 2

	Case A	**Case B**	**Case C**
Initial pressure (bars)	90	30	90
Initial temperature (°**C**)	260	233.8	300
Initial water saturation	1.0	0.65	1.0
Porosity	0.2	0.15	0.2
Permeability (md)	10	240	10
Thickness (m)	100	100	100
Producing Rate (kg/s)	14.0	16.7	14.0
Rock Compressibility	0	0	0
Rock thermal conductivity	0	0	0

The Corey curves were used as the relative permeability relationships:

$$k_{rl} = (S^*)^4$$

$$k_{rg} = ((1 - S^*)^2(1 - (S^*)^2) \quad (6)$$

$$S^* = \frac{S_w - 0.3}{0.65}$$

where k_{rl} is the relative permeability of liquid is water and k_{rg} is the relative permeability of the steam.

The same discretization scheme was used as in the code comparison study where the radius of each segment was:

$$r_n = 0.5 \times 2^{\frac{n-1}{2}} m, n = 1,2,3, \dots ,26 \quad (7)$$

Where r is the radius of the block center for the blocks numbered n, where the index 1 is the block closest to the well and 26 is at the outer most radius.

4.2.2 Results

Each of the different sub test cases either has an analytical or semianalytical solution to the problem. The semianalytical solutions were solved using a similarity variable of t/r^2 (O'Sullivan 1981). To verify the results from AD-GPRS these solutions are compared with the results from the simulator as a function of t/r^2.

Case 2a)

For this case 2a) the Theis solution (Theis, 1935) is used for comparison. Figure 2 shows the pressure as a function of t/r^2. As can be seen, there is a very good match between AD-GPRS and the Theis solution. This shows that the simulator is able to model the production from a well and the pressure changes associated with it.

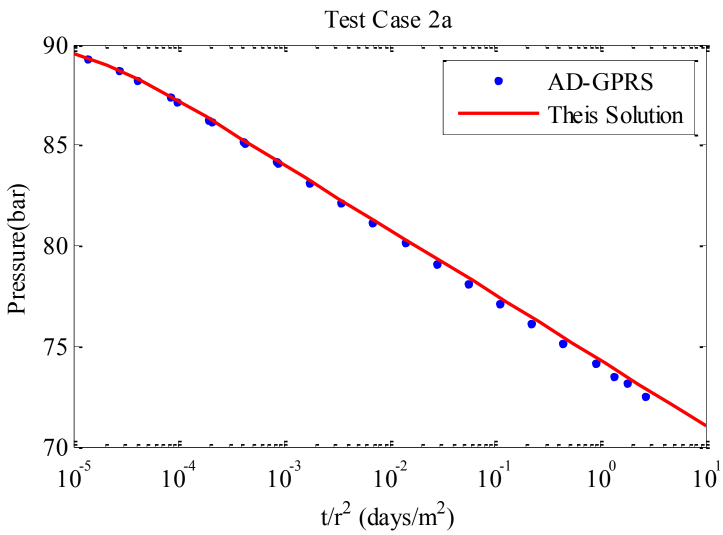

Figure 2: Pressure (bars) plotted with respect to t/r^2 (days/m^2) (Plotted at radius 0.5 m and 0.707 m)

Case 2b)

For both case 2b) and 2c) a similarity solution to the model (O'Sullivan, 1981) is available for comparison. This similarity solution transforms the governing mass and energy balance partial differential equations into ordinary differential equations and numerically integrates the ordinary differential equations. Figure 3 shows an acceptable match between the semianalytical results and AD-GPRS. The slight deviation between the two results can be attributed to the slight deviation in thermodynamic parameters.

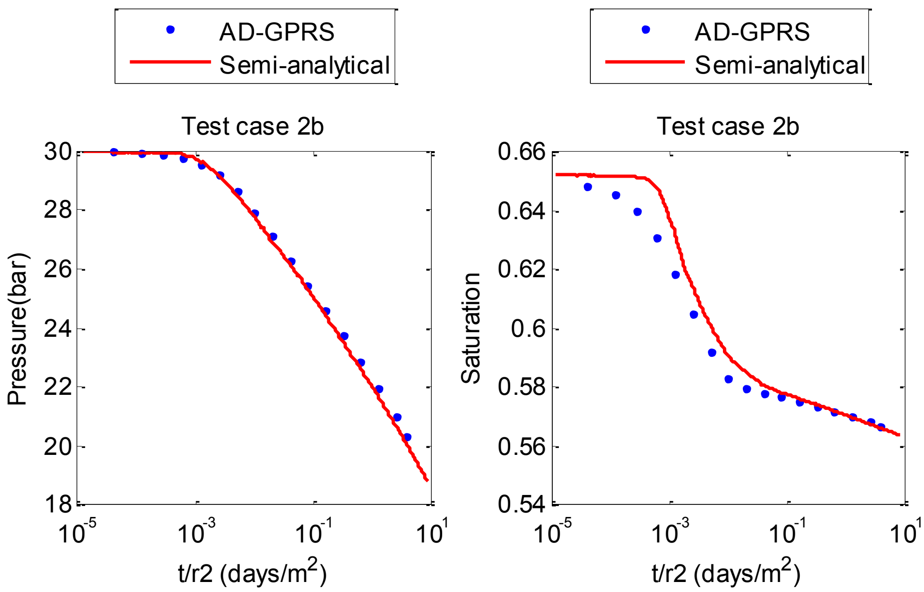

Figure 3: Pressure (Left) and Saturation (Right) plotted with t/r^2 for Case 2b

Case 2c)

Again, a semianalytical solution (O'Sullivan 1981) is available for case 2c). This simulation involves the propagation of a flash front moving outwards from the production well. Initially, the reservoir begins as completely filled with liquid water, approximately 5 bars above the saturation pressure at a temperature of 300°C. This results in boiling occurring 10 m from the well after about 1 day. Numerically, this problem is more difficult than the previous case due to the phase change behavior. In Figure 4, it can be seen that this match is not as close as the earlier cases. However, it is important to note that AD-GPRS did agree and follow the same results as the numerical codes presented in the Code Comparison study. This suggests that this deviation from the semianalytical solution is just a limitation of the numerical method that was used.

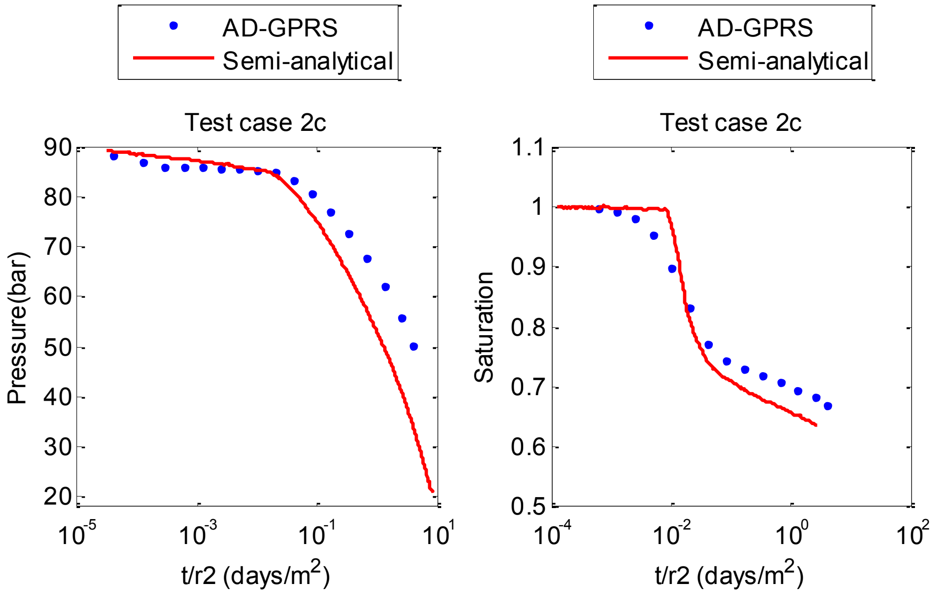

Figure 4: Pressure (Left) and Saturation (Right) plotted with t/r^2 (Case 2c)

4.3 Test Case 3 (Expanding two-phase region with drainage)

4.3.1 Problem Specification

This test case problem involves one-dimensional vertical single phase and two-phase flow. The reservoir is split into two 1km thick layers with a total of 20 grid blocks. The upper layer is less permeable than the lower layer (exact details shown below). The initial temperature in the upper layer linearly varies from 10°C to 290°C to the interface and the lower layer varies from 290°C at the interface to 310°C at the bottom of the model. The initial pressure condition in the reservoir is to reflect a hydrostatic pressure distribution.

The reservoir is being produced at a rate of 100kg/(s km^2) from the bottom of the model. The grid was chosen to be 20 equally sized blocks being simulated for a 40 year period.

Table 4: Table containing model parameters for test case 3

	Upper Layer	**Lower Layer**
Rock Density	2500kg/m^3	2500 kg/m^3
Porosity	0.15	0.25
Permeability (md)	5	100
Rock Specific Heat Capacity (J/g°C)	1.0	1.0
Rock Thermal Conductivity (W/m°C)	1	1

The relative permeability relationships were identical to that of Test Case 2 (Equation 6).

It is expected that a boiling zone will form near the interface in the lower layer of the reservoir. The boiling zone is expected to begin at the block closest to the interface and spread downwards. This problem could present some difficulties as the flow mechanism involves both gravity and convection effects. Also, this would test the simulator's ability to handle a large amount of boiling (multiple blocks changing phase).

4.3.2 Results

Due to the complexity of this problem, a semianalytical or analytical solution does not exist for this problem set up. Thus, a comparison with the results with TOUGH2, a widely used simulator was conducted instead. Figure 5 shows the pressure profile for three different blocks at decreasing depths. It can be seen that the pressure profiles for each of the blocks have a very close match to the results obtained from TOUGH2. It is important to note that these results are also in agreement to the results obtained in the Code Comparison study. From this result it is clear that AD-GPRS is able to handle the expansion of the boiling zone in a reservoir and the counter-flow of steam and water. This complex process is evident in geothermal reservoir fields such as Wairakei (Mannington 2004). The saturation (Figure 6) also shows a reasonable match with TOUGH2 over the simulated period. For a two phase system, the pressure and saturation fully defines the thermodynamic state of the fluid, it can be concluded that the other thermodynamic parameters such as temperature, enthalpy, etc. should also produce a reasonable match and any deviations would only due to fluid property calculations.

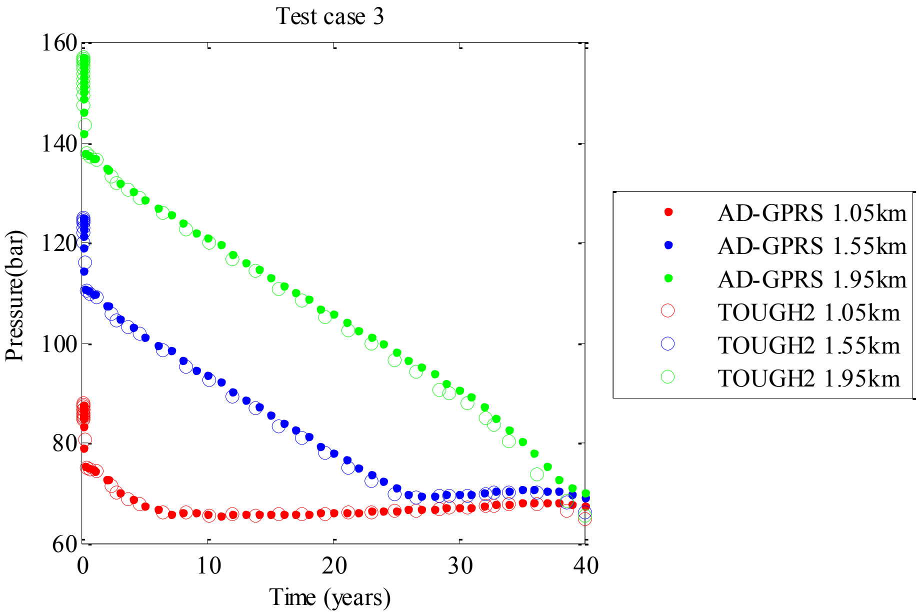

Figure 5: Pressure profiles for three different blocks at specified depths

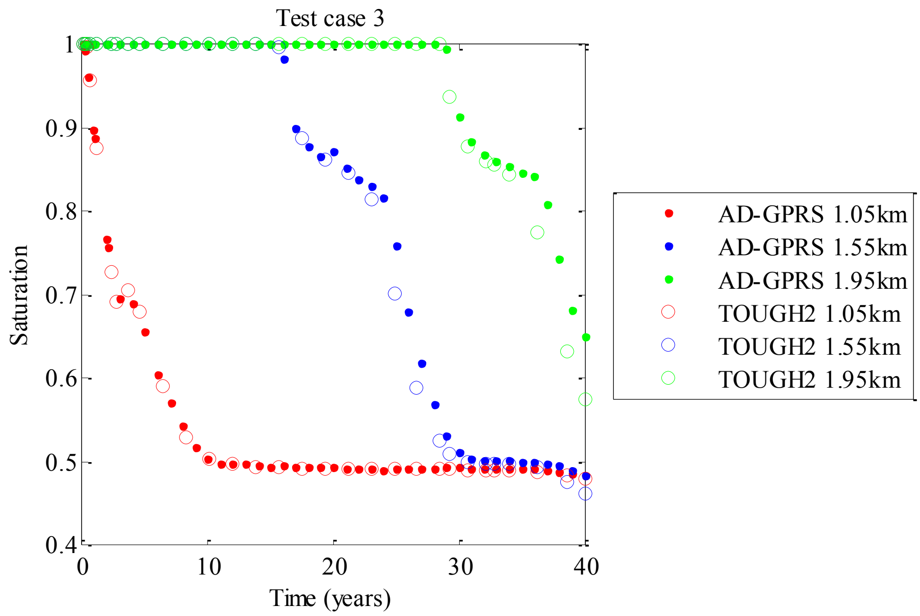

Figure 6: Saturation profiles for three different blocks at specified depths

5. CONCLUSIONS

A new geothermal reservoir simulator has been developed using the AD-GPRS simulation framework. Through the automatic-differentiation capability in AD-GPRS, this presents the opportunity to investigate many of the numerical issues related with reservoir simulation. Basic comparisons with AD-GPRS and analytical, semianalytical and TOUGH2 solutions have been performed to verify the solutions obtained from AD-GPRS. These solutions have all been in good agreement and provide confidence in the solutions from AD-GPRS.

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