A TESTBED FOR A NEW-GENERATION GEOTHERMAL SIMULATOR

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ABSTRACT

This paper describes a testbed code (TGNS) for a new-generation geothermal simulator. This is a fully operational simulation code which contains most of the functionality of TOUGH2 but is designed to explore new ideas and test new capabilities for a future, more complete simulator. Here, the background to the code and some of its features are described. Amongst others, TGNS can use different thermodynamic formulations, invoke a non-Darcy flow law and uses a simple unformatted input file. A number of validation problems are presented which show that TGNS and TOUGH2 produce similar results for a number of 1-D and 2-D problems. Also, some of the new capabilities of TGNS, including non-Darcy flow modelling and the use of continuous and time-dependent permeabilities are presented.

1. INTRODUCTION

The simulator TOUGH2 (Pruess, 1991) has been used by the geothermal industry for more than 25 years to model fluid and heat flows in geothermal systems and for other earth-science and industrial applications which involve non-isothermal multi-phase transport of water and dissolved species in porous materials. However, despite its widespread use and longevity, TOUGH2 has a number of limitations which have to be addressed to meet the needs of the geothermal/earth-science research communities in the future. These may be broadly (but not exclusively) described as follows:

a) Handling of model input and output is time consuming and error prone

b) Model specification is limited and could be generalised to allow for (e.g.) time dependent boundary conditions, permeabilities and porosities

c) The numerical algorithms for time integration, steady state calculations, fracture flow and phase-changing are not always robust

d) The thermodynamic functions used are inefficient and are limited to temperatures less than 350°C and pressures less than 1000 bar

e) The 'physics' is restricted to Darcy flow. This may not be the best description of some high-speed flows – e.g. in near-well locations with high permeabilities

The aim of the 'Geothermal Supermodels' research programme is to develop a new-generation simulator to address these and other issues. This paper describes work toward this aim.

In section 2 we give a general description of TGNS and some of its more novel features. In section 3 the results of some validation problems run with TOUGH2 and TGNS are presented. Then in section 4 we present some examples of problems that cannot be solved using TOUGH2.

2. THE TESTBED SIMULATOR, TGNS

2.1 Basic ideas

A testbed simulator has been developed to explore some of the issues outlined in section 1.1. The code, (TGNS - Testbed for New Geothermal Simulator) while still in the early stage of development, can represent the same single/two-phase processes as TOUGH2, but has several features which are foreign to the TOUGH2 modus operandi. Some of these include

a) A simplified, unformatted input file. There is no need to specify element names or other properties separately.

b) Output files which can be read directly into a graphics package.

c) A choice of several thermodynamic formulations is available, and this choice can be made from the input file.

d) The definition of the problem geometry has been simplified. The type of geometry (e.g 2-D Cartesian, radially symmetric) is specified in the input file and only a small number of other parameters are needed to define the model.

e) There is no concept of rock types. Instead, permeabilities (and in future other properties) can be defined as general functions of position and time.

f) Fixed pressure and temperature boundary conditions can specified separately as functions of time and do not require the use of large-volume model elements.

g) A 'Forcheimer' flow regime can be invoked. This is a more appropriate model to use than Darcy flow in situations such as near a discharging well where the fluid velocities can be very high.

Despite these new features, a number of concepts from TOUGH2 have been retained. TGNS has not been designed to test new algorithms for solving the mass and energy conservation equations relevant to geothermal systems. Rather, it is a tool for exploring new concepts in geothermal simulators, with the added bonus of being able to solve some types of problems that TOUGH2 cannot.

TGNS is an implementation of a standard finite volume numerical method, and uses an algorithm almost identical to that of TOUGH2 to discretise and solve the non-linear difference equations for the pressure, temperature (or

saturation) at each model element. Future adaptions of TGNS might be used to explore new time-integration methods for the equations, or the difficult problem of determining steady states. But for the moment the emphasis is on new modelling concepts and including new physical processes.

2.2 Input File

Below is an example of an input file. This specifies everything that is needed to model the withdrawal of fluid from the centre of a radial, horizontal domain. Many of the entries are self-explanatory and will be familiar to regular TOUGH2 users. However, the file very different in concept to a TOUGH2 input file.

The most noticeable feature is that the file is unformatted and contains a lot of commentary. This is in fact only partly true – the lines containing numerical inputs are unformatted, but the lines of commentary must always be in the same place in the file, and there must be no more or no fewer of them than shown here. Note also that there are no obligatory keywords – the lines of text are simply comments that relate to the input on the next line. They can be changed to add extra information if needed, provided that they do not extend over more than one line. After the 'END OF INPUT' (which is not a keyword) as much further commentary as needed can be added.

Part of the reason why the file is so different to an equivalent TOUGH2 input file is that the specification of the model domain and grid does not require that the grid blocks and their connections do not need to be specified explicitly. This will be described in more detail in section 2.3, but it highlights the general philosophy of keeping the input as simple as possible. This can be achieved by 'hiding' as much of the detail as possible, but comes at the cost of having to supply that detail elsewhere, for example in additional subroutines or data files.

```
Input for comparison problem 5 - radial geometry
ngeom: 4 = radial mesh
 4
ntherm: 1 = UKST1970,  2 = iapws97
 1
nperm: 1 = use kx,ky,kz below OR 2 = use general function
 1
grid parameters: nr,ntheta,nz,rmin,rmax,dz
 50 1 1 0.1d0 1000.d0 10.d0
rock properties: rho, phi, kx,ky,kz (mD!!!), K, cp, cf
  2650.d0  0.1d0  10000.d0 5.d0 5.d0 2.d0 1000.d0 0.5d0
initial conditions: P (bar) & T(C)
 100.d0  200.d0
source terms: nsource, then iel, qm, hm
 1
 1  -90.d-2 0.7e6
simulation parameters: t(final), initial dt, max timesteps
  0.1d06  5.d0  10000
increments of P (Pa) & T (C) for Jacobian calculation
  0.1d0  0.0001d0
END OF INPUT - can add comments after this..

radial domain to 1000 m, 10 m thick
initially 200C, 25 bar
withdraw/inject fluid at center element
```

2.3 Geometry

Specifying the geometry of the model domain is very simple. In the input shown above, the sections prescribing the geometry is as follows:

```
ngeom: 4 = radial mesh
 4
```

and

```
grid parameters: nr,ntheta,nz,rmin,rmax,dz
 50 1 1 0.1d0 1000.d0 10.d0
```

Because a radial geometry has been specified (ngeom=4), the code interprets the input parameters in terms of a radial mesh. Specifically, the mesh contains 50 elements (labeled 'nr in the comment), with only a single element in each of the 'theta' and 'z' directions ('ntheta'='nz'=1). The central element of the mesh extends to a radius of rmin (0.1 m), and the complete mesh to rmax (1000 m). The thickness of the mesh, dz, is 10 m. With this information, the code will generate a geometric progression so that the specified number of elements will precisely cover the model domain.

For Cartesian geometry, the relevant lines of input are:

```
ngeom: 1,2,3 = Cartesian mesh in 1,2, or 3-D
 2
```

and

```
grid parameters: nx,ny,nz,dx,dy,dz
 50 10 1 10.d0 10.d0 10.d0
```

Notice that the comments have been changed to better suit the problem being solved, and that the parameter labelled 'ngeom' plays a special role – it is the number of dimensions in the model domain. Also note that the general format is identical to that of the radial model– three integers followed by three real numbers. Here, the integers represent the number of elements in each of the x, y and z directions, and the three real numbers are the corresponding block dimensions.

TGNS can at present only handle very simple mesh geometries. More specifically, this means uniform meshes in Cartesian geometry and meshes where the elements increase in size according to a geometric progression in radial geometries. In these cases, the additional information needed for the finite volume algorithm (the volumes of the elements and the connections between them) can be generated internally and need not be specified in the input file as it must be in TOUGH2. This is an obvious limitation of the present version of TGNS because refined or unstructured meshes are a very necessary tool for modelling the complex multi-scale geological structures which occur in many earth science applications.

2.4 Thermodynamics

TGNS contains implementations of both the UK Steam Tables (1970) and the more recent IAPWS97 (Wagner et al., 2000) formulation for the properties of water and steam. The code includes four 'master' thermodynamic subroutines which calculate all of the fluid properties required to solve the conservation equations and which

point to the appropriate Equation of State (EOS) according to the value of a single parameter (ntherm) in the input file.

This feature of TGNS will facilitate the development and testing of new EOS's. An important part of the Supermodels programme is to implement new and highly efficient EOS's. As an example, in the near future a new supercritical module is planned for use in geophysical applications at extremely high temperatures and pressures. Only small changes are required in TGNS itself (in each of four master subroutines) to make use of any new thermodynamic functions.

Another application of this is the development of approximate EOS's. One idea is to use splines to calculate the thermodynamic properties of the fluids (Mike O'Sullivan, personal communication). The advantage of this is speed - properties could be evaluated using only a few arithmetic operations, resulting in a significant gain in performance. Development and testing of this technique would proceed exactly as described above for the new supercritical module, and in this way any number of distinct EOS modules can be included in TGNS in a simple and transparent way.

2.5 Rock Properties

The lines in the input file relevant to specifying the rock properties are as follows:

```
nperm: 1 = use kx,ky,kz below OR 2 = use general function
 1

and

rock properties: rho, phi, kx,ky,kz (mD!!!), K, cp, cf
  2650.d0  0.1d0  10000.d0 5.d0 5.d0 2.d0 1000.d0 0.5d0
```

The first of these provides a flag (labeled 'nperm') that controls how the permeabilities are defined. In this example this is set to 1, which means that the components of the permeability supplied in the input file will be used for all elements in the model. This is obviously very limiting if more than one permeability is required, and for this reason a second more general option is available. This is invoked by setting the flag to any negative number. This allows the permeability to be specified as a general function of position and time. This is done by providing a separate subroutine, which is linked with the basic TGNS code. This is one of the more experimental capabilities of the code, and in the future will be extended to the other rock properties.

The second part of the input (after 'rock properties') is where the permeabilities (if uniform everywhere in the model) and other rock properties are specified. These are largely self-explanatory except to note that the permeabilities are specified in milli-Darcy, a more familiar and convenient unit of permeability than the SI unit 'm^2'. The parameter labeled 'cf' (here with value 0.5) is the coefficient of the quadratic drag term (Joseph et al., 1982) which has been included in the flow law used by TGNS. The provision of non-Darcy flow terms as the default is a new feature and one which is not available in TOUGH2. In TGNS, setting this coefficient to zero restores the standard Darcy flow law.

2.6 Output files

TGNS has two main output files, one containing 'PTS' information, and one containing flow information. Both files are in the form of TecPlot input files and can be loaded directly into that package for visualisation. These data are also written in text files to give easy access to numerical values should they be needed for other post-processing. An example of this might be the determination of the integrals of density for micro-gravity studies.

3. VALIDATION PROBLEMS

The first requirement for a new code such as TGNS is to ensure that it gives results consistent with those from other codes which solve the same problems – in this case TOUGH2. In this section three such comparison problems are presented.

3.1 Single-phase, 1-D

The simplest validation problem involves a 1-D model domain and fluid which remains as a single-phase liquid throughout the simulation. Here we model the withdrawal of water (1 kg/s) from one end (X=0) of a domain 1000 m in length containing 100 10 m x 10 m x 10 m elements. The initial conditions are fixed at P=50 bar and T=200°C everywhere, and these conditions are held fixed at the far end (X=1000 m) of the model domain. The permeability is 500 mD and the porosity is 0.1. Other rock properties are the thermal conductivity (2 W/m/K), the specific heat (1000 J/kg/K) and density (2650 kg/m^3). The model setup is identical for both TGNS and TOUGH2. In this example (and all others in this paper) TGNS uses the UK Steam Tables thermodynamic functions.

Figure 1 shows the temperature distributions calculated by the two codes after 20,000 s. The small temperature reduction (about 0.06°C) occurs because of a weak 'thermodynamic' coupling between the rates of change of pressure and temperature. The codes clearly give very similar results.

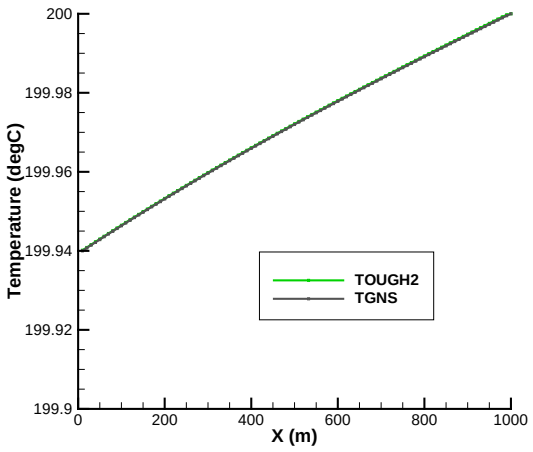

Figure 1: Comparison of temperature profiles for a single-phase, 1-D problem calculated with TOUGH2 and with TGNS.

Figure 2 shows the corresponding pressures. Again, these are in good agreement and are indistinguishable on the scale of the plot.

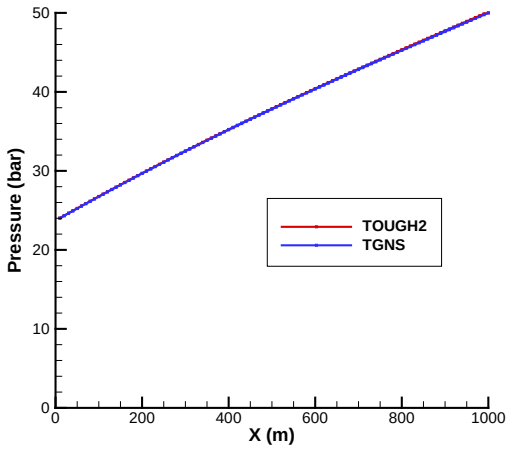

Figure 2: Comparison of pressure profiles for a single-phase, 1-D problem calculated with TOUGH2 and with TGNS.

3.2 Two-phase, 1-D

For the second comparison problem, the same model domain, rock properties and thermodynamics are used, but the initial conditions are changed to P=170 bar and T=350°C, and the withdrawal rate is increased to 5 kg/s. In this case, the initial conditions still correspond to a liquid state, but the increased withdrawal rate results in a greater pressure drop, with boiling taking place as soon as this reaches ~5 bars. As most boiling occurs within 250 m of the point of withdrawal, only this portion of the domain is shown in the Figures. Because this region is boiling (two-phase) comparison plots for this problem are shown for pressure and saturation.

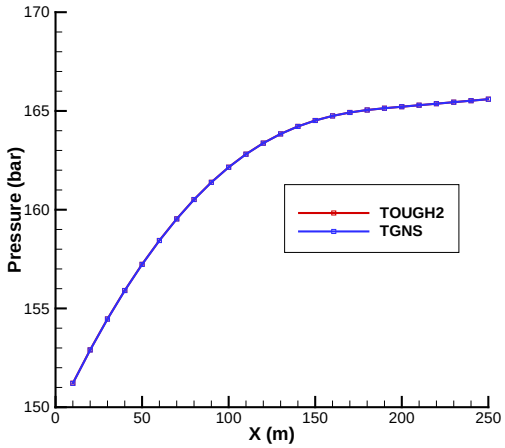

Figure 3: Comparison of pressure profiles for a two-phase, 1-D problem calculated with TOUGH2 and with TGNS.

Figure 3 shows a comparison of the pressures calculated by TGNS and TOUGH2, after a simulation time of 50,000 s. Figure 4 shows the distribution of liquid saturation at the same time. Again the agreement between the two codes is excellent, with the curves being indistinguishable in both figures.

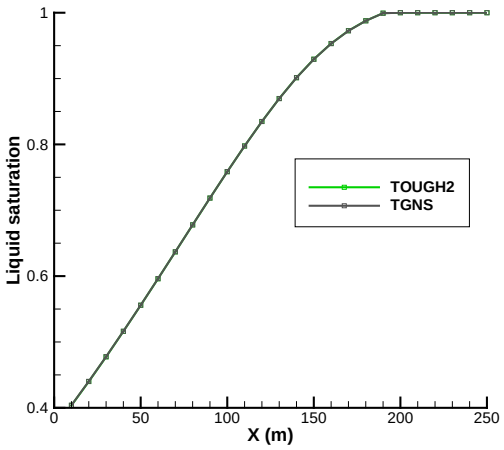

Figure 4: Comparison of saturation profiles for a two-phase, 1-D problem calculated with TOUGH2 and with TGNS.

3.3 Multi-phase, 2-D

As a final example, we consider injection of liquid water into a 2-D model domain initially filled with dry steam.

The model domain is 200 m x 200 m x 10 m and consists of 400 identical elements arranged in a 20x20 array. The permeability and porosity of the rock are uniform, at 5 mD and 0.1 respectively. The domain is initially at a pressure of 15 bar and a temperature of 200°C, and these conditions are fixed along one side of the domain. On the opposite side, fluid is injected into a central element at a rate of 0.01 kg/s with enthalpy 700 kJ/kg.

The injected fluid is cooler than the steam, and this leads to both a pressure increase and a fall in temperature at the point of injection. This first creates a small two-phase region due to the pressure rise and simultaneous drop in temperature. With further injection this zone expands and becomes wetter (higher liquid saturation), leading eventually to another phase change, this time to pure liquid.

Some idea of the subtleties of this problem is seen in Figures 5, 6, and 7, which show the pressure, temperature and liquid saturations at the injection point as a function of time. Generally, the comparison between TGNS and TOUGH2 is qualitatively satisfactory, although there are some clear differences. The initial pressure rise at the injection point occurs rapidly, but terminates as soon at the conditions there become two-phase. Then the subsequent pressure decay (until time = 8×10^6 s) is slower, with the element becoming progressively wetter in this interval. Until this point the three graphs show very similar results from TGNS and TOUGH2.

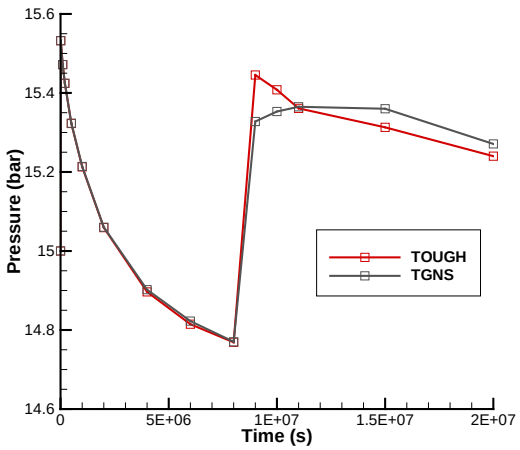

Figure 5: Comparison of pressure vs time at the injection point for a multi-phase, 2-D problem calculated with TOUGH2 and with TGNS.

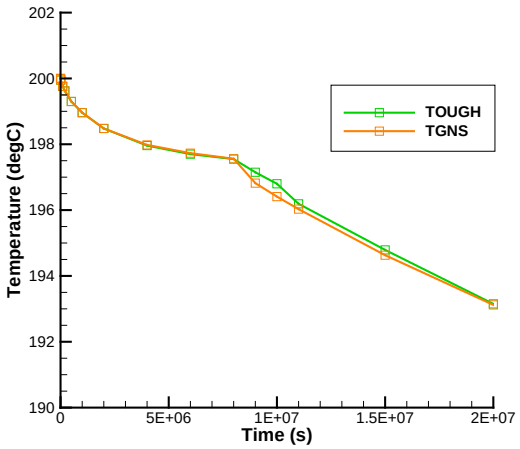

Figure 6: Comparison of temperature vs time at the injection point for a multi-phase, 2-D problem calculated with TOUGH2 and with TGNS.

At time = 8×10^6 s the injection element makes the transition to pure liquid (Figure 7), and this is accompanied by a large pressure rise (Figure 5). Beyond this point, the pressure and temperature curves differ slightly, by of order 0.1 bar and 1°C respectively, but there is little difference between the saturation curves. The differences between the pressure (or equivalently the temperature) curves occur largely because of the different time step histories in the two simulations.

TOUGH2 and TGNS have similar but not identical time stepping algorithms, and some differences in the sequence of time steps taken to reach the end of the simulation do occur. This affects the time when phase changes occur in particular elements and consequently there is a 'chaotic' effect on the remainder of the simulation. Experiments confirm that scatter similar to that in Figures 5 and 6 (~0.1 bar, 1°C) occurs in this model with both codes with different time step histories, as will happen (for example) when a different initial time step or maximum time step is specified.

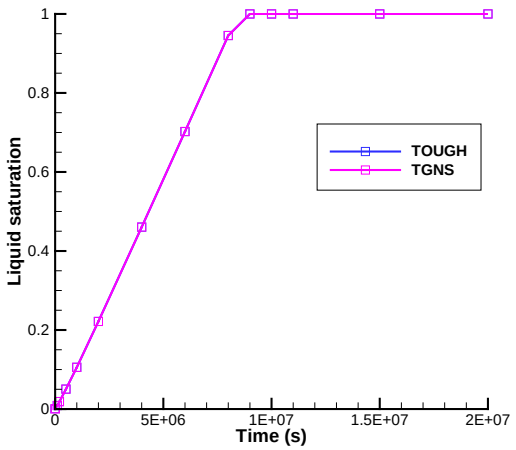

Figure 7: Comparison of liquid saturation vs time at the injection point for a multi-phase, 2-D problem calculated with TOUGH2 and with TGNS.

4. 'BEYOND-TOUGH2' PROBLEMS

In this section, a number of problems are presented which cannot be easily modelled using TOUGH2.

4.1 Continuous permeability

One concept which is not available in TOUGH2 is that of a continuous permeability. This capability is useful when (for example) a geological unit in a model is subjected to conditions which alter its permeability so that it varies continuously with position. To solve this problem in TOUGH2 would require an inconveniently large number of distinct rock types (although this can be overcome using PyTOUGH – Adrian Croucher, pers. comm.). With TGNS it is a simple matter to define the appropriate function of position, as described in section 2.5.

Figure 8 shows the pressure distribution in a 1-D domain identical to that described in section 3.1, except that now the permeability, rather than being a constant, is a function of position. The withdrawal rate at X=0 has also been increased to 0.4 kg/s. For each curve (at time = 1×10^7 s), the permeability varies linearly from the value indicated in the legend at X=0, to 500 mD at X=1000 m. Thus the green curve corresponds to a uniform permeability, the blue and black curves have higher permeability at the 'withdrawal' end, and the red curve has lower permeability there. As expected, with higher permeabilities the pressure drop is less than in the case where the permeability is uniform, and vice-versa.

The curves show the pressures at a time when they should be close to their 'steady state' values. Thus, the green curve is the only straight line – here the permeability is uniform through the model domain at 500 mD. Conversely, the other curves are not linear, highlighting the effect of the continuously varying permeability.

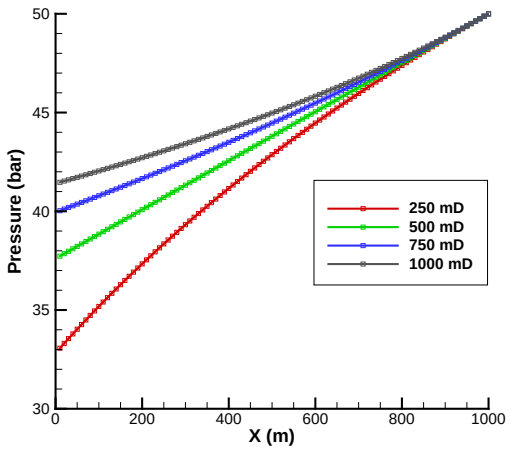

Figure 8: Comparison pressure distributions for problems where the permeability varies linearly from the value indicated in the legend at X=0 to 500 mD at X=1000 m. This type of problem cannot be conveniently solved with TOUGH2.

4.2 Time-dependent permeability

Another 'non-TOUGH2' concept in TGNS is allowing the permeabilities to be time-dependent. One application of this is the modelling of the flows in a fault or fault systems (e.g. Kissling et. al., 2013) following fault rupture. Fault permeabilities can increase markedly on rupture, and then decay back to 'ambient' values on timescales ranging from days to years (Ingebritsen & Manning, 2010). This type of behaviour is difficult to model using TOUGH2 but is straight forward with TGNS.

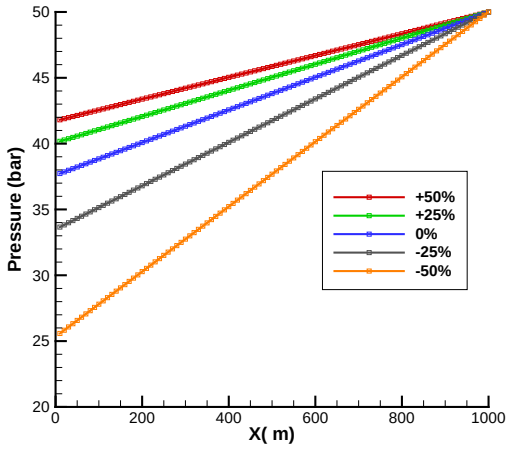

Figure 9: Pressure distributions for problems where the permeability varies linearly with time. The initial permeability is 500 mD and the values in the legend indicate the percentage change in permeability which occurred by 10^7 s.

Figure 9 shows a series of pressure profiles where the permeability is varied with time. The initial parameters and setup of the model are identical to those used in section 4.1. In this example, the permeability, initially 500 mD, varies linearly with time and at $t=10^7$ s has changed by the amount indicated on the plot. Again, as expected, decreasing permeability leads to greater pressure changes, and vice-versa. The profiles are close to linear because the pressure diffusivity is large (~1 m^2/s) and so the pressure changes equilibrate across the domain rapidly compared to the simulation time.

More interesting behaviour is observed if the permeability is changed in only one part of the model domain. In the following example, the section of the model domain between 450 m and 550 m has a permeability which reduces with time exponentially with a time constant of 10^6 s. In the remainder of the domain the permeability remains at 500 mD. This is a simple model for the behaviour of a fault (or other arbitrary flow path) which becomes blocked due to chemical deposition or some other process, while the forcing for the flow remains unchanged. This is compared to the case where the permeability is left unchanged.

The result is shown in Figure 10. The red and green profiles show the behaviour of the model for very short times, with the red curve at 10^3 s displaying the characteristic early time curvature. For these times the profiles with and without the blocked permeability are indistinguishable on the scale of the plot. The blue curve represents the steady state for constant permeability, and the curves below this show the increasing effect of the permeability reduction in the centre of the model domain. This is visible as early as 5×10^5 s (black curve), and by 2×10^6 s (purple) the permeability has dropped to a factor of $1/e^2$ or 14% of its original value and the pressure difference across the 'plug' is 10 bars. Slightly beyond this time the pressure drops further, boiling occurs and the elements near the origin boil dry and the simulation fails.

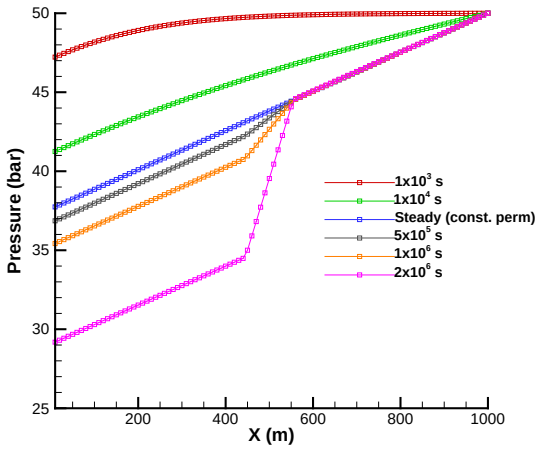

Figure 10: Comparison pressure distributions for problems where the permeability decays exponentially with time between X=450 m and X=550 m.

4.3 Non-Darcy flow

The normal 'Darcy' flow law is a linear relationship between the fluid velocity and pressure gradient, and applies where that velocity is small, i.e. the local Reynolds number (based on pore size) is of the order of one or less. As the fluid velocity increases, an additional term is necessary to describe the drag forces which arise. Joseph et al., (1982) and Nield & Bejan (1992) advocate the use of the 'Forcheimer equation' which contains an extra term which is quadratic in the fluid velocity

$$\mathbf{v} = - k/\mu\nabla(P - \rho g)/(1 + c_F k^{½}\mu^{-1}\rho|\mathbf{v}|), \qquad (1)$$

where the numerator represents the normal Darcy flow law, and the magnitude of the correction for quadratic drag is governed by the second term in the denominator. The quantity c_F is known as the form-drag coefficient and should be on the order of 1.

This extended flow law has been implemented in TGNS, and to demonstrate the extreme situations where it has an effect, a further 1-D example is presented. The model domain and setup are the same as those used previously. Initial conditions are P = 50 bar and T = 200°C and a uniform permeability of 125 mD is used. Withdrawal of fluid takes place at the origin at a rate of -0.1 kg/s. This time however the quadratic drag coefficient is non-zero.

Figure 11 shows a series of steady state pressure profiles for different values of the drag coefficient. This shows that as the c_F increases the pressure drop across the model domain remains linear, and its magnitude (or equivalently the pressure gradient) also increases. Thus, when accounting for the drag, a larger pressure gradient is needed to maintain the same flow rate. This is consistent with Equation (1), which expresses the fluid velocity as the Darcy flow velocity divided by a quantity which is always positive and greater than one. It should be noted that the drag coefficients used to achieve these large pressure changes are too large to be physically correct. In 'normal' geothermal applications, the quadratic drag is negligible, and permeabilities of the order of 100 Darcy or more are needed to render the quadratic drag correction significant.

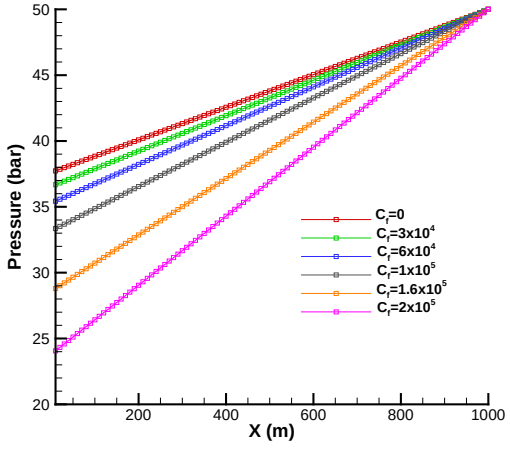

Figure 11: Comparison of pressure distributions for problems with quadratic drag. The legend indicates the size of the drag coefficient for each curve.

5. CONCLUSIONS AND OUTLOOK

In this paper we have described a testbed code (TGNS) for a new generation geothermal simulator. TGNS is an implementation of a standard fully implicit finite-volume algorithm for multi-phase flow in porous media and shares many 'algorithmic' features with TOUGH2. However, the philosophy behind TGNS is to test new ideas, and the code also has some capabilities which are not available in TOUGH2. To highlight both 'old' and 'new' capabilities, the paper presents a number of validation problems where results are compared with those from TOUGH2, and then some models where 'new' capabilities are used.

One of the most important features of TGNS is the use of a simple, 'short-hand' unformatted input file to define the problem being solved. This allows, amongst other things, to define the model domain and geometry very easily, the choice of thermodynamic functions to be used or how the permeability and other rock properties are to be defined. While this is extremely convenient, using the short-hand input comes at the cost of limiting the complexity of the problems that can be solved. A good example of this is defining the problem geometry. TGNS can at present only work with models which have simple geometry - regular Cartesian meshes and radial meshes where the element sizes change according to a geometric progression. These geometries can be described completely by a small number of parameters and so are well suited to the short-hand input format. It is not yet clear what the best method is to define more complex meshes within this context and this will be the subject of further research.

TGNS includes a number of other features which are quite foreign to TOUGH2. For example, there is no concept of 'Rock types'. Properties of the rock are instead defined as functions of position and time. TGNS also has the capability to use time-dependent boundary conditions for pressure and temperature independently. Again, it is not clear how to best implement these features while maintaining the concept of a simplified input file.

Some future developments for TGNS include the implementation of new EOS modules including additional components, for example the systems H_2O-NaCl and H_2O-CO_2. The phase-changing algorithms used in TOUGH2 are not always robust for systems like these (e.g. Kissling, 2005) and we plan to use TGNS to understand this problem and find a more general approach. It is also hoped to use TGNS to model the flows in fractured reservoirs in a manner independent of the assumptions of the commonly used MINC-like models. Direct simulation of fracture-block interactions seems possible and would lead to more realistic models of these systems than have been possible in the past. Finally, TGNS is well suited to being combined with a rock mechanics code to study thermo-hydrological-mechanical (THM) problems. In particular we are keen to pursue studies of the brittle-ductile transition in the TVZ (e.g. Kissling and Ellis, 2011) and the role it plays in controlling the large scale fluid circulation and formation of geothermal systems in that system.

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