Comparison of reservoir simulator DC3D (based on ROSIM input files) to other simulators

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1 Introduction

1.1 General remarks

In this report a benchmark of the TNO in-house software tool ROSIM is described, which contains the TNO tool DoubletCalc 3D (DC3D). ROSIM creates static 3D subsurface models which are subsequently used for flow simulation. There are two options for flow simulation: DC3D and OPM flow. DC3D is a thermal, single phase simulator for geothermal and heat storage applications, an in-house TNO development. OPM flow is an open-source, black oil simulator with thermal capabilities, part of the OPM project [1].

For simple configurations, the output can be compared to analytical solutions. For more complex geometries, a comparison to other simulators is given, in this case a commercial tool with coupled flow-thermal solution, which is an industry standard in the petroleum industry. However, the commercial simulator is not developed for an HT-ATES (high temperature storage) setting, with shallow depths, very high permeabilities and a yearly injection/production schedule. The commercial simulator deck is based on the input decks for OPM flow by ROSIM. However, due to differences between OPM flow and the commercial simulator adjustments are necessary. These are described in Appendix C. The benchmark is focused on showing suitability of ROSIM and DC3D for simulating reservoir conditions and inflow into wells for geothermal applications. Heat storage applications will only be addressed briefly.

The following versions were used:

- ROSIM 0.4 build 11/10/2022
  (= ROSIM 1.0 - Dec 2022, with some GUI updates)
- DC3D (November 2022)
- OPM flow 2022.10

Several DoubletCalc 3D features are currently in development. Therefore functionality is more limited compared to the commercial simulator. For example faults and pinching out layers are currently not included as grid options. Also pressure drop inside the well is not supported. Appendix A gives a very brief comparison of the differences in functionality between the simulators. The ROSIM installation, graphical user interface (GUI) settings, input/output and DoubletCalc 3D technical background are described in the ROSIM manual [2].

The simple cases are also runs using the 2D version of DoubletCalc (DC2D) [3]. The version of DC2D that has been used in this reports is the version compiled in August 2019 as used in-house at AGE (Advisory Group Economic Affairs). OPM flow is included in only a few cases, because currently (v2022.10) the implementation of the thermal modelling is relatively immature and can be unstable. The thermal modelling functionality used here has only recently been added to OPM flow and is still in the development phase. In general the flow runs are more stable when the solver settings below are used. Also reducing the time step size can help. The file ending with '_ONEPHASE.DATA' should be used rather than the '.DATA' file which will use the 3-phase flow simulator.

Solver settings used for running OPM flow:

```
flow <name>.DATA --linear-solver-reduction=0.03 --tolerance-mb=1e-7 --tolerance-cnv-relaxed=0.01
```

Settings for reducing the time step:
Additional run time option: --enable-tuning=TRUE
Keyword in SCHEDULE section:

```
TUNING
 0.1 10.0 0.001 /
 /
 /
```

1.2 Analytical solution

The analytical solution to which the results of the different simulators are compared is given below.

The pressure drop Δp_{inj} for the injector:

$$\Delta p_{inj} = Q \frac{\mu_{inj}\left(\ln\left(\frac{L}{r_w}\right) + S_{inj}\right)}{2\pi k H}$$

The pressure drop Δp_{prd} for the producer:

$$\Delta p_{prd} = Q \frac{\mu_{prd}\left(\ln\left(\frac{L}{r_w}\right) + S_{prd}\right)}{2\pi k H}$$

Where
Q : production / injection rate [m^3/s]
μ : viscosity of the producer/injector [Pa s]
L : well distance [m]
r_w : well outer diameter [m]
S : skin of the producer/injector [-]
k : permeability of the reservoir [m^2]
H : height of the reservoir [m]
inj/prd : subscript denoting injector and producer respectively.

The total pressure drop is calculated as the sum of pressure drop for the injector and for the producer.

The approximation of the inflow into a deviated well is calculated following the approach in DC1D using eq. 29 from the manual of DoubletCalc 1D [4].

1.3 Simulation time

Simulation times vary significantly: DC3D is the faster simulator if annual time steps are used. The finer the times steps, the longer the run takes, because every time steps is equally long irrespective of the length of the step. This is different from most simulators in which the calculation of a time step is generally faster for a shorter time step (overall run time does increase). The commercial simulator takes around 10 to 20 minutes for most of the models run here. The exception is the model with the sub-horizontal well, which did not run well and required very small time steps. Tests show that currently OPM flow is slower: a 30 year run can take many hours depending on the settings.

1.4 Structure of the report

In chapter 2, the results for cases are compared, most with a geothermal doublet. First a number of cases is compared for which an analytical solution is available, these are without under- and overburden. Next, different well configurations are compared in a reservoir which includes an under- and overburden. Finally, a tilted reservoir, heterogeneity in the permeability and a heat storage case (HT-ATES High Temperature Aquifer Thermal Energy Storage) are compared.

In Chapter 3, options available for DC3D are tested. Finally, Chapter 4 discusses the conclusions. Appendix A provided a very high level overview of functionality of the different simulators. Appendix B gives a detailed comparison of the functionality of DC2D and DC3D. In Appendix C, the keyword changes are listed that are required to change the OPM flow decks generated by ROSIM to decks for the commercial simulator.

2 Results comparison

2.1 Without under- and overburden

2.1.1 Vertical well

A simple model was constructed for comparison with the analytical solution: without over- and underburden and with no-flow and no-heat-exchange boundaries on all sides and top and bottom. For comparison with the analytical solution, temperature-dependent density was not included in the simulations for the commercial simulator, which was implemented by decreasing the dependence with a factor of 100 rather than setting it to zero, because that is more stable numerically. The DC3D runs are all with temperature-dependent density. The wells are vertical and fully penetrating. Further input settings can be found in Table 2.1.

Table 2.1. Input settings for comparison with the analytical solution

Reservoir thickness	60 m
N/G	0.9
Permeability xy	150 mD
Permeability z	15 mD
Por	0.2
Rock compressibility	1E-5 1/bar *
Model size	5 km x 5 km x 60 m
Grid resolution	50 x 50 x 3 m
Injection rate	100 m^3/hr
salinity	70000 ppm
Well distance	Defined as 605 m, but results in 650 m because wells are always modelled in the middle of a grid block.
Well diameter	8.5 inch
Injection/production rate	100 rm^3 for DC and OPM flow 100 sm^3=99.2 rm^3 for the commercial simulator
Boundary conditions	No-flow and no heat exchange

* Rock compressibility does not affect the results in this section, because only (semi) steady state conditions are analysed.

Because the settings for the different models are not entirely identical, an analytical solution was calculated for each simulator separately. In Table 2.2, the simulator results are compared with the analytical solution. For all simulators, the difference with the analytical solution is less than 0.5%.

For injection with a different temperature, the total pressure difference changes significantly. The analytical solution is most appropriate when the thermal front is halfway between the two wells. Visually this was identified to be after ~10 years of injection. From the results in Table

2.3, it is clear that all simulators underestimate the pressure drop. This is probably because at 10 years, the front is not exactly in the middle between the two wells. All results however, are close together. Figure 2.1 shows the thermal breakthrough. The results of all simulators are close together. The commercial simulator doesn't have an exact production temperature of 80°C, because the energy equations are solved simultaneously with the flow equations assuming constant enthalpy. This means that temperature changes when pressure changes.

Table 2.2. Δp results for an injection temperature of 80°C (results after 3 years).

	Δp_{total}	% difference
Analytical solution for DC2D	46.78 bar	
DC2D (visc. is Batzle and Wang instead of Kestin*)	46.90 bar	0.24
Analytical solution for DC3D	39.81 bar	
DC3D	39.92 bar	0.30
Analytical solution for commercial	39.59 bar	
commercial	39.63 bar	0.09
Analytical solution for OPM flow	39.81 bar	
OPM flow	39.90 bar	0.24

* Because the used viscosity it not exported with the solution, the values used in the analytical solution might be slightly different than the ones used in the simulator.

Table 2.3. Δp Results for an injection temperature = 30°C (results after 10 years).

	Δp_{total}	% difference
Analytical solution for DC2D	69.26	
DC2D (visc. is Batzle and Wang instead of Kestin)	66.10	-4.56
Analytical solution for DC3D	62.79	
DC3D	60.18	-4.16
Analytical solution for commercial	62.80	
commercial	60.38	-3.85
Analytical solution for OPM flow	62.79	
OPM flow	60.28	-4.00

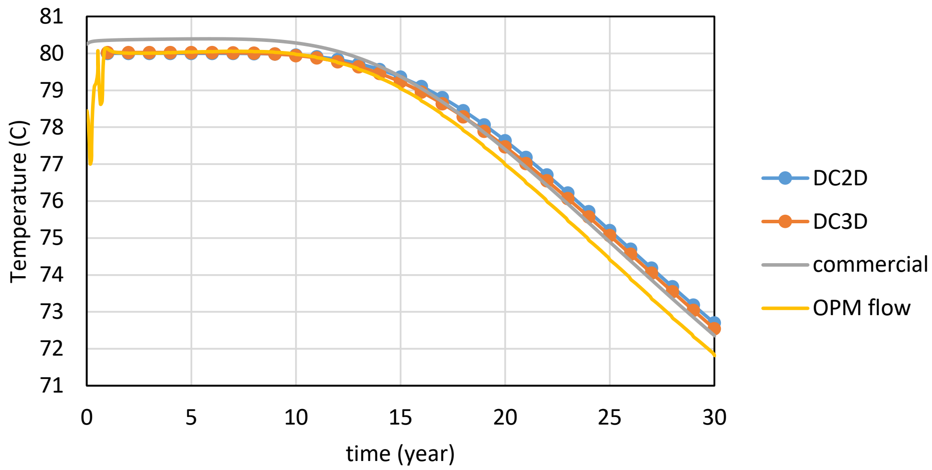

Figure 2.1. Thermal breakthrough at the production well for injection at 30°C. (OPM flow v2023.04 used for these results)

For the commercial simulator, an option is available to reduce the numerical dispersion: 9-point numerical solution. Figure 2.2 shows the impact of this on the thermal breakthrough which is small. For thermal runs, the impact is not that large, because the thermal conductivity is relatively large and also smooths the front.

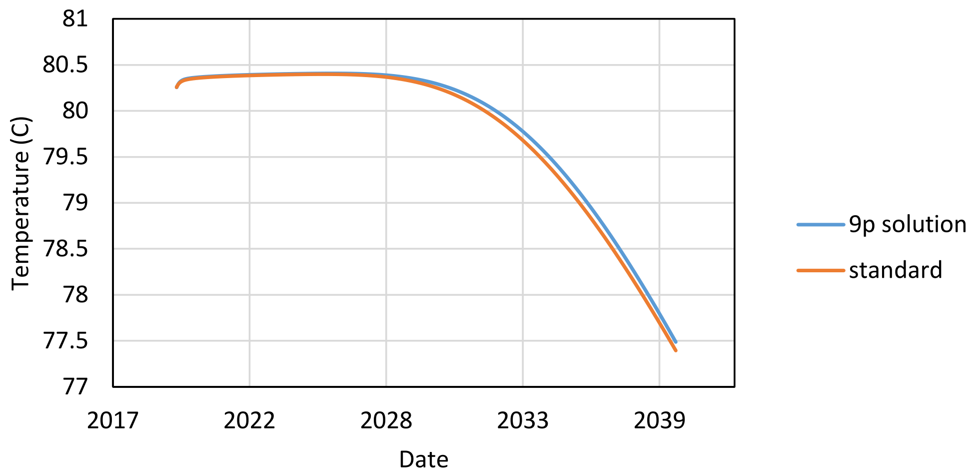

Figure 2.2. Impact of the 9-point solution on the thermal breakthrough calculated by the commercial simulator.

2.1.2 Deviated well

A well with a deviation of 45° is simulated in the same reservoir as in the previous section. An approximate analytical solution is used in which a skin is used to represent the inclination of the well following the approach in DC1D [4]. For the given conditions, the skin is estimated at -0.28. The results are presented in Table 2.4. For all simulators the required pressure difference is smaller than that resulting from the analytical solution. Because the analytical solution is also an approximation, it is not possible to state which solution is more accurate. This comparison only can show the consistency of the different solutions.

Table 2.4. Δp results for an injection temperature = 80°C (results after 3 years).

	Δp_{total}	% difference
Analytical solution for DC2D		
DC2D (visc. is Batzle and Wang instead of Kestin*)	Not done	
Analytical solution for DC3D	38.53 bar	
DC3D	37.19 bar	-3.46 %
Analytical solution for commercial	38.32 bar	
commercial	36.83 bar	-3.88 %

For the vertical well, the pressure drops in de different parts of the system (well to reservoir and through the wells) were consistent between the simulators (numbers not shown). For the deviated well, some differences occur (Table 2.5). It is not clear at this point what the cause is for these differences. However, the differences are not substantial.

Table 2.5. Breakdown of the total pressure drop in pressure drop (bar) in different parts of the system

Pressure (bar)	Injector to reservoir	Flow through the reservoir	Reservoir to producer	Total
commercial	9.03	18.79	9.01	36.83
DC3D	9.39	18.40	9.40	37.19
Difference commercial (%)	3.77	-2.10	4.17	0.97

2.1.3 Partially penetrating well

For the analytical solution, a fully penetrating vertical well is assumed. However, in some case a partially penetrating well can occur. This means that not the entire reservoir is perforated. This cannot be simulated with DC2D, therefore a comparison between DC3D and the commercial simulator only was done. Only the top 30 m of the well was perforated and the rate reduced to 80 m^3/hr. Simulation time was increased to 30 years to see a longer breakthrough. The figures below show the bottom hole pressure (BHP) and temperature of the production well. Agreement between the simulators is good. The main differences are in early time. The higher production temperature for the commercial simulator is caused by a difference in input conditions. In the commercial simulator, the enthalpy of the water is calculated based on the specified initial pressure and temperature. In the simulation, constant enthalpy is assumed and the actual temperature depends on the pressure.

Larger differences occur if we look at the detailed temperature distribution: in Figure 2.6, the temperature distribution is presented in a cross-section which is centered on the well. The largest difference occurs just below the well, where the commercial simulator cools faster than DC3D (max difference is about 8.5°C). It is still visible after 5 years of injection (Figure 2.7), but disappears later because the entire near well area cools to 30°C. This difference is partially due to the large time steps used in DC3D, namely annual time steps. If smaller time steps are used (for example monthly or bi-weekly) the difference in the temperature field reduces. Another effect is that the injection temperature is lower for the commercial simulator, because it depends on the injection pressure. On average, the injection pressure is ~1 Bar lower.

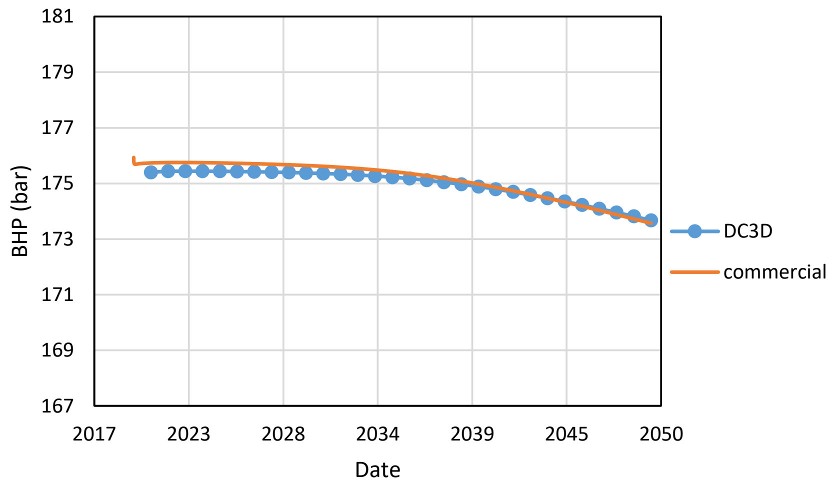

Figure 2.3. Bottom Hole Pressure (BHP) of the production well for the commercial simulator and DC3D.

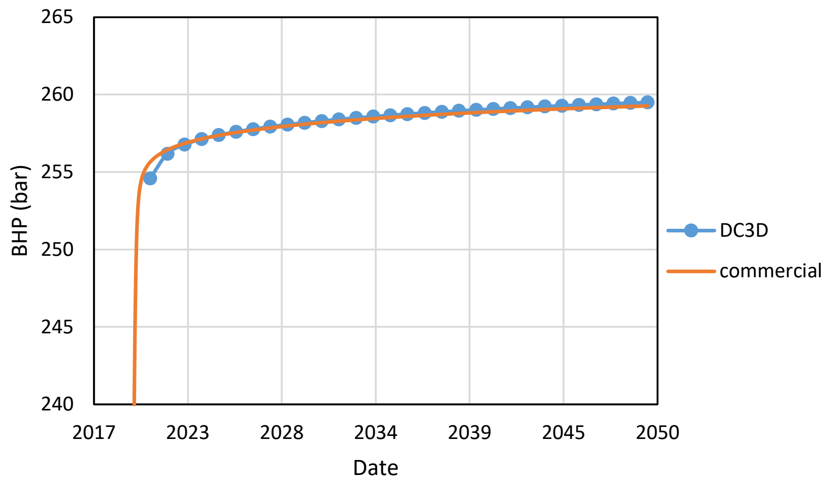

Figure 2.4. Bottom Hole Pressure (BHP) of the injection well for the commercial simulator and DC3D.

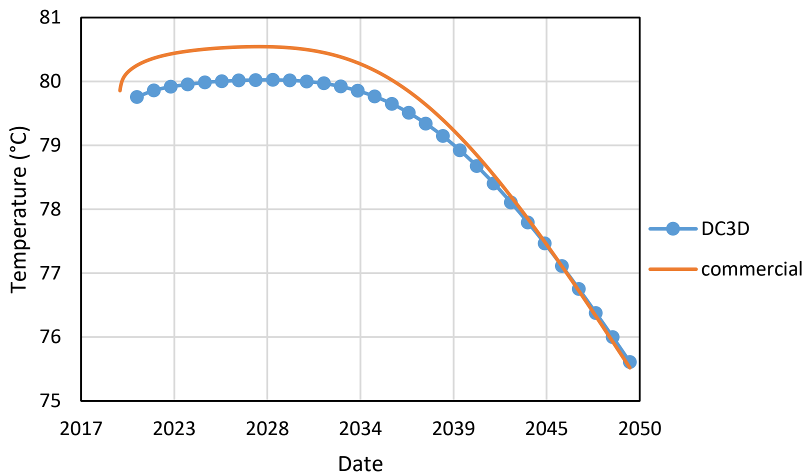

Figure 2.5. Temperature of the production well for the commercial simulator and DC3D.

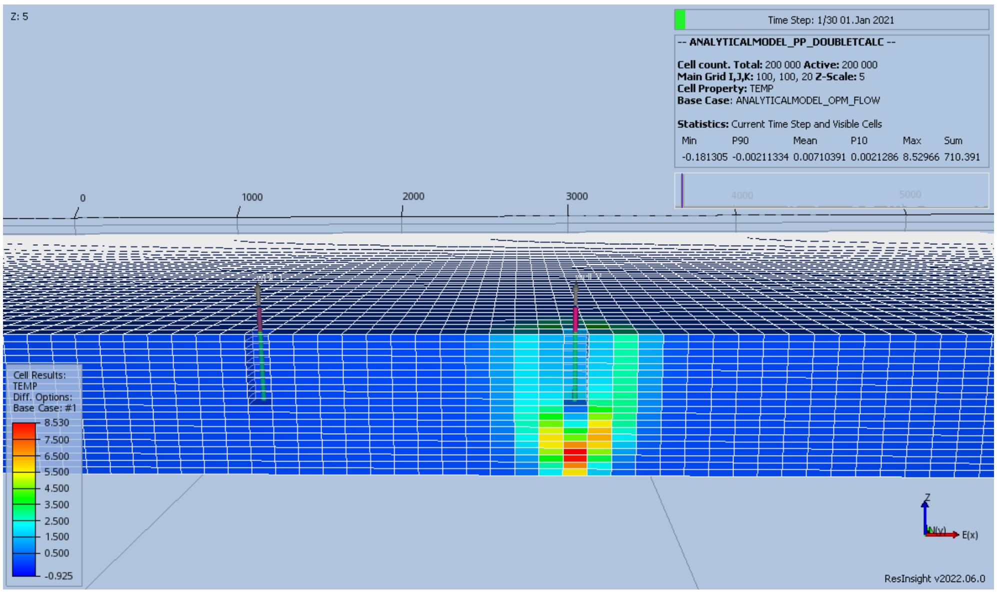

Figure 2.6. Temperature difference between DC3D and the commercial simulator after 1 year of injection at 30°C in a partially penetrating well (difference is calculated as DC3D-commercial: cold water penetrates less deep in DC3D).

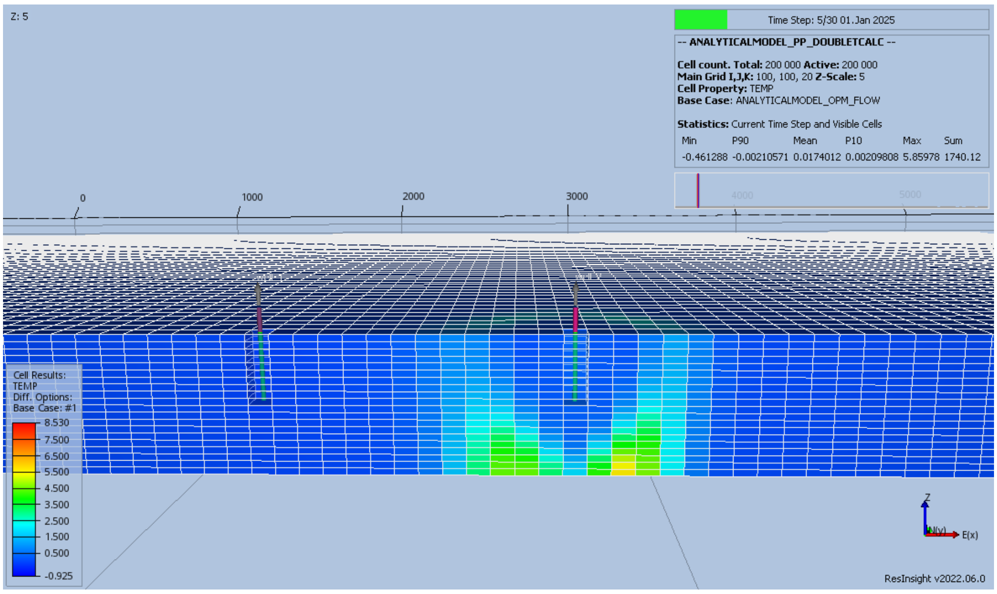

Figure 2.7. Temperature difference between DC3D and the commercial simulator after 5 years of injection at 30°C in a partially penetrating well.

2.2 With under- and overburden

In the next step, it will be investigated if different well configurations are simulated accurately. In this section a model is used with under- and overburden, because this is more appropriate for simulation of geothermal reservoirs and is the default setup in ROSIM.

2.2.1 Deviated well

On top of the reservoir a low permeability overburden is assumed. The underburden below the reservoir has a moderate permeability. All input settings are given in Table 2.6.

- Simulations of DC3D are done with temperature dependent density. The commercial simulator is simulated without the temperature dependent density. The reason for not including temperature dependent density is the combination with the no flow boundary. For the commercial simulator the reduction in volume due to cooling reduces the pressure in the model, making a comparison of pressure results impossible. See section 3.5 for more information. The impact of temperature dependent density on the flow is very small for these conditions. (~0.1 °C after 30 years).
- For this case a deviated well (40°), fully perforated over the depth the reservoir was used.
- Injection temperature is 30°C.
- No flow boundary conditions.
- DC2D is not included in this comparison, because it cannot handle an over- and/or underburden in which fluid flow occurs.

The thermal breakthrough (Figure 2.8) and the total pressure drop in the system (Table 2.7) both show good agreement between the commercial simulator and DC3D. Also a check was done on the pressure drop in the reservoir and the pressure drop between the reservoir and the well and the differences between the commercial simulator and DC3D were found to be small (Table 2.7). This is similar as was found for the deviated well without under and overburden (Table 2.5).

Table 2.6. Input settings for a model with over- and underburden.

	overburden	reservoir	underburden
Thickness	40 m	60 m	40 m
N/G	0.5	0.9	0.5
Permeability xy	0.1 mD	150 mD	10 mD
Permeability z	0.01 mD	15 mD	1 mD
Porosity	0.05	0.2	0.12
Grid resolution	50 x 50 x 3 to 20 m	50 x 50 x 3 m	50 x 50 x 3 to 20 m
Model size	3 km x 3 km x 100 m		
Salinity	70000 ppm		
Well distance	Defined as 605 m, but results in 650 m because wells are always modelled in the middle of a grid block.		
Well diameter	8.5 inch		
Injection/production rate	150 rm^3 for DC 150 sm^3 = 152.4 rm^3 for the commercial simulator		

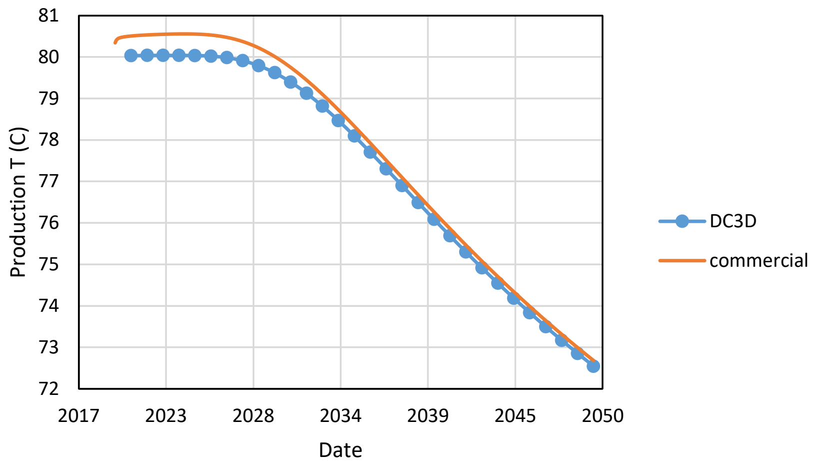

Figure 2.8. Thermal breakthrough prediction for a model with over- and underburden.

Table 2.7. Breakdown of the total pressure drop in pressure drop (bar) in different parts of the system for injection rate: 150 m³/d, injection temperature 30°C; values after 3 yrs of injection.

	dP inj2res	dP reservoir	dP res2prd	dP total
commercial	30.86	39.26	14.53	84.65
DC3D	31.40	37.50	14.57	83.47
Difference commercial (%)	1.76	-4.48	0.25	-1.39

The main pressure difference between the commercial simulator and DC3D occurs in the over- and underburden (Figure 2.9). The pressure above and below the production wells is lower for DC3D than for the commercial simulator. Above and below the injection well, the pressure is higher in DC3D than in the commercial simulator. The temperature distribution in the over- and underburden also differs (Figure 2.10) with a similar difference as for the partially penetrating well (Section 2.1.3): the area below the injection well shows less cooling for DC3D than for the commercial simulator.

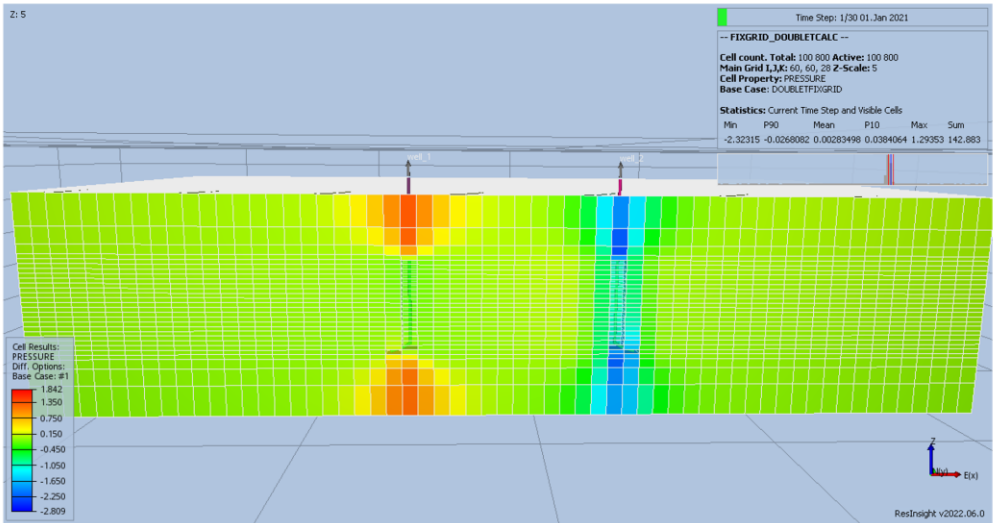

Figure 2.9. Pressure difference between DC3D and the commercial simulator (DC3D-commercial) after 1 year of injection.

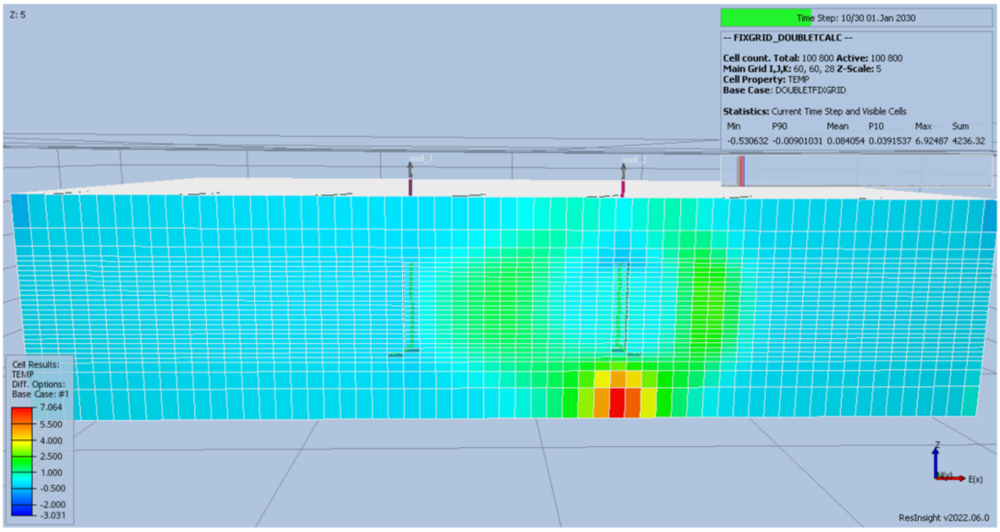

Figure 2.10. Cross section with temperature difference (°C) between DC3D and the commercial simulator (DC3D-commercial) after 10 years. Max difference is 7 °C.

2.2.2 Horizontal well

In this section, the inflow into a sub-horizontal well has been simulated using the commercial simulator and DC3D. The model size is adjusted to 3 x 3.6 km. In Figure 2.11 and Figure 2.12, the bottom hole pressure (BHP) in the wells is presented. Overall, the results are very similar. The BHP in the producer decreases a bit more for the commercial simulator than for DC3D, but the difference is only 0.4 bar. The thermal breakthrough is somewhat faster in the commercial simulator than in DC3D (Figure 2.13, Figure 2.14 and Figure 2.16). In part this is caused by the difference in time steps. If DC3D is run with monthly time steps instead of annual time steps, the front moves a bit faster, but that effect is less than the difference with the commercial simulator. After 10 years, the difference is much more diffuse and now the largest difference is in the underburden (4°C). The pressure difference after 1 year is shown in Figure 2.15.

Please note for accurate simulation the model size used here is too small. The purpose of this model is not to get accurate simulations, but to compare the output and functionality of the software tools.

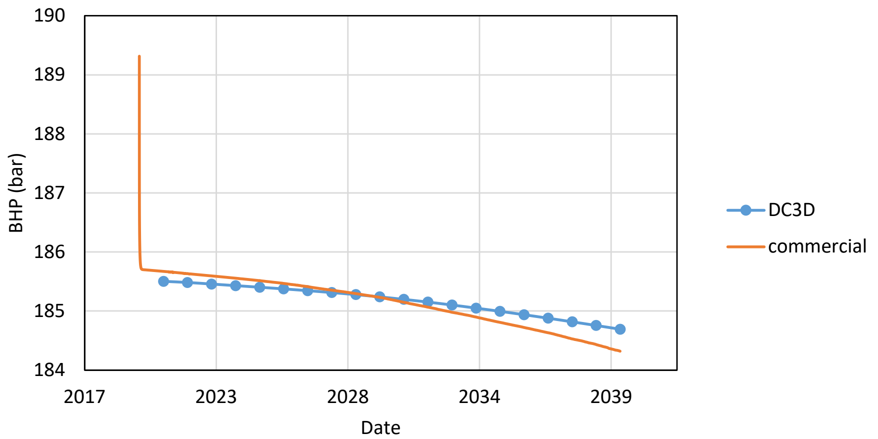

Figure 2.11. BHP of the sub-horizontal producer

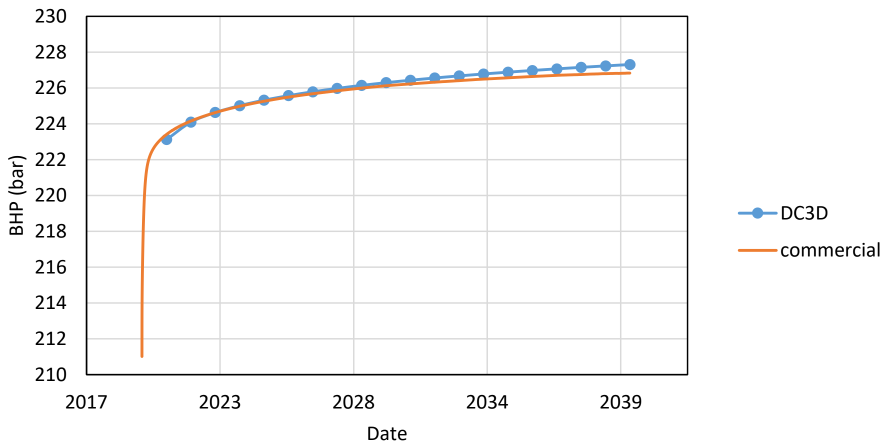

Figure 2.12. BHP of the sub-horizontal injector

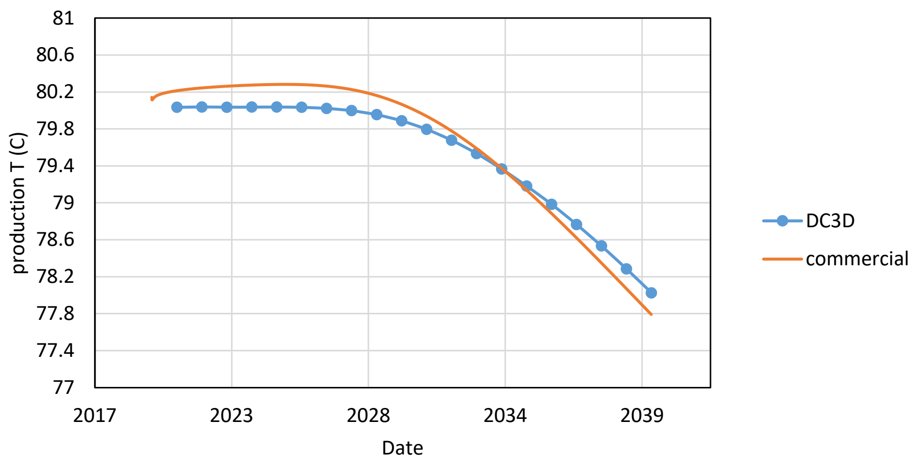

Figure 2.13. Temperature of the sub-horizontal producer (°C).

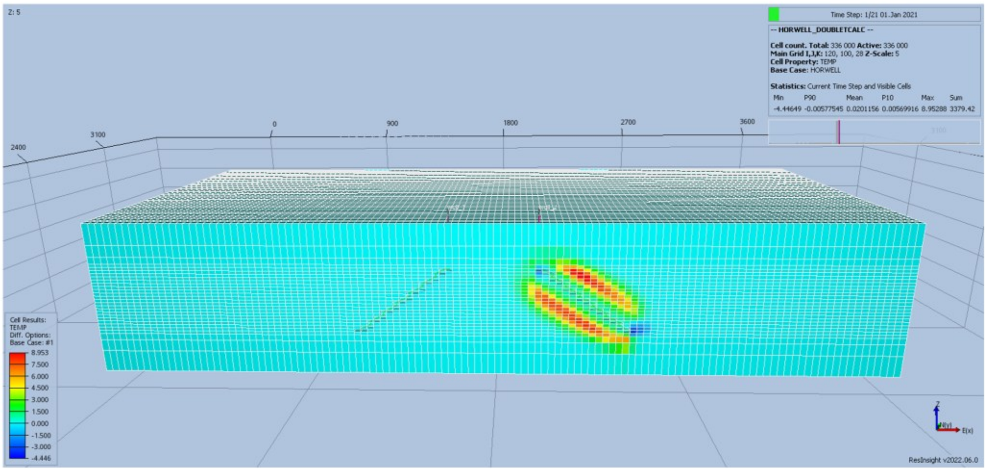

Figure 2.14. Temperature difference (°C) after 1 year between DC3D and the commercial simulator (DC3D-commercial). Cold front advances faster in the commercial simulator. Max. difference is 8.9 °C.

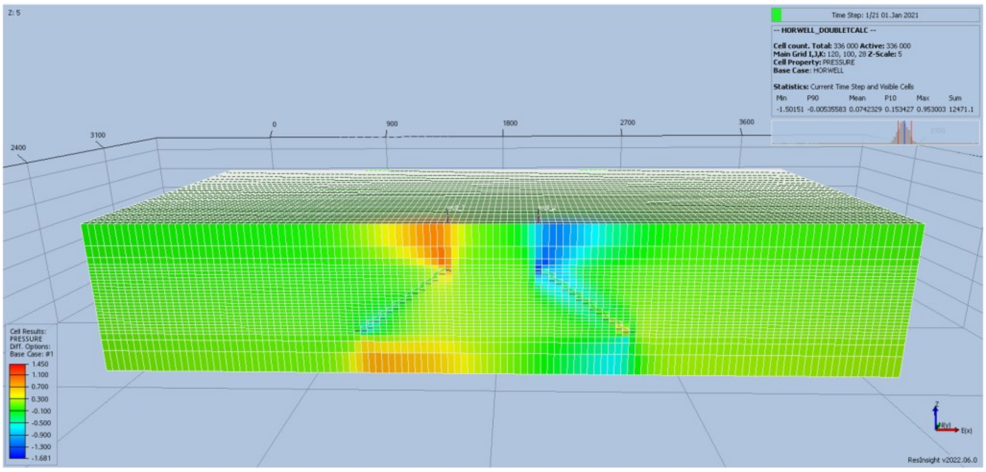

Figure 2.15. Pressure difference (DC3D-commercial) after 1 year.

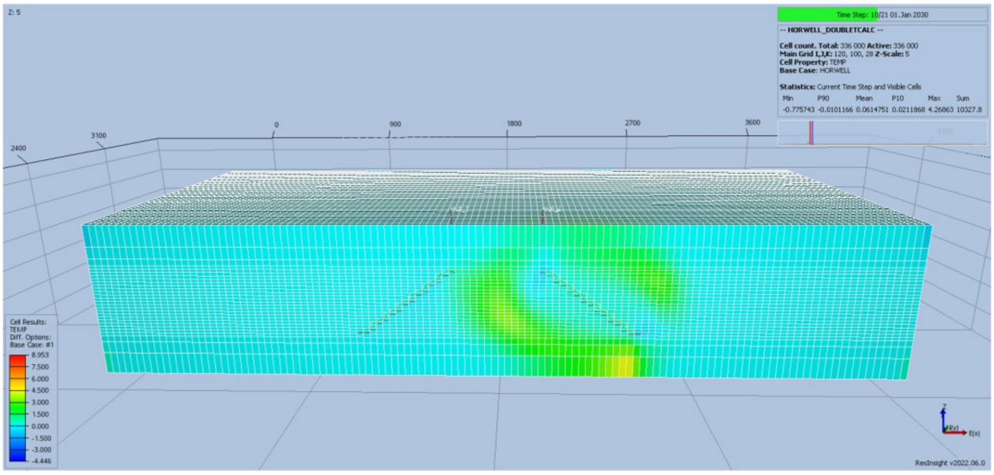

Figure 2.16. Temperature difference (°C) after 10 years between DC3D and the commercial simulator (DC3D-commercial).

2.2.3 Triplet

In this test, a triplet is simulated with one producer and two injectors. The total injection rate is equally distributed between the two injectors. All other settings for the model are the same as used in Section 2.2. The results are shown in Figure 2.17 (for the production well) and Figure 2.18 (for the injection wells). The results show excellent agreement between the two models.

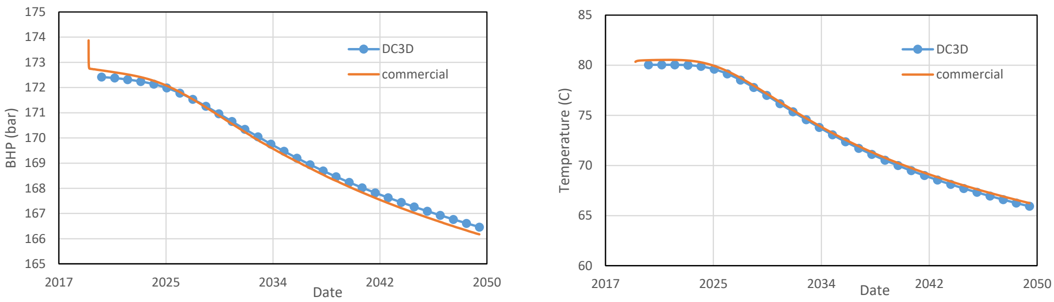

Figure 2.17. Bottom hole pressure (left) and production temperature (right) of the production well for DC3D and the commercial simulator.

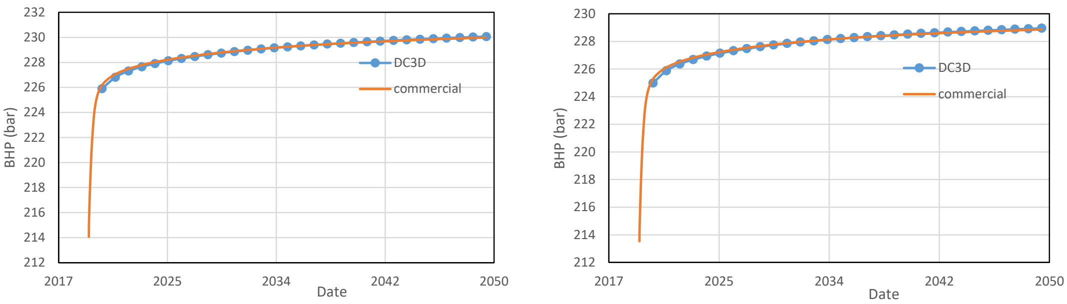

Figure 2.18. Bottomhole pressure of the two injectors of a triplet for DC3D and the commercial simulator.

2.3 Tilted reservoir

Many geothermal reservoirs are not completely horizontal, but have a dip. It can be important to include this dip, both for simulating the correct production temperature, the reservoir pressure and for the thermal breakthrough. To study this, a reservoir model with a tilt of 3° was simulated. The reservoir permeability was increased to 500 mD and flow rate is 200 m^3/hr. Production is in the lower of the two wells of the doublet to get a higher production temperature. The wells have a deviation of 40°C. The over- and underburden have a permeability of 0.01 mD (0.001 mD in vertical).

The thermal breakthrough is presented in Figure 2.19 for the commercial simulator and DC3D[1] with and without temperature dependent density. Please note that the option to run DC3D without temperature dependent density is only available in the beta version of ROSIM. It shows the thermal breakthrough for both the commercial simulator and DC3D with and without temperature dependent density. The results look very similar and the effect of the density is small for both simulators. In Figure 2.20 the thermal breakthrough of OPM flow is added (without temperature dependent density). The OPM flow run took very long (> 3 days). The thermal breakthrough is very similar to the other two simulators. The total pressure difference over the system was also close between the models (~1.3% difference)(Figure 2.21).

Figure 2.22 shows the temperature difference after 20 years of injection between DC3D and the commercial simulator (both without temperature dependent density). The results are in line with earlier results. Figure 2.23 and Figure 2.24 show the impact on the temperature distribution of the temperature-dependent density for DC3D and the commercial simulator respectively. The impact is very similar for both simulators and small overall: approximately 0.75 °C max.

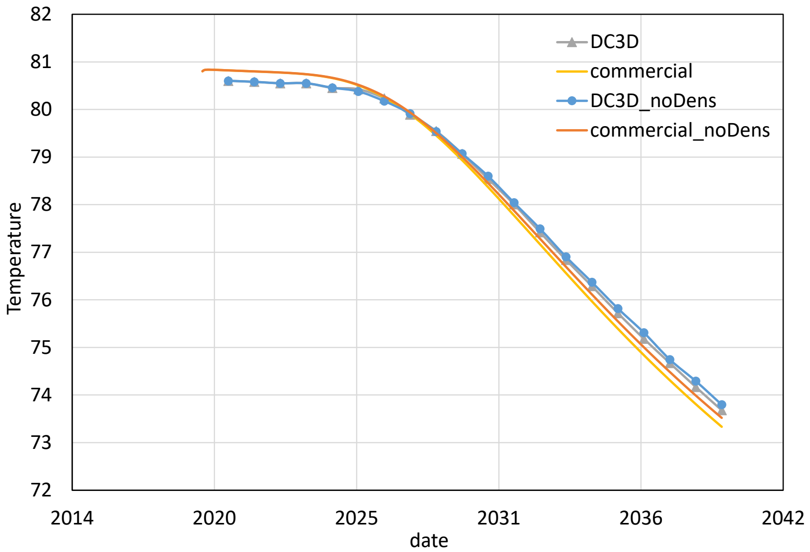

Figure 2.19. Thermal breakthrough for a tilted reservoir for DC3D and the commercial simulator both with and without temperature-dependent density (noDens = no temperature-dependent density).

[1] The results in this section were generated in the first phase of the benchmark in January 2022 with slightly earlier versions of DC3D (from dec 2021) and OPM flow (2021.4). Because no changes were implemented in the meantime which would affect these results, the simulations were not repeated.

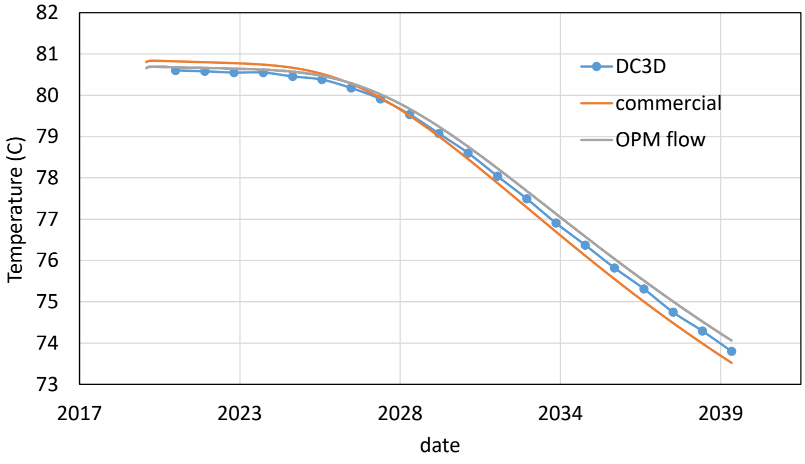

Figure 2.20. Thermal breakthrough for a tilted reservoir for DC3D, the commercial simulator and OPM flow without temperature-dependent density

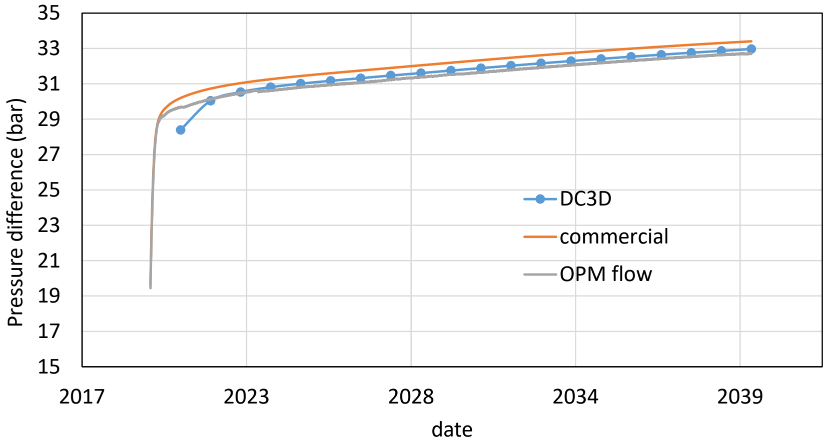

Figure 2.21. Pressure difference between the injector and producer for DC3D, the commercial simulator and OPM flow.

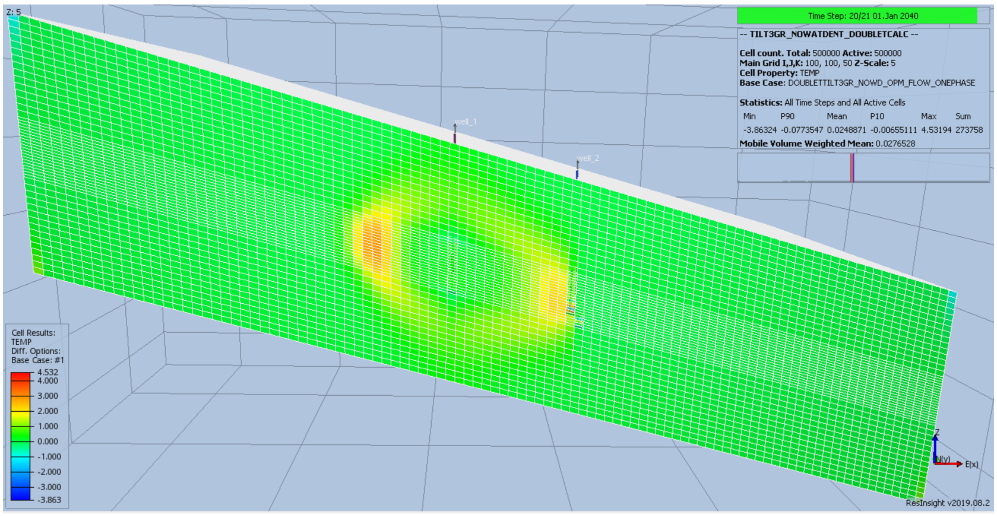

Figure 2.22. Difference in temperature between DC3D and the commercial simulator (DC3D-commercial) after 20 years of injection (30°C).

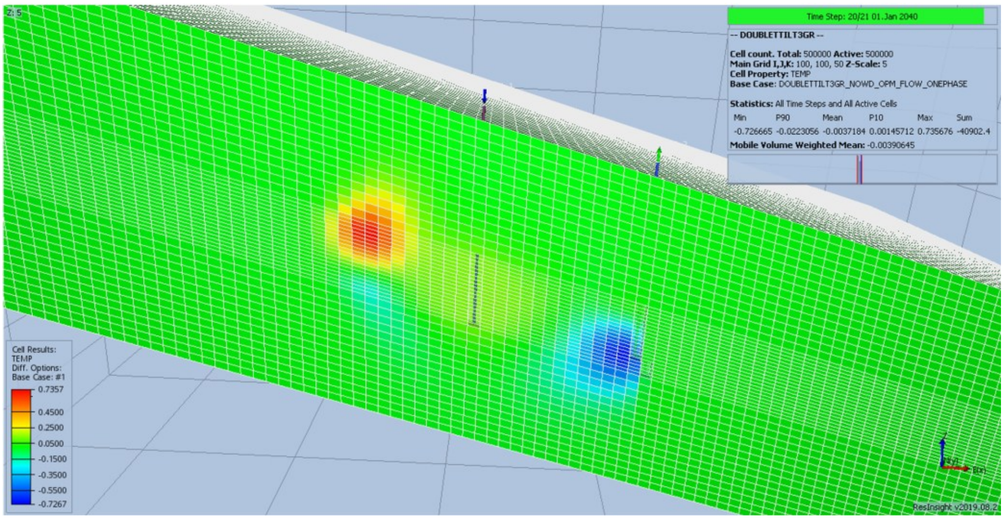

Figure 2.23. Difference in temperature for the commercial simulator with and without temperature-dependent density (after 20 years of injection with 30°C).

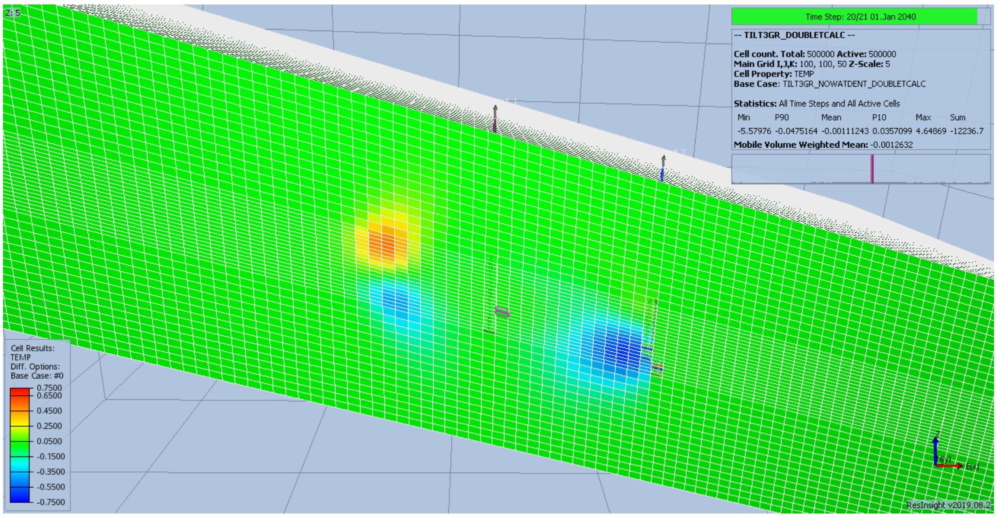

Figure 2.24. Difference in temperature for DC3D with and without temperature-dependent density (after 20 years of injection with 30°C).

2.4 Heterogeneity

Heterogeneity in the reservoir properties is common in geothermal reservoirs. In ROSIM, layered reservoirs can be created. To run models with lateral heterogeneity, a custom .grdecl file needs to be created outside of ROSIM. To test a layered model, a case with a single high permeability layer (HPS) was included. The permeability of the HPS was a factor of 10 higher than the permeability of the rest of the aquifer. The results are presented in section 2.4.1. To test if DC3D can handle lateral variations in permeability, half of the model was reduced in temperature. This is reported in section 2.4.2.

2.4.1 High perm streak

Both simulators shows the faster breakthrough compared to the results in section 2.2, which the breakthrough for the same rate and well distance for a homogeneous reservoir. For the homogeneous reservoir, the production temperature is constant for almost 10 years, whereas with the HPS, the temperature starts to decline after some 3 years.

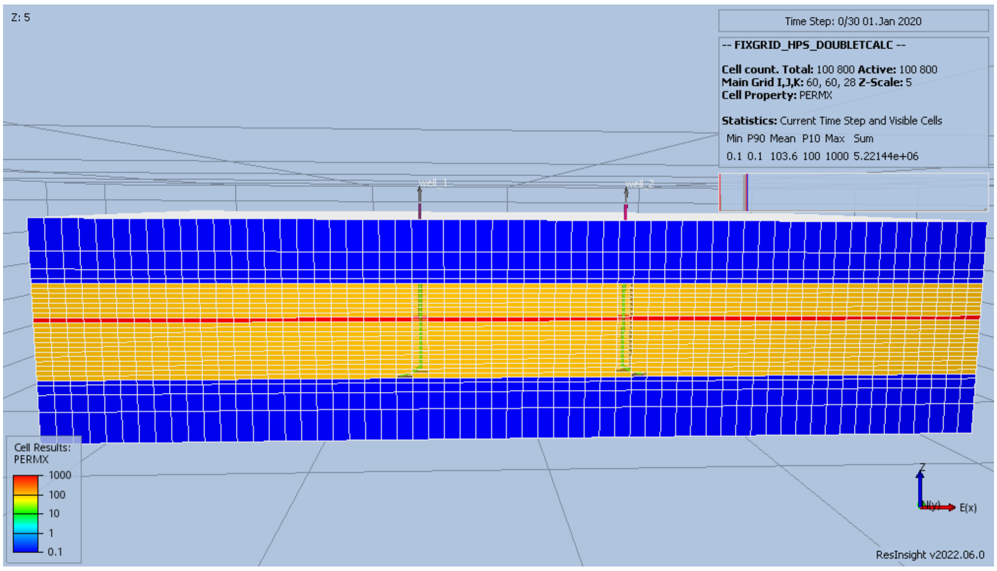

Figure 2.25. Illustration of the permeability showing the HPS (high permeability layer).

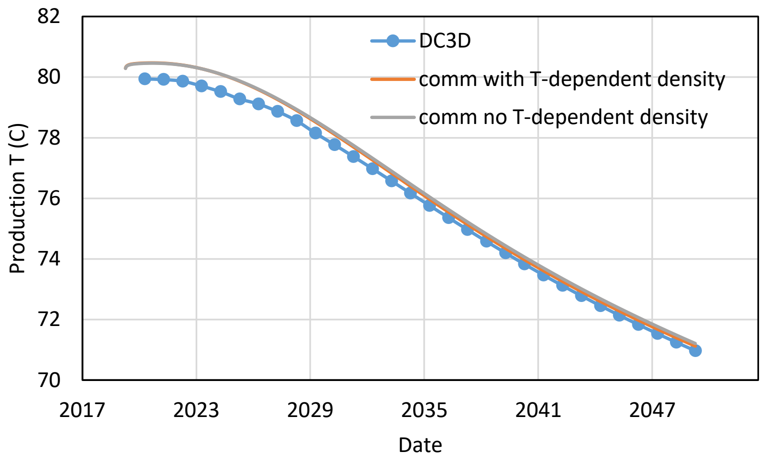

Figure 2.26. Production temperature for DC3D and the commercial simulator with and without temperature dependent density for a reservoir with HPS.

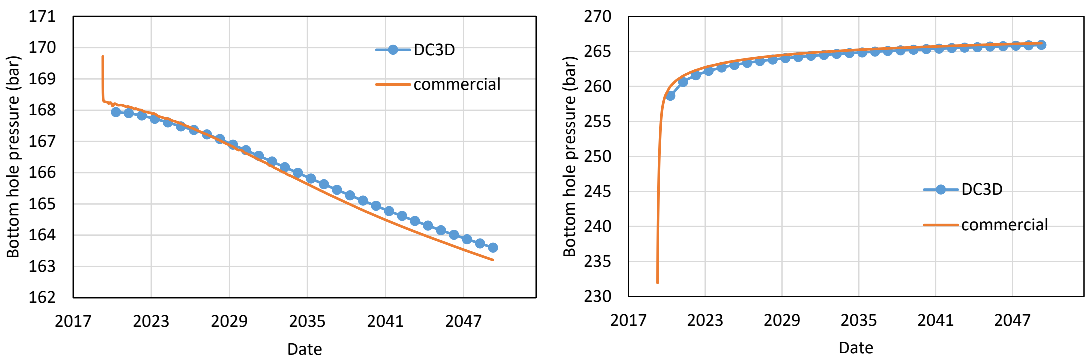

Figure 2.27. Bottom hole pressure in the producer (left) and the injector (right) for DC3D and the commercial simulator with temperature-dependent density for a reservoir with HPS.

2.4.2 Lateral variability in permeability

To simulate lateral variability in the permeability, the grid input .grdecl file needs to be created outside of ROSIM. Once created, it can be used by selecting the option to use a custom .grdecl file. The input in the .grdecl file has to contain all the information on the “Input 3D static model tab”, which is more than the .gredecl normally contain. This information can be added manually to an existing .grdecl file (e.g. from Petrel).

In this case, the permeability on the injection side has been set to 200 mD. On the producer side, it has been reduced to 75 mD (Figure 2.28).

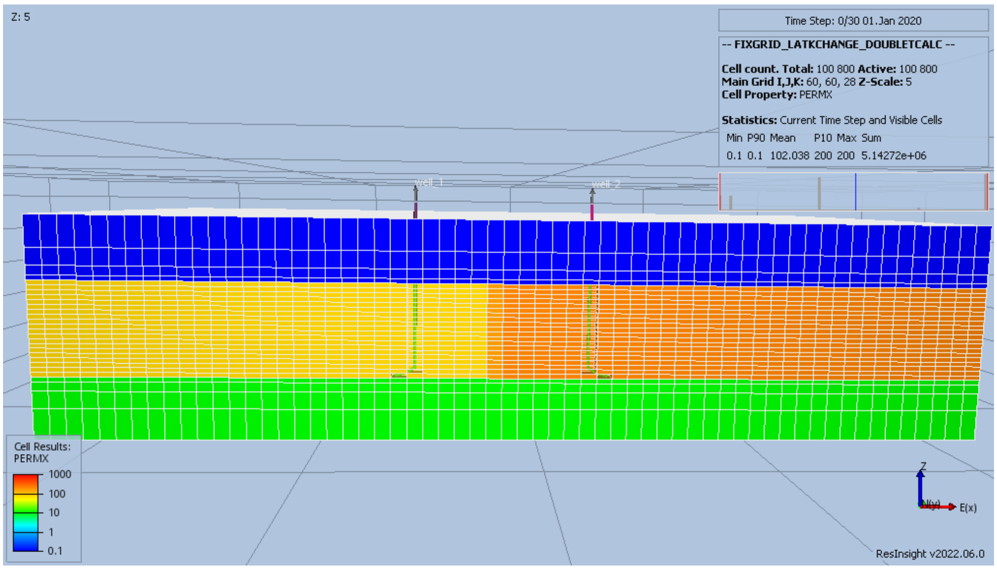

Figure 2.28. illustration of the lateral variation in permeability.

The production temperature and bottom hole pressure are presented in Figure 2.29 and Figure 2.30, respectively. This is the first case in which the pressure is consistently different. Although the initial pressure is equal, after production start the pressure in the entire reservoir is approximately 1 bar higher for the commercial simulator than for DC3D and remains that way throughout the simulation run. This is likely related to a difference in input settings, but it is not clear at this point which input this would be.

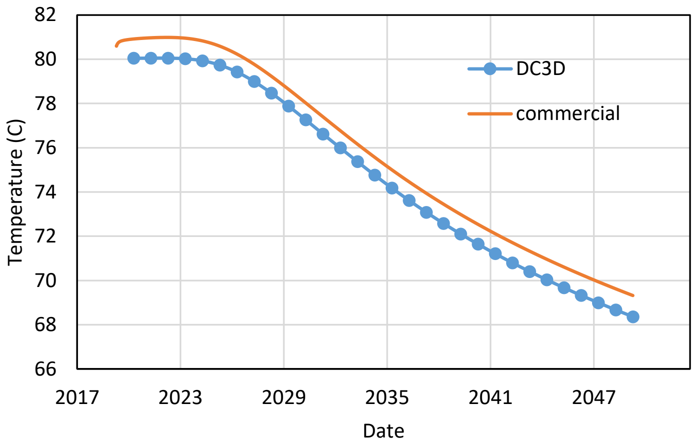

Figure 2.29. Production temperature for DC3D and the commercial simulator for a reservoir a lateral change in permeability.

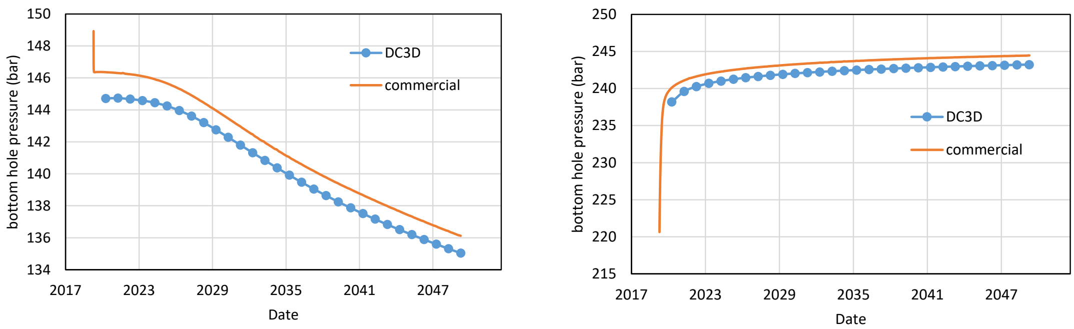

Figure 2.30. Bottom hole pressure (in bar) for the producer (left) and injector (right) for a reservoir with a lateral change in permeability.

2.5 Heat storage example

The last case for which the results of the commercial simulator and DC3D are compared is a heat storage case (HT-ATES: High Temperature Aquifer Thermal Energy Storage). In this case, hot water (90°C) is injected during 3 months of the year (summer), followed by 3 months without injection or production (autumn). Then the injector and producer are switched and the hot water is produced back during 3 months (winter). Finally the last 3 months are again without injection and production (spring). This is a very challenging simulation problem due to the low pressure gradients (high permeability and relatively low rates), strong density driven flow effects and the alternation of injection and production in the same well. Because this is a challenging problem, a fine grid (5 x 5 x 2 m grid block) and small time step size was used. Time step size was taken as 1 week for DC3D. In the commercial simulator, time step size is determined by the simulator and is around 5 to 10 days. The reservoir in this case is smaller than for the geothermal applications (600 x 600 m) and shallower (top of the model is at 280 m depth). Further input is given in Table 2.8.

Setting the boundary conditions for this case is important, because the model is relatively small. No flow (heat and fluid) boundary conditions were set for the top. Choosing no flow boundary conditions on the lateral boundaries results in a rise in pressure in the reservoir for the commercial simulator due to heating up (density dependent flow is required for simulating HT-ATES). Constant pressure boundaries are therefore more convenient for the comparison. However for the commercial simulator, this also requires setting the temperature constant, because pressure and temperature are solved together assuming constant enthalpy. However, this assumption is not made in DC3D and there the pressure is set constant without fixing the temperature. Since the temperature changes on the lateral boundary are smaller than 0.1°C, this constant temperature should not affect the results much. In the following, both results from no flow as well as constant pressure boundary conditions are discussed.

For the constant pressure boundary condition, the temperature in the cold well and hot well are presented in Figure 2.31 and Figure 2.32 respectively. Please note that the commercial simulator shows constant values for temperature during shutin, whereas DC3D shows no values during shutin. The back production temperature in the hot well is very similar for DC3D and the commercial simulator. However, the production temperature in the cold well differs considerably, with a maximum difference in the second year of around 5 degrees. If the time step for DC3D is reduced from 1 week to 1 day, the difference decreases. In general, with decreasing time step, DC3D shows more change in the shape of the hot water bubble due to upward flow of the lower density, hot water and a faster thermal breakthrough because of that (results not shown).

In Figure 2.33, a cross section through the models is given, which shows the shape of the hot-water bubble after 3 months of injection. On the right the difference in temperature is shown (DC3D- the commercial simulator). This shows that the front of the commercial simulator has advanced further in the top part especially in the direction of the production well. It can also be seen that the front is wider for the commercial simulator than it is for DC3D. It is not clear at this point which solution is better. DC3D has a sharper front which might be more accurate. Another difference is that the fluid heat capacity of DC3D is temperature dependent and specific for the fluid salinity. The thermal version commercial simulator on the other hand, uses internal tables which are for pure water only (the more simple temperature option of the commercial simulator can use the temperature dependent specific heat, but not the thermal option). This could account for some of the differences in thermal breakthrough.

The bottom hole pressure (BHP) for both wells is very similar for DC3D and the commercial simulator and is shown in Figure 2.34 and Figure 2.35 for the cold well and hot well respectively. Pressure is only shown when the well is in operation. During shutin no value is shown. Injection pressure in the hot well show a rapid decrease in injection BHP due to the growth of the hot water bubble (less pressure required due to lower viscosity). During back production, the production BHP shows the same effect in reverse.

For the no flow boundary, the temperature in the well is shown in Figure 2.36 and Figure 2.37. For both simulators, thermal breakthrough occurs faster with no flow boundary conditions than with constant pressure boundary conditions. This is particularly pronounced for the commercial simulator in the first time step. Pressure cannot be compared because of the pressure increase resulting from heating up in the commercial simulator.

Test runs were also done with coarser models. Both simulators showed faster thermal breakthrough with coarser models (results not shown).

Table 2.8. Input settings for reservoir simulation model of heat storage.

	overburden	reservoir	underburden
Thickness	20 m	30 m	20 m
N/G	0.5	1.0	1.0
Permeability xy	20 mD	18000 mD	20 mD
Permeability z	2 mD	4500 mD	2 mD
Porosity	0.6	0.3	0.6
Grid resolution	5 x 5 x 2 m		
Model size	600 m x 600 m x 70 m		
Salinity	70000 ppm		
Well distance	150 m		
Well diameter	13 inch		
Injection/production rate	150 rm³ for DC 150 sm³ = 150 rm³ for the commercial simulator		
Injection temperature	90°C injection into the hot well 30°C injection into the cold well		

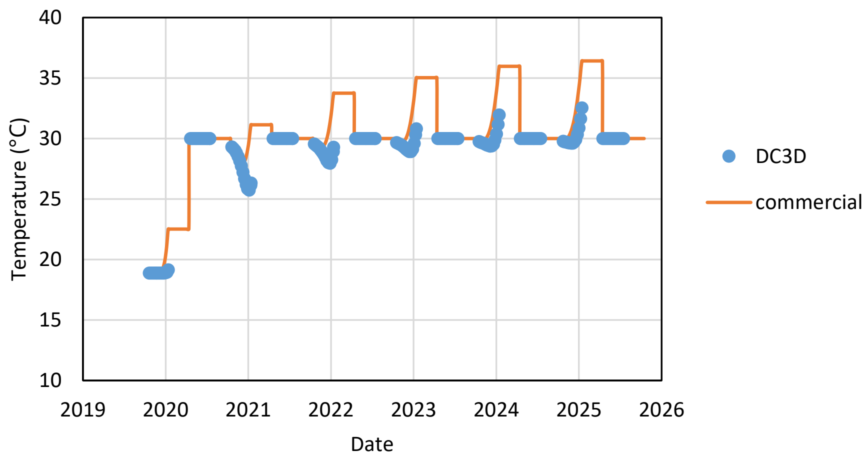

Figure 2.31. Temperature (°C) in the cold well for DC3D and the commercial simulator with constant pressure/temperature boundary. DC3D with weekly time steps.

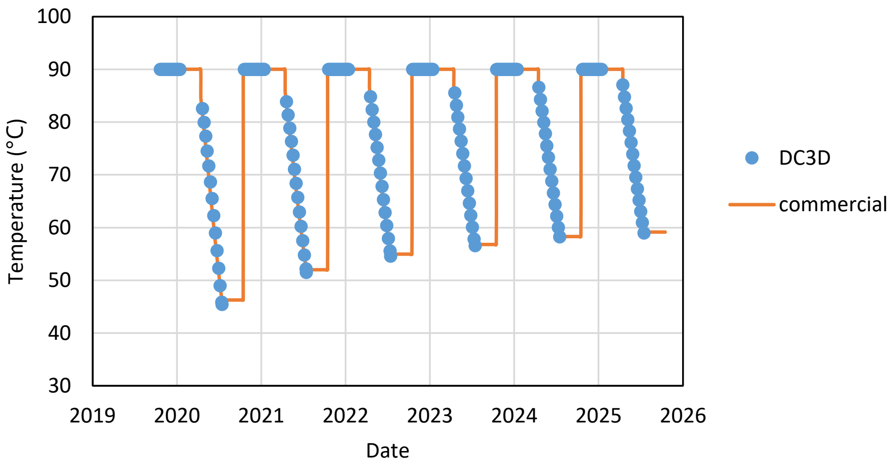

Figure 2.32. Temperature (°C) in the hot well for DC3D and the commercial simulator with constant pressure/temperature boundary. DC3D with weekly time steps.

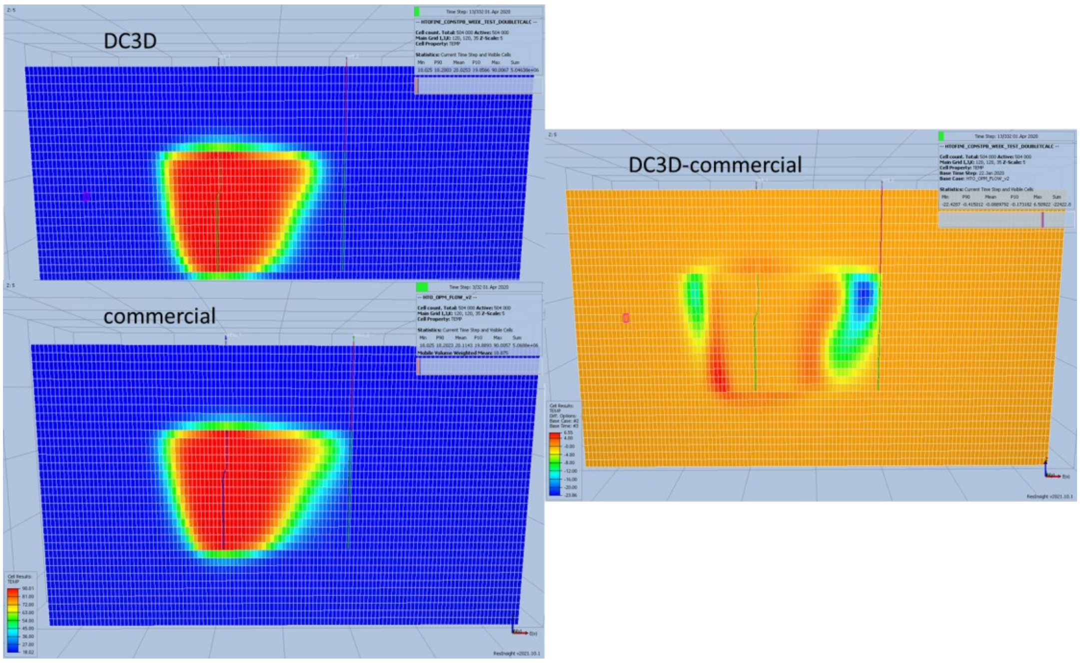

Figure 2.33. Temperature distribution in a cross section of the model for DC3D and the commercial tool with constant pressure boundary (left) and the difference (DC3D-commercial) on the right after 3 months of injection at 90°C.

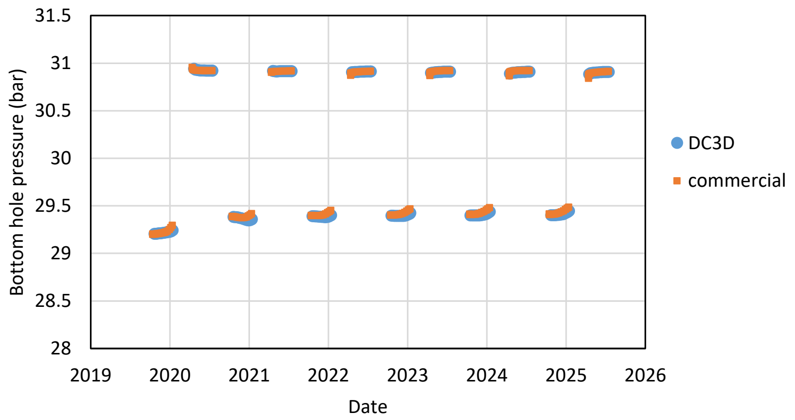

Figure 2.34. Bottom hole pressure (bar) in the cold well for DC3D and the commercial tool with constant pressure/temperature boundary (values only shown when well is open).

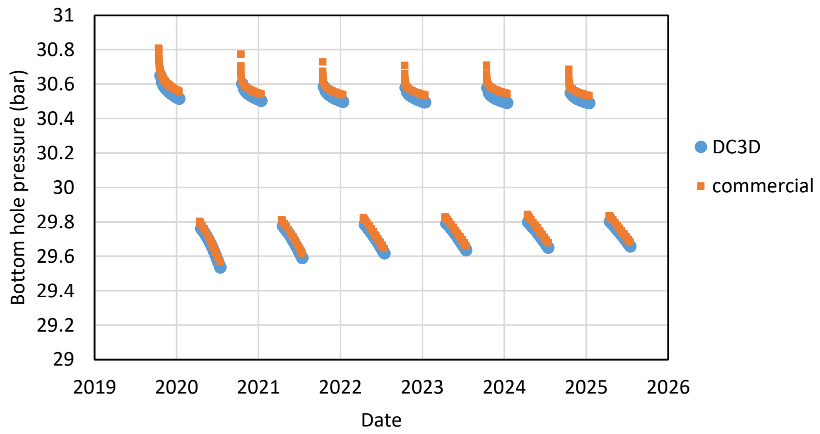

Figure 2.35. Bottom hole pressure (bar) in the hot well for DC3D and the commercial simulator with constant pressure/temperature boundary (values only shown when well is open).

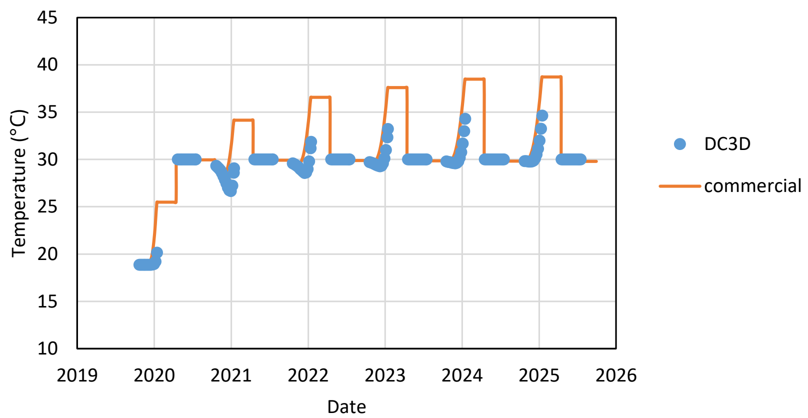

Figure 2.36. Temperature in the cold well for DC3D and the commercial simulator with no flow boundary conditions.

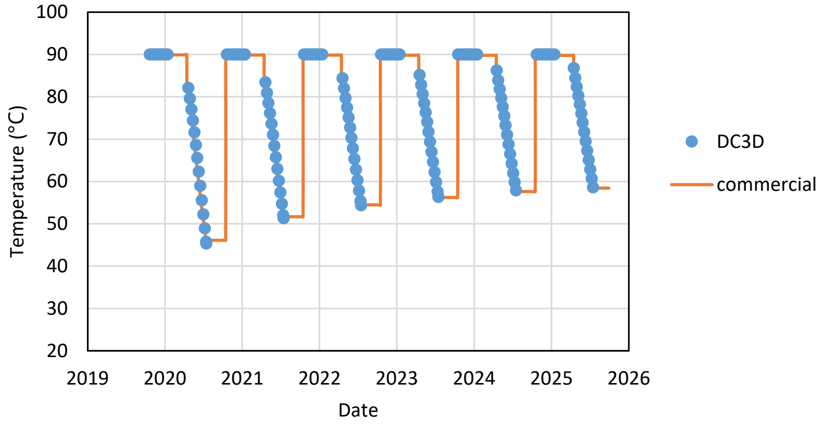

Figure 2.37. Temperature in the hot well for DC3D and the commercial simulator with no flow boundary conditions.

3 Options in ROSIM / DC3D

3.1 General

ROSIM and DC3D provide a number of options, for input specification and/or simulation. Not all options were tested in detail. The most important options are discussed in the following sections. The option for reading custom .grdecl and layer grid has been tested only for a simple case.

Although tested during the development of ROSIM and DC3D, the following options were not included in the tests for this report:

- Option to include a custom compdat file.
- Skin on the wells

3.2 Local grid refinement around the well

ROSIM gives the option to refine the grid around the well. This is not done as a typical local grid refinement, but as a tartan type of grid (Figure 3.1). The local grid refinement option around the well was tested for the case of a reservoir with over- and underburden with deviated wells (Section 2.1.2). The xy grid size target was set to 10 m and the grid refinement range to 5 grid cells. The number of grid cells increased from 100800 to 224000.

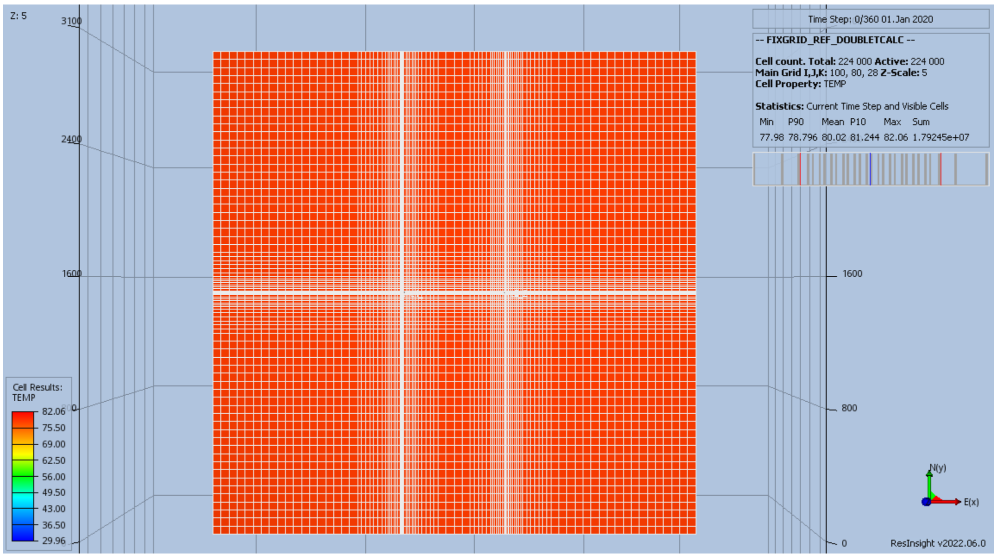

Figure 3.1. Example of a tartan type grid that is created using ROSIM (top view). White lines indicate the boundaries between grid cells.

With the presence of grid refinement, the simulation can become unstable and produce oscillating results. Changing the settings of the refinements or reducing the calculation time step size (in this case to a month instead of a year) solves this problem. The same problem occurred for the commercial simulator: adding the refinements caused serious numerical problems. Because of these numerical problems, it might be that the coarse grid provides better answers than the locally refined grid.

The thermal breakthrough with and without refinements is shown in Figure 3.2 for DC3D. The thermal breakthrough is slightly slower with refinements which was also observed for the commercial simulator (data not shown). The impact on the BHP is small (Figure 3.3).

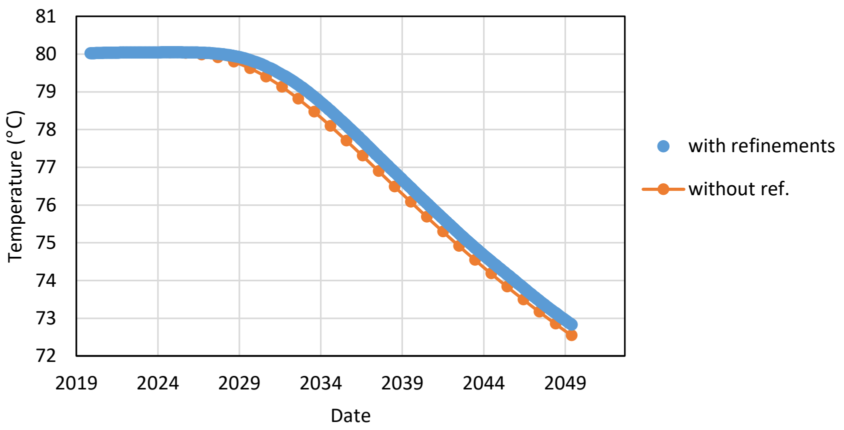

Figure 3.2. Impact of adding refinements on the temperature in the production well for DC3D.

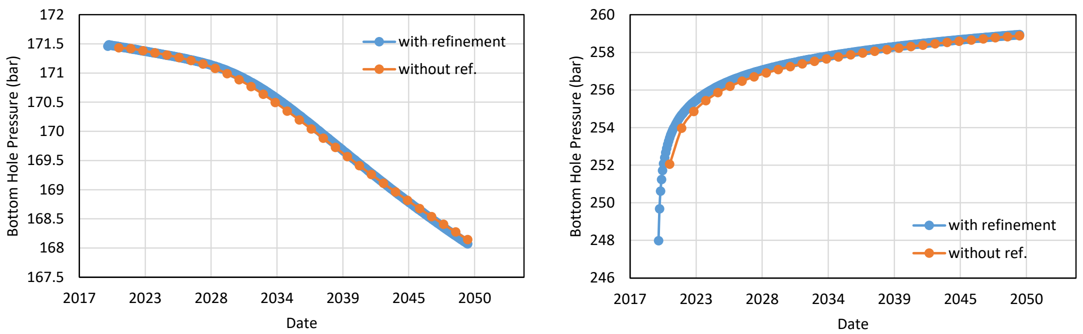

Figure 3.3. Bottom hole pressure (bar) for the producer (left) and injector (right) with and without refinements around the well.

3.3 Flow boundary conditions

For fluid flow, two types of boundary conditions are available in DC3D: no-flow boundaries and constant pressure boundary condition. The top and bottom of the model are always no-flow boundary conditions for DC3D.

For the runs with the commercial simulator, the choice of boundary condition has a large influence on the pressure if the density depends on the temperature. Due to the cooling (or heating for HT-ATES) of the in situ fluids, the pressure declines (increases for heating). Even though the model area is considerable (5 x 5 km or 3 x 3 km), in case of no-flow boundary conditions, the pressure declines. This is further discussed in section 3.5. The result of this is that the simulation results with temperature-dependent density in combination with no-flow boundary conditions are difficult to compare between DC3D and the commercial simulator. Not only for the pressure but also the temperature, which is affected by the pressure via the enthalpy.

The constant pressure boundary for both the commercial simulator and DC3D is implemented by increasing the pore volume. The commercial simulator also has other options for boundaries such as analytical or numerical aquifers, but increasing the block volume is more in line with DC3D. For the commercial simulator, this requires two additional settings in case of THERMAL runs. For thermal runs the default is that if the pore volume of a grid block is larger than the bulk volume, the pore volume is maximised on the bulk volume of the grid block. In the settings of OPTIONS3, this behaviour can be disabled (in the RUNSPEC section):

```
OPTIONS3
 322*0 1 /
```

In addition, increasing only the pore volume does not result in stable pressure on the boundary. In addition the rock volume should also be increased. This will result in a constant temperature boundary as well, which is different from DC3D.

The implementation of the flow boundary conditions was compared for the model with under- and overburden (Section 2.2) and for the HT-ATES example (Section 2.5), which is more sensitive to the boundary conditions than the geothermal applications. The changes resulting from the change in boundary conditions was consistent between the two simulators (Figure 3.4). For the geothermal application, a constant pressure boundary results in a smaller pressure difference between the two wells (higher BHP in the production well and lower BHP in the injection well) and slower thermal breakthrough than no flow boundary condition For the HT-ATES application, the trend is the same with slower thermal breakthrough for constant pressure boundary conditions than for no flow boundary conditions.

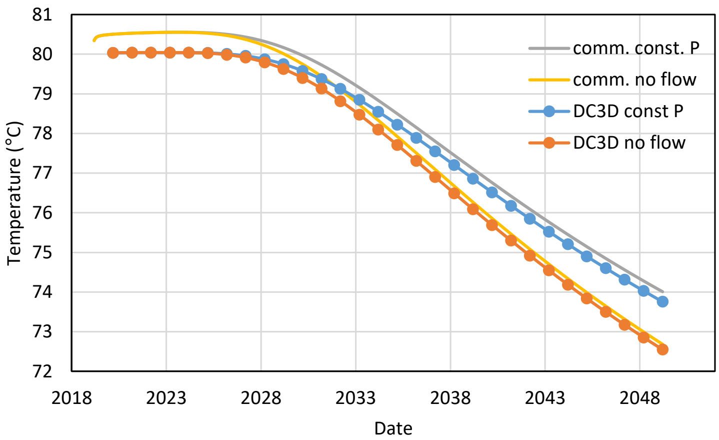

Figure 3.4. Temperature in the production well for the setup in section 2.2 for the commercial simulator and DC3D with no flow boundary conditions and constant pressure boundary conditions.

3.4 Thermal boundary conditions

Thermal boundary conditions may be required for specific geothermal applications, for example to calculate how long it takes to heat up an area cooled due to geothermal production. In ROSIM the default setting for heat flow is a no-heat-flow boundary. Since heat is exchanged with the over- and underburden, a normal ROSIM model includes this explicitly. Laterally the model should be large enough to avoid any cooling or heating up near the boundary.

If no over- and underburden are implemented (top and bottom), cooling in the reservoir is overestimated and due to thermal diffusion the thermal gradient will be reduced over time. For the usually relatively thin geothermal and heat storage reservoirs (~20 to 200 m), these effects can be considerable.

The Beta version of ROSIM offers additional boundary conditions, namely a fixed top and bottom temperature and an option to analytically calculate the temperature exchange with the over- and underburden. This last option can potentially replace the explicit simulation of the over- and underburden. However, this option is not fully tested yet and not included in the ROSIM v 1.1.0.

For the commercial simulator several options are available for thermal boundary conditions, but they all need to implemented explicitly. The default is also a no-heat-flow boundary conditions. This is the same for OPM flow, although fewer options for thermal boundary conditions are available.

3.5 Temperature dependent density

Although the density of the brine is temperature dependent, the changes are not very large and in many cases can be ignored. There a few exceptions:

- In a very small reservoir, for example one which is enclosed in sealing faults, the reduction in volume can impact the pressure in the reservoir considerably. Since the volume change is in the order of a few percent and the compressibility of brine and formation is generally two orders of magnitude lower, a considerable volume is required to buffer the volume changes.
- For flow with very low pressure gradients (low flow rates and/or high permeability), density-driven flow is relatively more important. This sort of conditions are more likely to be found in high-temperature heat storage than in geothermal production.

The temperature-dependent density in DC3D is implemented differently than in the commercial simulator. For DC3D only the impact on the flow is included. In the commercial simulator also the effect on the volume in the reservoir is included. This means that for a model in which all boundaries have no-flow conditions, the pressure in the reservoir will go down since the volume of water decreases due to cooling (or increases due to heating in HTO applications). This is a real effect, however in realistic subsurface conditions, no-flow boundaries are usually further away and also the compressibility of the rock mitigates this effect.

Another remark on including temperature-dependent density for the commercial simulator is the impact on under- and overburden. If these are used with zero permeability, just for thermal boundary conditions, no temperature-dependent density should be used. Pressure will decrease to zero and the numerical solution will become problematic.

4 Conclusions

4.1 Conclusions

The results presented in this document show that for the configurations of geothermal doublets tested here, ROSIM with DC3D performs well. Both in terms of the pressure and temperature, the results are in line with the analytical solution and the commercial simulator. An advantage of DC3D is the fast run time, in particular for annual time steps. DC3D is in particular useful for evaluating long-time behaviour. ROSIM allows to quickly setup a simple 3D subsurface model and flow input files.

The single phase flow version of OPM, with temperature dependence for the density and viscosity can be unstable at times and can require long run times (for version 2022, more recent versions are more stable). The results of OPM flow are close to the commercial simulator and DC3D.

The reporting/calculation time unit in most geothermal cases does not have much influence on the conditions in the well. The results of the model used for comparison with the analytical solution were virtually identical for yearly and monthly reporting time steps.

Most of the runs in this report were done with considerable pressure differences (tens of bars), which is representative for most geothermal reservoirs. These cases can well be simulated with relatively coarse grids and coarse timesteps. However, if the permeability is high or flow rates are small and small pressure differences are required for production and injection, simulation is more complicated. Density driven flow becomes relatively more important and higher resolution both in space and time are required. Generally, reducing the grid size without reducing the time step size does not improve the results.

One consistent difference was observed between the results of the commercial simulator and DC3D: directly above and below the well head and toe, the pressure and the temperature differs between the two simulators. This is seen for partially penetrating wells and in under- and overburden in both horizontal, deviated and vertical wells. This affects the results very little.

4.2 Further developments

Although DC3D performs very well for basic setups simulated here, improvements would allow the simulator to be applicable to a wider range of conditions:

- For geothermal applications, a very useful addition would be the incorporation of faults in the simulator (this has been implanted for v1.1.0).
- For horizontal wells, the possibility to add pressure drop in the well would be useful.
- For HTO applications, the possibility to have cross flow in the well would be very useful. During the shutin phase, temperature differences can cause vertical flow in the well redistributing the heat around the well.

Links and references:

[1] The Open Porous Media Initiative, „OPM | The Open Porous Media Initiative,” [Online]. Available: https://opm-project.org/.

[2] TNO, „ROSIM manual v1.0,” 2022.

[3] TNO, „DoubletCalc2D: Tools | NLOG,” [Online]. Available: https://www.nlog.nl/en/tools.

[4] TNO, „DoubletCalc1D: Tools | NLOG,” [Online]. Available: https://www.nlog.nl/en/tools.

[5] SLB, „Petrel,” SLB, [Online]. Available: https://www.software.slb.com/products/petrel.

Appendix A: Overview table of functionality of the different simulators

	DoubletCalc3D	OPM	Commercial
Water viscosity temperature dependent	✓	✓*	✓
Water density temperature dependent (HTO)	✓	✓*	✓
Simultaneous Rate & Pressure flow constraint	×**	✓	✓
Handle faulted grids	×	✓	✓
Enthalpy/temperature-based	temperature	enthalpy	enthalpy
Heat capacity temperature dependent	✓	✓	×

Appendix B: Comparison of functionality of DC2D and Rosim/DC3D

Differences between DC2D (version 2019 used by AGE) and Rosim/DC3D:

	DC2D	Rosim / DC3D
Grid dimensions	2D	3D
Grid discretization	Variable grid size not possible. Heterogeneous properties only in horizontal direction for depth and thickness of the cells and actnum	Variations in vertical layering supported in Rosim; grid refinement around the wells supported in Rosim; variations in horizontal direction via custom grid.
Fluid viscosity (P,T,S)	Batzle and Wang (1992)	Kestin (1981)
Fluid density (P,T,S)	Batzle and Wang (1992)	Batzle and Wang (1992)
Fluid thermal properties (heat capacity (T,S), conductivity)	Conductivity constant, heat capacity following Batzle and Wang (1992)	Conductivity as heterogeneous grid property, heat capacity following Batzle and Wang (1992)
Fluid salinity (S)	constant	Heterogeneous properties
Rock properties (porosity, permeability,N/G)	Heterogeneous properties only in horizontal direction	Heterogeneous properties
Thermal rock properties (conductivity, heat capacity and density)	Constant	Heterogeneous properties
Pore volume compressibility	As constant storage (m^3/Pa)	Not supported
wells	Only fully-penetrating vertical wells (other configurations implemented via skin)	All well configurations possible
Thermal boundary condition top and bottom	Version 2015 (download NLOG): 2 options: no heat flow and wall cooling. 2019 version: no heat flow only	no heat flow and no wall cooling**
Flow boundary conditions top and bottom	No flow	No flow
Thermal boundary conditions lateral	Not specified as user option, depends on the top and bottom thermal boundary	Not specified as user option, depends on the top and bottom thermal boundary

Flow boundary conditions lateral	No flow or constant pressure	No flow or constant pressure
Initial conditions	Initial T per grid cell; output pressures are expressed as relative changes to initial conditions.	Initial T calculated per grid cell based on user input of surface temperature and gradient; Initial P following hydrostatic gradient based on user input of depth and pressure.
Faults*	Implemented as cell permeability multiplier	Implemented as cell permeability multiplier.
Subsidence calculation*	Yes	Yes, (thermal) compaction averaged over vertical stack
Geomechanical rock properties*	Constant values for reservoir and overburden, (thermal) compaction parameters apply to reservoir only	Constant values for reservoir and overburden, (thermal) compaction parameters apply to reservoir and over and underburden and can vary

* not part of this benchmark yet; implemented for Rosim/DC3D in 2023.
** for version 1.1.0. Development versions have more options.

Notes:
- both simulators can handle multiple wells (>2)
- for Rosim/DC3D: variations in the properties in vertical direction can be implemented via Rosim. Heterogeneous properties In horizontal direction need to be implemented via a custom grid created outside of Rosim.

Comparison of boundary conditions
The lateral thermal boundary conditions cannot be set explicitly by the user, but depend on the choices for the thermal boundary conditions set for the top and bottom of the model. Thus, in DC3D if a no heat flow boundary condition or wall cooling has been set for the top and bottom, then a constant temperature is assumed on the lateral boundaries. The complete overview is presented in the tables below.

Settings for the lateral thermal boundary conditions for DC3D depending on the choice of top and bottom boundary condition.

Selected top and bottom thermal boundary condition	Lateral thermal boundary condition
No heat flow	Constant T boundary
Fix T at top and bottom	No heat flow
Wall cooling	Constant T boundary

Settings for the lateral thermal boundary conditions for DC2D depending on the choice of top and bottom boundary condition.

Selected boundary condition	Lateral thermal boundary condition
Constant pressure boundary on the lateral boundaries	Constant T boundary

All other situations	No heat flow

Appendix C: Overview of the changes made to the OPM flow deck for the commercial simulator.

Keyword	adjustment
RUNSPEC section	
EQLDIMS (defaulted for OPM flow)	EQLDIMS cannot be defaulted, EQLDIMS should be equal to PVTDIMS
DIMENS (not required by OPM flow)	DIMENS required
THERMAL BLACKOIL GAS OIL WATER	THERMAL DEADOIL GAS OIL WATER
	OPTIONS3[1]
GRID section (GRDECL file)	
	Add HEATCR
	Add THCOIL
	Add THCGAS
	EDIT or GRID section: MULTIPLY PORV and ROCKV[1]
PROPS section	
PVTW	Adjust PVTW: Bw has to be consistent with cw and not be defaulted to 1.0, otherwise, the pressure will not remain at the initial pressure set in EQUIL.
VISCREF	Remove
PVCDO	Remove
PVDG	Remove
	Add OILCOMPR
	Add OILSPECH
	Add OILMW
	Add OILVISCT
	Add WATDENT
	Add ROCKOPTS (set to PVTNUM)
SPECHEAT	Remove
SPECROCK	Remove
	Add ZMFVD

	Add TEMPVD
	WATDENT
REGIONS section	
	Add EQLNUM (copy of PVTNUM)
SOLUTION section	
TEMPI	Remove
	give EQUIL settings for all EQL/PVT regions
SUMMARY section	
WTPCHEA / WTICHEA	Replace with WTEMP
	Optional: add additional output like DENW and VWAT
SCHEDULE section	
WTEMP	Replace with WINJTEMP and add the pressure at which the temperature occurs.

[1] for constant pressure boundaries only.

Notes:

- The oil properties can be dummy values.
- The production/injection temperature in the wells cannot be read by ResInsight, only in Petrel.

Energy & Materials Transition

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