Draft Description:  
11th SPE Comparative Solution Project

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Changes 20.02.2023:

* Rounded off permeability and entry pressures to round numbers.
* Removed maximum value for non-wetting rel-perm.
* Introduced an extension of capillary pressure to saturations below immobile wetting.
* Added units in reporting section
* Corrected mistake in density of water with CO2 present.
* First draft of a performance data section

# Technical description CSP 11A

The CSP 11A is a 2D geometry, set at laboratory scale and conditions.

## Governing equations and constitutive laws

As governing equations, we state the standard isothermal two-phase, two-component extension of Darcy’s law. For a detailed description, Nordbotten & Celia, 2011 or Lake et al., 2014; the main equations are summarized below. We emphasize that all rock parameters and constitutive functions denoted by an asterisk () are treated as spatially dependent, and will be defined as constant within each facies (see the geometry description in the next section).

Multi-phase Darcy’s law for phases (CO2-rich non-wetting gas phase), and (H2O-rich wetting liquid phase):

|  |  |  |
| --- | --- | --- |
|  |  |  |

Here is the phase flux, is the phase pressure, and are the relative and intrinsic permeabilities, respectively, is the phase viscosity, is the phase density, and is the gravitational force, defined with three significant digits, , pointing “down”.

Component mass conservation for components and :

|  |  |  |
| --- | --- | --- |
|  |  |  |

Here is the porosity, is the component mass fraction in phase , is the time variable and is the sum of diffusive and dispersive fluxes.

Diffusive and dispersive flux for component in phase :

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| --- | --- | --- |
|  |  |  |

Here is the mutual diffusivity in phase , while is a linear and isotropic dispersion model, with dispersion coefficient .

Capillary pressure: The phase pressures are related depending on saturation:

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| --- | --- | --- |
|  |  |  |

Completeness of model: For phases and components :

|  |  |  |
| --- | --- | --- |
|  | and |  |

In addition to the governing equations provided above, the following constitutive laws are considered.

Brooks-Corey type relative permeability and capillary pressure: For primary drainage (initial period of injected gas displacing water) we consider normalized saturations:

|  |  |  |
| --- | --- | --- |
|  | and |  |

Where is the saturation below which the phase is immobile. The relative permeability curves are then given by:

|  |  |  |
| --- | --- | --- |
|  |  |  |

Here the exponents determine the non-linearity of the rel-perm curves. Similarly, the basic Brooks-Corey capillary pressure is given by

|  |  |  |
| --- | --- | --- |
|  |  |  |

Here is the entry pressure for the rock. We remark that the capillary pressure is only meaningful when the phases are essentially connected. For non-wetting saturations less than , the phase will exist as disconnected bubbles of various radii, and thus a unique non-wetting pressure may not exist. This has no impact on the flow calculations (since the non-wetting relative permeability is zero), but does impact the thermodynamical calculations. For this CSP, we therefore define an extended capillary pressure, valid for all saturations, as

|  |  |  |
| --- | --- | --- |
|  |  |  |

Here defines a maximum capillary pressure, while the error function ensures a smooth transition of the capillary pressure function to the maximum value. For completeness, we emphasize that as the error function is defined as the integral of the normal distribution, it is well-defined at infinity: .

Thermodynamics: The description of the thermodynamics is split into three parts: Phase partitioning, pure-phase properties, and mixture properties.

1. We define the phase partitioning of the pure CO2-H2O system according to Spycher, Pruess and Ennis-King (2003), see in particular section 4.3 and Tables 1 and 2.
2. The pure-phase CO2 and H2O properties defined according to the NIST database (<https://webbook.nist.gov/chemistry/fluid/>).
3. For the range of conditions considered herein, the solubilities are quite small. As a consequence, all mixture properties are considered as equal to that of the pure phase with the exception of water density, which takes the form (Garcia, 2001):

|  |  |  |
| --- | --- | --- |
|  |  |  |

In this expression, is the density of water containing , while is the pure-phase properties discussed in point 2) above. Finally, is the apparent density of CO2 dissolved in water (defined as in the notation of Garcia, 2001). This quantity is specified in Equation (3) of Garcia, 2001, and parameterized therein as:

|  |  |  |
| --- | --- | --- |
|  |  |  |

Where temperatures are measured in Celsius, and the molar weight of CO2 is .

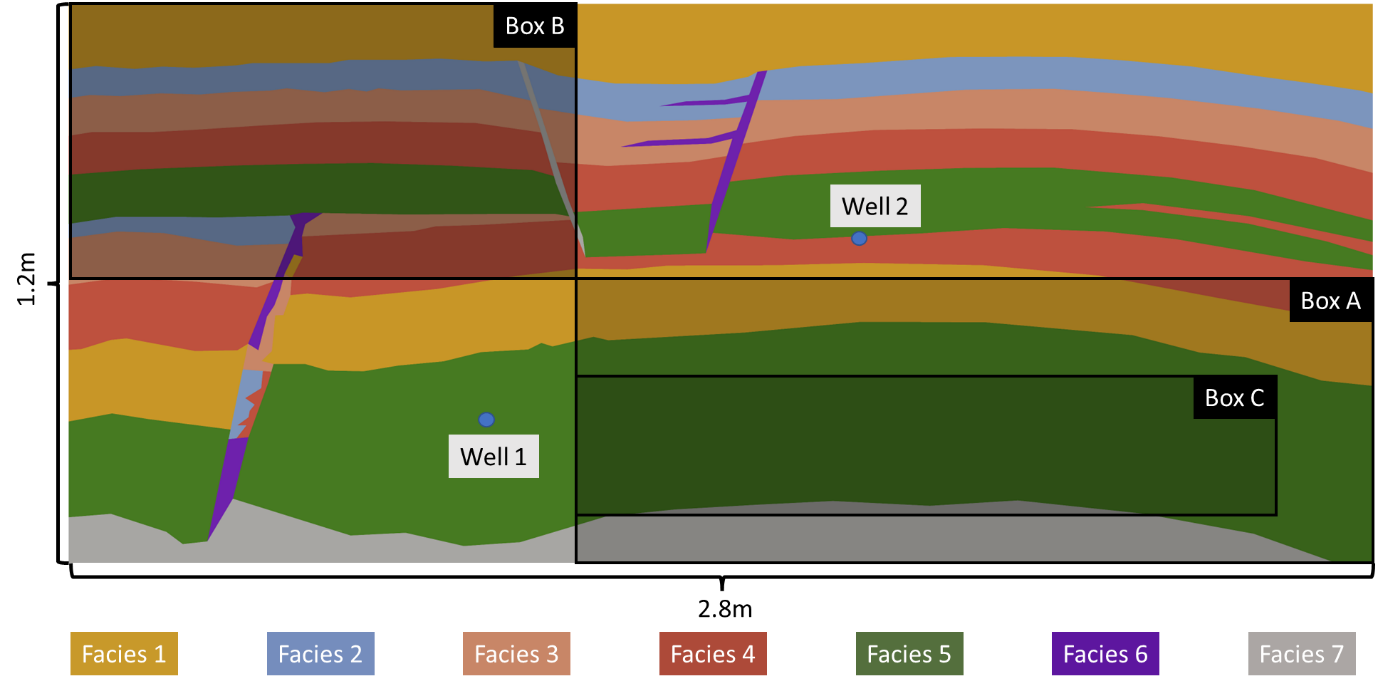
Rock compressibility: The rock is considered incompressible, thus does not vary over time.

## Geometry, boundary and initial conditions

The geometric description is motivated by laboratory experiments relevant for North Sea reservoirs, and has been developed in consultation with faculty and researchers at the Department of Geology, UoB[[6]](#footnote-7). The geometry presented here is a simplification of the geometry defined in Nordbotten et al., (2022).

The length of the porous media is 2.8 m and height is 1.2 m. The CSP v1 is 2D, but in order to present quantities in common units of “mass per volume”, we consider a uniform depth in the third dimension of 0.01 m. The porous domain consists of the full porous media, except for the two injection wells, as specified below.

Figure 1 provides a sketch of the geometry, a precise definition is given in the gmesh compatible file draft\_spe11.geo\_unrolled. As evident from the figure, the geometry contains six facies, all of which are considered to be internally homogeneous. The facies properties are given in the next section.



**Figure 1:** A sketch of the benchmark geometry. The geometry includes an anticline (right side) where CO2 accumulation is anticipated. There are three fault-like structures in the geometry, with different permeability (two high and one low). The lower fault (left side) is heterogeneous and consists of several facies. The upper left fault is a homogeneous sealing fault. The upper right fault is homogeneous consisting of a single facies. There are two CO2 injection points (blue circles), with locations given in the text. Box A, B and C indicated in the figure correspond to regions of interest motivated in Section 1.2, and further detailed in Section 2.5, with positions defined in the text. The facies are identified by colors, and further detailed in Section 2.3.

The figure contains three boxes that are used for reporting. Their (x,z) coordinates are measured relative to the lower left corner of the domain and are specified in terms bottom left and top right corners:

Box A: Bottom left (1.1, 0.0), top right (2.8, 0.6)

Box B: Bottom left (0.0, 0.6), top right (1.1, 1.2)

Box C: Bottom left (1.1, 0.1), top right (2.6, 0.4)

The figure also indicates the presence of the two injection wells, with (x,z) coordinates:

Well 1: (0.9, 0.3)

Well 2: (1.7, 0.7)

Temperature: Isothermal conditions of 20° C are considered for CSP 11A.

Boundary conditions: The left, right, and bottom boundaries are impermeable, i.e.:

|  |  |  |
| --- | --- | --- |
|  | and |  |

Where is the (outward) normal vector to the boundary.

The top boundary is considered a constant pressure boundary in contact with pure water, i.e.

|  |  |  |
| --- | --- | --- |
|  | , and |  |

Here is the boundary pressure, defined as .

The two injection wells, , are also defined as (internal) boundary conditions. Both wells are defined to have a radius of , centered at their respective coordinates. We refer to the respective well-to-reservoir circular boundaries as , where we impose the boundary conditions:

|  |  |  |
| --- | --- | --- |
|  | , , and |  |

Here are the injection rates, specified in the section “Operational conditions”.

Initial conditions: The initial conditions is a water-filled medium at rest, compatible with the boundary conditions, i.e.

|  |  |  |
| --- | --- | --- |
|  | , and |  |

## 2.3 Facies properties

The geometry contains seven facies, one seal (facies 1), five permeable reservoir sands (facies 2-6) and one impermeable (facies 7). These provide the definition of the material properties (all quantities marked by in section 2.1).

**Table 3**: Facies properties in SI units (meters, seconds, kg, Pascal, etc.)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | Isotropic Intrinsic permeability | Porosity | Immobile wetting saturation | Immobile gas saturation | Shape exponents relperm |
| Facies 1 |  | 0.44 | 0.32 | 0.10 | 2 |
| Facies 2 |  | 0.43 | 0.14 | 0.10 | 2 |
| Facies 3 |  | 0.44 | 0.12 | 0.10 | 2 |
| Facies 4 |  | 0.45 | 0.12 | 0.10 | 2 |
| Facies 5 |  | 0.43 | 0.12 | 0.10 | 2 |
| Facies 6 |  | 0.46 | 0.10 | 0.10 | 2 |
| Facies 7 | 0 | 0 | N/A | N/A | N/A |

**Table 3 (continued)**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | Gas entry pressure | Max cap- pressure | Shape exponent capillary pressure | Diffusion constants | Diffusion constants | Dispersion constant |
| Facies 1 | 1500 |  | 2 |  |  |  |
| Facies 2 | 300 |  | 2 |  |  |  |
| Facies 3 | 100 |  | 2 |  |  |  |
| Facies 4 | 25 |  | 2 |  |  |  |
| Facies 5 | 10 |  | 2 |  |  |  |
| Facies 6 | 1 |  | 2 |  |  |  |
| Facies 7 | N/A | N/A | N/A | 0 | 0 | N/A |

We remark that the maximum capillary pressure is chosen to avoid any potential for phase transition from water to vapor.

## 2.4 Operational conditions

Tentative CO2 injection protocol:

1. CO2 injection in well 1 with rate for s (continuous injection for 5 hours).
2. CO2 injection in well 2 with rate for s (start after 2.5 hours, end 2.5 hours later).
3. Monitor CO2 flow and transport until final time s (total run time of 5 days).

To exemplify the injection conditions, the specified mass rate corresponds to a volumetric rate of about 4.8 cubic centimeters per minute at 20C and .

## 2.5 Measurables

In addition to spatial maps of the field variables, the following measurables shall be reported, details of which, including time resolution, are described in Section 2.6. These measurables corresponds to proxies for the motivating questions in section 1.2.

### 2.5.1 Pressure (Proxy P1)

Pressure shall be reported at each of the two pressure observation points (labeled [15, 5] and [17, 11] in Figure 1) in [N/m2].

### 2.5.2 Phase composition (Proxies P2 and P3)

The distribution of the CO2-phase shall be reported within boxes labeled A and B in Figure 1. The phase distribution (in ) shall be reported in the following categories: 1. Mobile free phase (CO2 at saturations for which the relative permeability exceeds 0), 2. immobile free phase (CO2 at saturations for which the relative permeability equals 0), 3. dissolved (CO2 in water phase) and 4. seal (CO2 in any form in facies 1). The sum of the three first categories (mobile, immobile and dissolved) shall equal the total mass of CO2 in the respective box.

### 2.5.3 Convection (Proxy P4)

For the box labeled Box C in Figure 1, the extent of convective mixing shall be reported as the integral of the magnitude of the gradient in relative concentration of dissolved CO2. In other words, if mass-fraction of CO2 in water is denoted , and the dissolution limit is denoted , then the following quantity shall be reported

This quantity corresponds to the normalized total variation of the concentration field within box C, and has units of meters.

### 2.5.4 CO2 in sealing units (Proxy P5)

Similar to section 2.5.2, the total mass of CO2 in all sealing units (CO2 in any form in facies 1) shall be reported in .

## 2.6 Data reporting

All result data will be uploaded by the participants to XXX. Each participant will get write access to a dedicated repository named after his/her institution, e.g., XXX. At the end of the CSP, corresponding to the release of the final report, the relevant repositories will be turned public.

The reported data will be analyzed in two respects: Both in terms of an intercomparison of general numerical simulation capability (global spatial maps), but also in terms of our ability to correctly assess key properties of the system (the measurables outlined in Section 2.5). Consequently, we establish both a “dense” and a “sparse” reporting protocol.

Groups are encouraged to submit up to four results, if they deem it interesting, of which at least one should be representative of a computation that is reasonable within common reservoir engineering practice.

## 2.6.1 Sparse data

All measurables identified in section 2.5 shall be reported at 600s (10-minute) intervals starting at the initial injection and lasting s (5 days). The data is expected in csv format in the repository in a file time\_series.csv of the form

# t [s], p1 [Pa], p2 [Pa], mobA [kg], immA [kg], dissA [kg], sealA [kg], <same for B>, M\_C [m], CO2tot [kg]  
0.000e+00, 1.234e+56, 1.234e+56, <…>  
6.000e+02, 1.234e+56, 1.234e+56, <…>  
...

according to the measurables defined in section 2.5, with CO2tot denoting the total CO2 mass inside the computational domain.

## 2.6.2 Dense data

A spatial map of all field variables (pressure, saturation, phase composition) shall be reported for each hour from injection start. While the computational grids are generated by the participants individually, and should be chosen by each group as they find most appropriate, for cross-group comparison the spatial maps shall be reported on a uniform Cartesian grid of 280 by 120 cells (.01 m by .01 m grid cells from the bottom of the domain). For each temporal snapshot indicated by X hours, X = 0, 1, 2, …, cell values should be provided in csv format in a file spatial\_map\_<X>h.csv of the form

# x [m], y [m], presssure [Pa], gas saturation [-], CO2 concentration in water [kg/m3], H20 concentration in gas [kg/m3]  
5.000e-03, 5.000e-03, 1.234e+56, 1.234e+56, 1.234e+56, 1.234e+56  
1.500e-02, 5.000e-03, 1.234e+56, 1.234e+56, 1.234e+56, 1.234e+56  
…  
2.795e+00, 5.000e-03, 1.234e+56, 1.234e+56, 1.234e+56, 1.234e+56  
5.000e-03, 1.500e-02, 1.234e+56, 1.234e+56, 1.234e+56, 1.234e+56  
1.500e-02, 1.500e-02, 1.234e+56, 1.234e+56, 1.234e+56, 1.234e+56  
… …  
2.785e+00, 1.195e+00, 1.234e+56, 1.234e+56, 1.234e+56, 1.234e+56  
2.795e+00, 1.195e+00, 1.234e+56, 1.234e+56, 1.234e+56, 1.234e+56

The origin of the coordinate system should be located in the lower left corner with the x-axis positively oriented towards the right and the y-axis positively oriented towards the top.

## 2.6.3 Performance data

Reporting of performance data is strongly encouraged to the extent possible, but not mandatory. Note that several reporting quantities may not be relevant for certain participating groups, depending on their choice of numerical method and solution strategy. Performance data should be reported in three categories: As time-series (similar to sparse data in section 2.6.1), as spatial maps (similar to dense data in section 2.6.2) and as a questionnaire. These are detailed below.

The participants are encouraged to provide time-series at 600s (10-minute) intervals starting at the initial injection and lasting s (5 days). The data is expected in csv format in the repository in a file performance\_time\_series.csv of the form

# t [s], t\_step [s], mass [kg], dof[-], nl\_iter [-], lin\_iter [-]  
0.000e+00, 1.234e+56, 1.234e+56, <…>

The reporting quantities provided as time-series are defined as:

* t\_step: Average time-step size over the last 600s.
* mass: Mass balance, i.e. total mass of CO2 in the domain plus any mass that has crossed the boundaries.
* dof: Average number of degrees of freedom per time-step over the last 600s.
* nl\_iter: Average number of non-linear iterations per time-step over the last 600s.
* lin\_iter: Average number of linear iterations per non-linear iteration over the last 600s.

The participants are encouraged to provide spatial maps for each hour from injection starts. For cross-group comparison the spatial maps shall be reported on a uniform Cartesian grid of 280 by 120 cells (.01 m by .01 m grid cells from the bottom of the domain). For each temporal snapshot indicated by X hours, X = 0, 1, 2, …, cell values should be provided in csv format in a file spatial\_map\_<X>h.csv of the form:

# x [m], y [m], dx, max\_res\_error, tot\_error  
5.000e-03, 5.000e-03, 1.234e+56, 1.234e+56   
1.500e-02, 5.000e-03, 1.234e+56, 1.234e+56  
…  
2.795e+00, 5.000e-03, 1.234e+56, 1.234e+56  
<…>

The reporting quantities provided as spatial maps are defined as:

* dx: Average grid diameter within 1cm x 1cm reporting box at latest time-step.
* max\_res\_error: Maximum residual error within 1cm x 1cm reporting box at convergence of latest time-step.
* tot\_error: A posteriori estimate of total error within 1cm x 1cm reporting box at convergence of latest time-step. Please specify how total error is defined in the questionnaire.

The reporting quantities above are supplemented by the following questionnaire (also available separately as questionnaire\_A.xls):

|  |  |  |
| --- | --- | --- |
| Question | Numerical value  (where applicable) | Free-form text response  (where applicable) |
| Spatial discretization |  |  |
| Time discretization |  |  |
| Linear solvers (incl. preconditioner) |  |  |
| Notable aspects of solution strategy |  |  |
| … |  |  |
|  |  |  |
|  |  |  |

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