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# **A workflow for handling heterogeneous 3D models with the TOUGH2 family of codes: Applications to numerical modeling of CO<sub>2</sub> geological storage**

Pascal Audigane, Christophe Chiaberge, Frédéric Mathurin, Julie Lions, Géraldine Picot-Colbeaux

Corresponding author email adresse: [p.audigane@brgm.fr](mailto:p.audigane@brgm.fr)

BRGM: Water Division,  
3 Av. Claude Guillemin, BP 36009  
45060 ORLEANS Cedex 2 (FRANCE)  
tel: +33(0)2 38 64 33 72  
fax: +33(0)2 38 64 3719

## **Abstract**

This paper is addressed to the TOUGH2 user community. It presents a new tool for handling simulations run with the TOUGH2 code with specific application to CO<sub>2</sub> geological storage. This tool is composed of separate FORTRAN subroutines (or modules) that can be run independently using input and output files in ASCII format for TOUGH2. These modules have been developed specifically for modeling of carbon dioxide geological storage and their use with TOUGH2 and the Equation of State module ECO2N, dedicated to CO<sub>2</sub>-water-salt mixture systems, with TOUGHREACT, which is an adaptation of TOUGH2 with ECO2N and geochemical fluid-rock interactions, and with TOUGH2 and the EOS7C module dedicated to CO<sub>2</sub>-CH<sub>4</sub> gas mixture is described. The objective is to save time for the pre-processing, execution and visualization of complex geometry for geological system representation. The workflow is rapid and user-friendly and future implementation to other TOUGH2 EOS modules for other contexts (e.g. nuclear waste disposal, geothermal production) is straightforward. Three examples are shown for validation: i) leakage of CO<sub>2</sub> up through an abandoned well, ii) 3D reactive transport modeling of CO<sub>2</sub> in a sandy aquifer formation in the Sleipner gas Field, (North Sea, Norway), and iii) an estimation of enhanced gas recovery technology using CO<sub>2</sub> as the injected and stored gas to produce methane in the K12B Gas Field (North Sea, Denmark).

**Keywords:** TOUGH2, pre and post processing, CO<sub>2</sub> geological storage, 3D visualization, multiphase flow, reactive transport modeling

## **1. Introduction**

The capture and geological storage of carbon dioxide (CCS) has been under consideration as one technical option for greenhouse gas emission mitigation since the Intergovernmental Panel on Climate Change published its Special Report on Carbon Dioxide Capture and Storage (CCS) (IPCC, 2005). The elaboration of a legal

framework for CCS requires pertinent estimates of storage feasibility, efficiency and safety during and after injection, and numerical modeling is increasingly being used for a better understanding in the preparation, approbation and elaboration stages of pilot sites for CCS. Extrapolation of laboratory results from core to reservoir scale can be done by numerical modeling with correct implementation of the identified relevant physical processes. Modeling of carbon dioxide geological storage requires at least the implementation of multiphase flow and phase partitioning (dissolution of supercritical CO<sub>2</sub> in the brine and vice versa). The CO<sub>2</sub> is to be injected deep enough (> 800 m) so that it will stabilize in its supercritical state with a high density and therefore with a better storage efficiency. This injection will have a huge impact on local and regional hydrogeology and hydrogeochemistry. Since the CO<sub>2</sub> will be injected for several years, a large volume of water will be displaced and the integrity of the storage zone must be assessed in order to avoid any upward migration of the supercritical CO<sub>2</sub> due to over pressure or buoyancy.

The TOUGH2 family of codes is one of several numerical models dedicated to CCS that is capable of handling identified trapping mechanisms (Bachu *et al.*, 1994) when CO<sub>2</sub> is injected and stored in saline aquifers (Pruess *et al.*, 1999, Pruess and García 2002, Pruess and Spycher, 2007). Implementation of geochemical fluid-rock interactions in the code extended its modeling applications to mineral trapping characterization (Xu *et al.*, 2003; Xu *et al.*, 2006). As a start, the 1D radial demonstration problem (one layer system centered around the injection well) provides a simplified but complete picture of gas bubble evolution, storage capacity, pressure build up, dissolution and mineral trapping (Xu *et al.*, 2003, André *et al.*, 2007). The 2D radial model better describes the gravity impact on pressure build up, CO<sub>2</sub> migration, induced convection effects and mineral trapping efficiency (Audigane *et al.*, 2007; Zhou *et al.* 2008, Zhang *et al.*, 2009). The weakness of the radial models is that they consider a flat geological formation, disregarding any dip or regional hydrogeology induced by the geometry of the system. Simulations of long term effects would require a better representation of layer horizons as well as the heterogeneity of the cap rock formation overlying the storage zone afforded by 3D models.

3D modeling and meshing of geological formations is a vast subject in itself, and is not the aim of the present paper. Our study deals solely with the use of TOUGH2 (and associated modules) to develop a 3D model of a geometrically complex system. The mesh maker (“*MESHMAKER*”) embedded in TOUGH2 generates numerical grids with Cartesian or radial geometrical configurations. Although the TOUGH family of codes has great flexibility in handling the wide variety of grid information required to describe complex objects, designing and generating a suitable irregular grid can be tedious and error-prone. For this reason, graphical user interfaces (GUI) have been developed specifically for TOUGH2 (O’sullivan and Bullivant, 2005; Sato *et al.*, 2003 ;

Burnell *et al.*, 2003; Swenson *et al.*, 2003; Alcott *et al.*, 2006, Pan, 2003 and 2008). These tools aim to provide efficient and user-friendly integrated gridding software with graphic interfaces and easy viewing. Though this creates a more convenient working environment for the TOUGH2 family of codes, various constraints remain. First, updating the TOUGH2 module requires a complete recompilation of the tool, making the user highly dependent on the GUI developers' technical support teams. Second, the option for editing results may be limited in comparison with the specific finite element mesh visualization tool. Finally, the GUI may have to be purchased.

Our objective was, therefore, to provide a convenient, user-friendly tool for modeling CCS with TOUGH2 on a geometrically complex geological system while preserving a maximum flexibility for updating and rapid release. Our strategy involved developing a set of separate modules (hereafter called a “workflow”) written as an executable FORTRAN subroutine aimed at providing specific tasks using only input and output files from a “standard” TOUGH2 run (Chiaberge and Audigane, 2009). The TOUGH2 code can then be easily modified or updated in one of the subroutines. The workflow outputs ASCII files in specific formats for two classical FEM visualization tools: Tecplot ([www.tecplot.com](http://www.tecplot.com)), a licensed computational fluid dynamics post-processing tool and ParaView ([www.paraview.org](http://www.paraview.org)), an open-source, multi-platform application designed to visualize small to very large data sets.

After briefly describing the TOUGH2 family of codes, focusing on the CCS application, we describe here in detail the structure of the input and output files needed for a “standard” run, and associated equation-of-state (EOS) routines. Mesh generation and boundary condition management is also addressed. Thereafter, we describe the workflow structure and its connection with TOUGH2 input and output files. Several other tools are also documented (Local Grid Refinement implementation, import from geo-modeler, streamline visualization). Three applications are presented. The first involves using the workflow in a benchmarking trial on a CCS model recently proposed by the University of Stuttgart (Class *et al.*, 2009). The second application is a case study of reactive transport modeling of CO<sub>2</sub> injection in the Utsira sand aquifer at the Sleipner Gas Field in the North Sea (Picot-Colbeaux *et al.*, 2009). The third concerns a pilot site for enhanced methane recovery by carbon dioxide injection in the K12B gas field, also in the North Sea (Audigane *et al.*, 2008).

## **2. General description of TOUGH2**

### **2.1 TOUGH2 and CCS**

TOUGH2 is a non-isothermal multiphase fluid flow simulator used extensively for modeling heat and mass transfer in various situations such as geothermal systems, nuclear waste disposal and basin hydrogeology. Recent developments enable its use in assessing CO<sub>2</sub> geological storage. The code's versatility is due to the development of a set of equation-of-state (EOS) modules adapted to various gas- and liquid-mixture behaviors. An EOS routine called ECO2N has recently been developed specifically for treating CO<sub>2</sub>-water-salt systems typically encountered in the case of CO<sub>2</sub> geological storage in saline aquifers (Pruess and Spycher, 2007). TOUGHREACT is an adaptation of TOUGH2 to reactive transport modeling considering geochemical fluid-rock interactions during multiphase fluid flow (Xu *et al.*, 2006). TOUGHREACT is designed to run with several EOS routines, including ECO2N.

Numerous publications (not all of which are cited here) describe studies of CO<sub>2</sub> geological storage done using TOUGH2/ECO2N and TOUGHREACT/ECO2N codes. One of these, involving a 1D model using radial geometry centered on the injection well in a single-layer porous geological formation, has been proposed as a code intercomparison study (Pruess *et al.*, 2004). In a similar fashion, Xu *et al.* (2003) developed a 1D reactive transport model of CO<sub>2</sub> geological storage in the Gulf Coast sediment using TOUGHREACT. Audigane *et al.* (2007) have studied a 2D model of short- and long-term evolution of a CO<sub>2</sub> gas bubble and the related geochemical reactions of the Utsira sandy aquifer in the North Sea. TOUGH2 and TOUGHREACT have also been used to predict near-well dry out induced by several years of CO<sub>2</sub> injection (Pruess and Muller 2009), along with salt precipitation (André *et al.*, 2007). Oldenburg *et al.* (2004) developed a specific EOS called EOS7C to study the injection of CO<sub>2</sub> in a depleted methane reservoir. Audigane *et al.* (2008) have used TOUGHREACT and TOUGH2/EOS7C to predict induced geochemical interactions during Enhanced Gas Recovery at the K12B site in the North Sea.

## **2.2 TOUGH2/ECO2N Input/Output files**

The TOUGH2 and TOUGHREACT User's Guides (Pruess *et al.*, 1999; Xu *et al.*, 2005) describe the TOUGH2 code structure in detail. We focus our attention, therefore, on the input and output files needed to run the workflow presented here, from a run using TOUGH2 and associated components.

The numerical scheme used in TOUGH2 is based on the Integral Finite Difference (IFD) method (Narasimhan and Witherspoon, 1976) with a fully implicit time discretization. The residual form of the system of equations is

solved using the Newton-Raphson iteration method. The IFD method offers the advantage of being applicable to regular or irregular discretization in three dimensions. In our study we will focus on the use of a hexahedral grid block commonly used in reservoir fluid flow simulators.

A set of primary variables, which differs depending on the EOS routine used, must be defined for each grid-block in order to initiate the simulation run. When TOUGH2 is run with the ECO2N module, four variables are needed: pressure, CO<sub>2</sub> amount (either as gas saturation in two-phase conditions or mass fraction in single-phase conditions), salinity (either as solid saturation or mass fraction of the dissolved part), and temperature. When the EOS7C module is used, the amount of methane (either as gas saturation in two-phase conditions or mass fraction in single-phase conditions) must be provided.

### **2.2.1 Input files**

The input files containing the parameters needed to run TOUGH2 and TOUGHREACT are (Figure 1):

- “*flow.inp*” This file mainly includes rock properties, time stepping and multi-phase fluid and heat flow simulation parameters. Each of these parameters is defined for a domain which can contain more than one grid block. This file also allows date selection for data editing.
- “*INCON*” This file includes initial condition for porosity, permeability, and the four primary variables (pressure, gas saturation (or mass fraction of the dissolved gas), salinity and temperature) for each grid-block.
- “*MESH*” This file includes all grid block geometric properties (volume, exchange area, distance between grid block centers, coordinates, definition of rock properties domain).

The structure of the input and output files in TOUGH2 (and associated EOS) is flexible. For example, information from the “*INCON*” and “*MESH*” files can be incorporated in the “*flow.inp*” file. We use the “*INCON*” and “*MESH*” files below as a basis in order to simplify the structure of the workflow.

The following files are needed for TOUGHREACT only.

- “*inchem*” This file includes initial condition for the geochemical system (aqueous species, solid mineral phases, etc.).

- “*chemical.inp*” This file is used for defining the general parameters of the geochemical system (kinetic rate of mineral species, secondary solid and aqueous phases, sorbed species, etc.).
- “*solute.inp*” This file includes transport and other run parameters such as diffusion coefficients, tolerance limits for convergence, printout flags, grid block attribution of a domain with a different chemical composition (in agreement with the definition supplied in the “*chemical.inp*” file), etc.

The structure of the “*inchem*” file depends directly on the geochemical system defined in the “*chemical.inp*” file. The assumed number of chemical species and mineral phases in the geochemical system will determine the number of variables to be calculated and stored in the “*inchem*” file. Although TOUGHREACT can run without the “*inchem*” file, in this study we use separate files for pre- and post-processing data treatment. In addition, it is very easy to generate the “*INCON*”, “*inchem*” and “*MESH*” files with TOUGH2 and TOUGHREACT (see User’s Guide).

### 2.2.2 Output files

The output files are:

- “*flow.out*” This file includes, for each date selected in the “*flow.inp*” file, the parameters calculated during the simulations for each grid block (pressure, temperature, gas saturation, salinity, gas and liquid density, gas and liquid velocity vectors, etc.).
- “*SAVE*” This file gives the values calculated for porosity, permeability, and the four primary variables (pressure, gas saturation, salinity, temperature) for each grid-block, at the end of the simulation. It can be used as a restart file by being renamed “*INCON*”. There is some redundancy in data editing between this file and the “*flow.out*” file.

The following output files are provided for the TOUGHREACT run only:

- “*savechem*” This file provides the result of the calculated variables initially in the “*inchem*” file at the end of the simulation. It can be used as a restart file by being renamed “*inchem*”.
- “*conc.dat*” This file includes all aqueous chemical species concentrations for each grid block for every selected date in the “*flow.inp*” file.
- “*min.dat*” This file includes all mineral phase concentrations for each grid block for every selected date in the “*flow.inp*” file.

Other files are produced during a TOUGHREACT/ECO2N run (“*chemical.out*”, “*runlogout.out*” etc.), but these files are not necessary, in our case, for a complete editing of the simulated variables. On the other hand they provide additional information very helpful for a better understanding of the simulation (run convergence, mass balances etc.).

### **3. The workflow tool**

Pre- and post-processing of data using TOUGH2 and TOUGHREACT are challenging for complex 3D models including geological heterogeneities and multi-domain geological facies with associated mineralogy. We, therefore, developed a workflow module as a set of Fortran subroutines able to handle (i) visualization of TOUGHREACT file results, (ii) grid block attribution of heterogeneous properties, (iii) boundary condition attribution, (iv) refinement and coarsening of 3D grid mesh. These modules can be broken down into three main categories (Figure 2):

- building or modification of existing mesh (GRID)
- physical property attribution to grid blocks (PROPERTY)
- 3D Visualization of the simulation results (RESULT)

The 15 workflow modules, along with their input and output files, are listed below by category. The flow-chart in Figure 3 describing the entire procedure can serve as a guide for using the workflow.

#### **3.1 GRID category**

##### ***“Mesh2visu”***

This module enables the visualization of the TOUGH2 mesh generated by MESHMAKER. It enables the conversion of “*MESH*” files to “*grid.dat*” files that can be opened with Tecplot or Paraview software. This file will be used by many other modules. Visualization of a mesh grid containing local refinement is also possible.

**Input file:** “*MESH*”

**Output file:** “*grid.dat*”

##### ***“Petrel2Tough”***



This module converts a mesh generated by the Petrel geomodeler (Schlumberger) to a “*MESH*” file, ready to be run with TOUGH2. The Petrel mesh file must be in ASCII format, readable by the ECLIPSE “black oil” simulator (Schlumberger). The “Petrel2Tough” module is programmed to identify ECLIPSE keywords such as ‘SPECGRID’, ‘COORD’ and ‘ZCORN’, to recognize grid block coordinates, as well as ‘PERMX’, ‘PORO’, ‘ACTNUM’ to identify active grid block properties.

It is important to notice that Petrel software can produce several types of mesh according the topological feature of the generated grid. For structured grid cartesian block centered or rectangular corner point geometry is required while unstructured grid models can be built with control volume finite elements, composite tetrahedral grids or PEBI (Perpendicular bisector or voronoi) element techniques (Palagi and Aziz, 1994). The IFD method assumed that node connections are orthogonal to interface surface which makes the PEBI method perfectly suited for the use of TOUGH2. In the present study we used grids provided with a cartesian block centered approach. Therefore, the mesh generated with Petrel2Tough module contain elements with identical volumes, identical surface area and identical inter-nodal distances with respect to the original grid, but the orthogonality between inter-nodal distance and surface area might not be preserved in agreement with the dip angle of the modeled geological formations.

**Input file:** ASCII Petrel Mesh file

**Output file:** “*MESH*”

### **“Coarser”**

This module enables the coarsening of a Petrel grid mesh in order to reduce the total number of grid blocks. It is often needed when importing large grid meshes from geological models that can contain up to several million grid blocks. Up-scaling of the reservoir properties is needed for assigning average property values to the new grid blocks of the coarse mesh. A separate input file is needed to define the selected zone of the mesh to be coarsened, and the degree of coarsening.

**Input files:** “*Coarser\_Change.itt*”, “*MESH*”

**Output file:** “*MESH*” (modified)

### **“LGR”**

This module is dedicated to “Local Grid Refinement” technique in mesh generation. Nested gridding is done in order to refine one part of the domain. This is often needed when addressing near well zone issues like scaling,

dry out or salt precipitation. An input file is needed to describe the domain to be refined, and also the degree of refinement. Several refinement levels are supplied with this option.

It is important to specify that for the LGR technique proposed in this study the node connections (parameters D1 and D2 in the CONNE block of the MESH file) of gridblocks generated for the sub-gridding decomposition is kept orthogonal to the interface surface. Therefore the real distance “D” between the nodes of two adjacent grid blocks (one in the sub-grid part and one from the initial mesh) is not preserved (D is not equal to D1+D2). The correct implementation of sub-gridding elements would require introduction of composite elements containing interpolated information and modification of the TOUGH2 source code files (as proposed by Garcià and Pruess, 2000). Based on several application case study recommendation of using the “LGR” module with a smooth transition for sub-gridding decomposition of a factor of 5 is reported (Wertz and Audigane, 2010).

**Input files:** “*Gigogne.itt*”, “*MESH*”

**Output file:** “*MESH*” (modified)

#### **“ActiveCell”**

This module enables the inactivation of mesh elements for the simulation. It is very efficient for reducing the total number of grid blocks. An input file is needed to select the domain where inactive elements should be removed from the original mesh file.

**Input files:** “*ActiveCell.itt*”, “*MESH*”

**Output file:** “*MESH*” (modified)

### **3.2 PROPERTY category**

#### **“Rocktype”**

This module enables the attribution of ‘ROCK’ domains as defined in the TOUGH2 “*flow.inp*” input file. In TOUGH2, several intrinsic rock properties, such as relative permeability function, capillary pressure, rock grain density, pore compressibility and specific heat, are defined for each domain. The attribution of a domain to each grid block defined in the “*MESH*” file becomes difficult when working with 3D mesh. This module requires an input file to select the geometrical coordinates of the domain under consideration.

**Input files:** “*Rocktype.itt*”, “*MESH*”

**Output file:** “*MESH*”

### ***“Chemtype”***

In much the same way, “Chemtype” assigns domains representing (i) initial water formation, (ii) boundary water formation and (iii) mineralogical assemblage. This is input in TOUGHREACT by the “solute.inp” input file. This domain attribution is independent of the ‘ROCK’ domain from a numerical point of view, but the “MESH” file is needed as an input in order to recover the grid block coordinates.

**Input files:** “Chemtype.itt”, “solute.inp”, “MESH”

**Output file:** “solute.inp” (modified)

### ***“Init\_P\_t”***

This is a tool for initializing a pressure and temperature field according to a hydrostatic and a geothermal profile along the depth. This is done by modifying the TOUGH2 “INCON” input file, which contains all pressure and temperature data for each grid block before the simulation begins. The “MESH” file provides grid block coordinates. A separate input file is needed for defining the imposed pressure and temperature gradient (linear according to depth).

**Input files:** “Init\_p\_t.itt”, “MESH”, “INCON”

**Output file:** “INCON” (modified)

### ***“Condinit”***

This is a tool for initializing all parameters in the “INCON” file (porosity, permeability, pressure, salinity, gas saturation field and temperature). This is done by entering values for each parameter by keyword (e.g. ‘PORO’ for porosity) for each grid block in the order defined in the “MESH” file. A separate include file is, therefore, needed, in addition to the “MESH” and “INCON” files, as an input.

**Input files:** “Condinit.itt”, “MESH”, “INCON”

**Output file:** “INCON” (modified)

### ***“Volinf”***

This module enables the implementation of Dirichlet boundary conditions on either existing grid blocks or new grid blocks. In TOUGH2, assignment of such conditions is implemented by considering large volume grid blocks, which implicitly keeps all grid block properties constant during the simulation run. We kept the same approach by imposing an arbitrary volume of  $1.0 \text{ E}^{+29} \text{ m}^3$  (easily modifiable). A separate input file makes it

possible to define the domain that contains either grid blocks for assignment, or grid blocks to which new grid blocks need to be generated and connected – in which case, these new grid blocks are not used for the final visualization of the simulation results. The “*MESH*” and “*INCON*” files are therefore needed for modifications.

**Input files:** “*Volinf.itt*”, “*MESH*”, “*INCON*”

**Output files:** “*MESH*” and “*INCON*” (modified)

### 3.3 RESULTS category

#### “*Visuflow*”

This module was specifically developed to visualize simulation results from the TOUGH2 “*flow.out*” file. The input files, “*flow.out*” and “*grid.dat*” (generated by the “*Mesh2visu*” module described in the GRID category above) are, therefore, needed. The output file, “*gridflow.dat*”, is in a Tecplot format and contains all properties calculated in “*flow.out*” for each date selected.

**Input files:** “*flow.out*”, “*grid.dat*”

**Output file:** “*gridflow.dat*”

#### “*Visuchem*”

In much the same way as for the “*Visuflow*” module, this module was developed to visualize simulations resulting from a TOUGHREACT run. Therefore, the “*grid.dat*” file (generated with the “*Mesh2visu*” module) must be supplied along with the files containing aqueous, mineral and gas phase concentrations – “*conc.dat*”, “*min.dat*” and “*gas.dat*”, respectively (default names). An output file, “*gridchimie.dat*”, in Tecplot format, is produced, which contains all chosen parameters (chemical species, minerals) for editing and for each date selected.

**Input files:** “*grid.dat*” and “*conc.dat*” and/or “*min.dat*” and/or “*gas.dat*”

**Output file:** “*gridchimie.dat*”

#### “*Visuvectflow*”

This module is specific to the edition of flow vectors which can be (optional) edited in the “*flow.out*” file. Flow through connected grid blocks is provided for liquid, gas and heat and for each selected date. Vector coordinates are calculated at the center of each grid-block averaging the vector components provided by TOUGH2 for each

**grid-block connection (interface).** As for the “VisufLOW” module, the “*grid.dat*” and “*gridflow.dat*” input files are needed to generate an output file, “*gridvect.dat*”, in Tecplot format.

**Input files:** “*grid.dat*” and “*gridflow.dat*”

**Output file:** “*gridvect.dat*”

#### **“Mass-balance”**

This module provides a mass balance of the CO<sub>2</sub>, salt and water system under aqueous, gaseous and solid phases for the entire model. This information is provided during a TOUGH2 run in the “*flow.out*” file for each selected date and for each domain defined in the ROCK block of the “*flow.inp*” file. The output is a text file easily manageable using any table editor for plotting history evolution of such mass balances.

**Input file:** “*flow.out*”

**Output files:** A list of text files for each data field (gaseous CO<sub>2</sub>, aqueous/liquid CO<sub>2</sub>, solid salt etc.) and for each rock domain.

#### **“Tec2Para”**

This module converts files in ASCII Tecplot format to ASCII Paraview format, because with Paraview software it is necessary to define a separate file for each parameter (pressure, temperature etc.) whereas Tecplot handles all parameters in one large file.

**Input file:** “*gridflow.dat*”

**Output files:** “*geometry.insight*”, “*ensight.case*”, list of files for each parameter

## **4. Application and case study**

The workflow has been tested with a 3D case of (i) Local Grid Refinement (“*LGR*”) and (ii) inactive grid block (“*Activecell*”) implementation for hydrodynamic multiphase modeling of a generic synthetic case, and two case studies with realistic data using reactive transport data modeling from real pilot sites.

### **4.1 Stuttgart Benchmark**

The University of Stuttgart recently published a code intercomparison study on CCS modeling (Class *et al.*, 2009). Three exercises were proposed and we participated in exercise 1 involving the leakage of CO<sub>2</sub> from a storage zone to an overlying aquifer by way of a leaky well (Figure 4). A semi-analytical solution has been

provided, to be compared with numerical modeling results (Nordbotten *et al.*, 2005), the rate of leakage being calculated in the middle section of the leaky well.

To develop the model, we first created a 3D grid with the TOUGH2 “MESHMAKER” tool. This 3D grid includes the storage aquifer, the overlying aquifer and the aquitard. Using the “LGR” module, we then refined the grid around the leaky well for the entire domain, and around the injection well only within the storage aquifer. Using the “Activecell” module, we removed all grid blocks defining the aquitard domain except those located within 1 m of the leaky well. “Mesh2Visu” shows of the final 3D grid mesh (Figure 5).

CO<sub>2</sub> is injected for 1,000 days at a constant rate of 8.87 kg/s (1,600 m<sup>3</sup>/day). Using the “Init\_p\_t” module, the pressure is initialized for the whole system (the temperature is assumed to be constant). Constant hydrostatic pressure is imposed on all sides of the grid with the “Volinf” module. The simulated leakage rate is then compared with the analytical solution (Figure 6). The results differ mainly because of the grid mesh resolution around the wells, although they are satisfactory in comparison with other simulation results (see Figure 5 in Class *et al.*, 2009). Visualization of the CO<sub>2</sub> gas bubble is possible with the “VisufLOW” module (Figure 7). Using “Visuvectflow”, a fluid flow vector field was built, enabling the visualization of the liquid and gas phase in the system (Figure 8).

#### **4.2 Case study 1: Injection of CO<sub>2</sub> in the Sleipner field (Saline aquifer)**

One of the first pilot sites for CO<sub>2</sub> injection into a saline aquifer is the Sleipner gas field operated by Statoil in the North Sea (Torp and Gale, 2004). The gas produced via several wells contains a relatively high CO<sub>2</sub> concentration ranging from 4.5 to 9% (Korbøl and Kaddour, 1995). As a result of financial deterrents (a Norwegian tax of \$55 per ton of CO<sub>2</sub> emitted), Statoil decided to store carbon dioxide underground in the Utsira formation located above the gas reservoir (Kongsjorden *et al.*, 1997). Injection started in 1996 at an approximate average rate of 1 million tonnes per year. The Utsira formation is a large sandy aquifer extending over 26,100 km<sup>2</sup> at a depth of between 700 and 1000 m. Several seismic surveys have been conducted since the start of the injection in order to visualize the evolution of the gas bubble (Torp and Gale, 2004; Arts *et al.*, 2004). Several modeling studies have also been done for history matching and for long-term predictions of the hydrodynamics and geochemical impacts of this injection (Lindeberg and Bergmo, 2002; Johnson *et al.*, 2001; Audigane *et al.*, 2007). BRGM has recently conducted a study to predict the multiphase flow and associated fluid-rock interactions induced by CO<sub>2</sub> injection at Sleipner (Picot-Colbeaux *et al.*, 2009). The geometry of the reservoir

was built from a geological 3D model elaborated by the Sintef Institute with a geo-modeler Petrel (courtesy of Bergmo from Lindeberg and Bergmo, 2002).

Using the “*Petrel2Tough*” module, the Petrel mesh deduced from the geological model is converted into a “MESH” file readable by TOUGH2 and TOUGHREACT (Figure 9a). However, this resulted in 428,400 grid blocks, which is definitely too many for running a reactive transport model with TOUGHREACT in a reasonable length of time. The number of blocks was, therefore, reduced by coarsening the mesh using the “*Coarser*” tool (Figure 9b).

Intra-shale layers were identified by seismic interpretation. This geological heterogeneity enables the local accumulation of CO<sub>2</sub> during its upward migration due to buoyancy. The mineralogical assemblage of the model was divided into two domains in order to consider both sand and shale formations in the system. Heterogeneous hydrogeological and geochemical properties were attributed to these two geological formations using the “*Rocktype*” and “*Chemtype*” modules.

Simulations were done with the coarser mesh (41,400 grid blocks) for a 3-year injection period. Visualization of both multiphase flow and fluid-rock interactions in a Tecplot format was done with the “*Visuflow*” and “*Visuchem*” modules. Results predict a rather low geochemical impact, as seen on a 2D cross-section of the change in porosity induced by CO<sub>2</sub> injection (Figure 9c). After three years of injection, the primary trapping process is the geological structure of the system – mainly the cap rock formation overlying the reservoir aquifer, which prevents the upward migration of the free CO<sub>2</sub> due to buoyancy. Solubilization has started but does not represent more than 10% of the injected mass of carbon dioxide.

#### **4.3 Case study 2: Injection of CO<sub>2</sub> in the K12B Field (Enhanced Gas Recovery)**

As part of the Dutch Climate Policy to implement the Kyoto protocol, the nearly depleted K12-B gas reservoir in the North Sea operated by Gaz de France Netherlands was chosen as a demonstration site for the Offshore Re-injection of CO<sub>2</sub> project (ORC project). The K12-B field is located in the Dutch sector of the North Sea (150 km from Amsterdam). Gaz de France Production Nederland B.V. has been producing gas with four wells (K12-B1, K12-B2, K12-B5 and K12-B7) since 1985 and the field is now almost depleted. Located at a depth of about 3,800 m, the gas field consists of a number of tilted fault blocks that are not, or only barely, in pressure communication. Fluid flow is strongly influenced by the presence of wrench fault tectonics resulting in some further compartmentalization of individual fault blocks (van der Meer *et al.*, 2004). The present study addresses CO<sub>2</sub> injection into compartment 3 of the gas field during phase 3 of the ORC project. We used the geological

model and the associated 3D grid mesh generated by Geel *et al.* (2006) in agreement with previous studies (Figure 10). This 3D model was built with Petrel and compartment 3 initially contained 27,747 grid blocks. A coarser 3D grid in a TOUGH2 "MESH" file format was built using the "*Petrel2Tough*" and "*Coarser*" tools in order to be able to run both hydrodynamic and reactive simulations with TOUGH2/EOS7C and TOUGHREACT, respectively. Four different geological formations have been identified in compartment 3. A clay cap rock formation (Ten Boer) with two sandstone formations (Upper and Lower Slochteren) separated by a clay layer near the cap rock unit (Ameland). We used the "*Rocktype*" and "*Chemtype*" modules to implement the heterogeneities on the final 3D grid containing 3,171 grid blocks (Figure 11).

The principal aim of the operator was to assess the efficiency of the Enhanced Gas Recovery technique using CO<sub>2</sub> injection. Carbon dioxide was injected in order to both reduce CO<sub>2</sub> emissions and recover CH<sub>4</sub>. This technology is often envisaged at the final stage of field production, which is the case in the K12B gas field. We used a specific EOS module for TOUGH2 called EOS7C (Oldenburg *et al.*, 2004), which can handle a CO<sub>2</sub>-CH<sub>4</sub> gas mixture. The injection rate of 10 kg/s corresponds to phase 3 of the research project considering a full-scale injection of about 310-475 Kton per year. K12-B1 and K12-B5 are production wells, while CO<sub>2</sub> is injected in K12-B6. We chose a production rate of 1 kg/s for each producer to limit the CO<sub>2</sub> breakthrough time. Enhanced Gas Recovery could be greater if the production rate was greater but this simulation was carried out as if the injection of large quantities of CO<sub>2</sub> was a primary objective.

Gas recovery and geochemical impacts were assessed and visualized with the "*Visuflow*" and "*Visuchem*" modules (Figure 12). Since the reservoir originally contained 13% of CO<sub>2</sub> in the gas phase, the aqueous phase was already in equilibrium with high carbon dioxide fugacities and therefore the initial brine was very acidic with a pH of around 4.7. Simulations predict, after 10 years of injection, a very small modification of pH in the entire reservoir causing very little geochemical fluid-rock interaction (Figure 13). Structural and solubility trapping are the two main carbon dioxide storage processes, as shown by the "*MassBalance*" module (Figure 14). Since the reservoir is a closed system, a large pressure increase of 50 bar is predicted, which is in agreement with the very great under-pressurization (from about 350 bar to 40 bar) previously induced by methane production. These results are discussed in greater detail in Audigane *et al.* (2008).

## 5. Conclusion

Modeling of carbon dioxide geological storage requires a precise description of the geological formation envisaged as a storage target in order to improve storage capacity prediction and risk assessment of such a new



technology. 3D geological modeling tools are now able to reproduce such a detailed geometry and pertinent geo-statistical simulations for modeling hydrogeological reservoir property fields. Multiphase flow modeling done with the TOUGH2 simulator, developed by the Lawrence Berkeley National Laboratory (LBNL) and recently used, along with other numerical tools, for CCS modeling, is poorly suited to handling complex mesh geometry and 3D heterogeneous porous media. Pre and post processing of such a tool is still lacking, though several attempts have been made to provide graphic-interface software.

The workflow proposed in this study is a set of Fortran subroutines that are easy to use and adapt for any TOUGH2 code up-date. This set of modules can generate TOUGH mesh and corresponding property fields to assess liquid and gas hydrodynamics as well as fluid-rock geochemical interactions. Post processing is provided as export in two classical mesh visualizer formats: Tecplot and ParaView. Additional options are also provided to handle boundary condition attribution and mesh refinement and coarsening. A converter of geo-modeler Petrel files in ASCII format into TOUGH mesh files has also been developed.

The workflow has been applied to different test cases in order to validate its use in a carbon dioxide geological storage context. An unstructured mesh geometry has been modeled to simulate an abandoned well linking a saline storage reservoir with an overlying aquifer. Import of the Petrel format and coarsening of the mesh in order to reduce the number of grid blocks enables the simulation of induced geochemical fluid-rock interaction associated with CO<sub>2</sub> injection in the sandy aquifer of the Utsira formation in the North Sea, Norway. Another context of carbon dioxide storage was tested in a context of methane production using reservoir data from the K12b gas field, also in the North Sea.

The flexibility of the workflow enables it to be easily extrapolated to other contexts such as nuclear waste disposal or geothermal production by adapting the workflow to specific equation of state modules (EOS1, EOS3...) developed by LBNL for TOUGH2.

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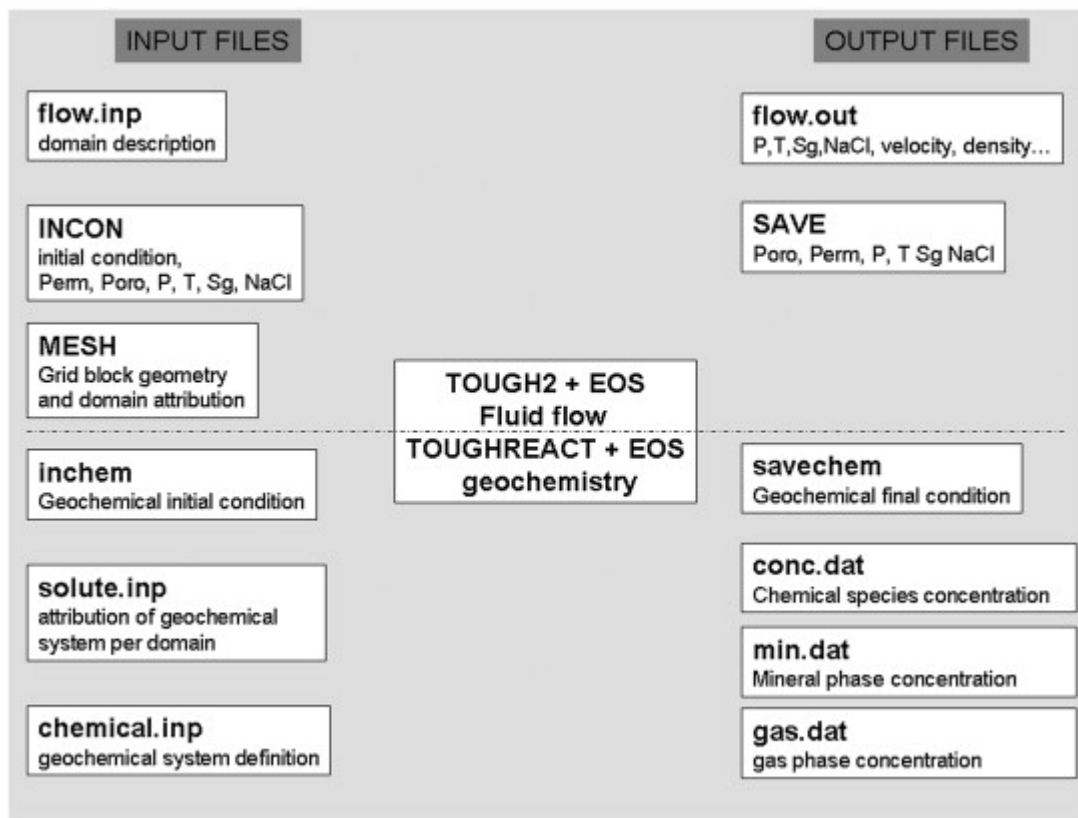
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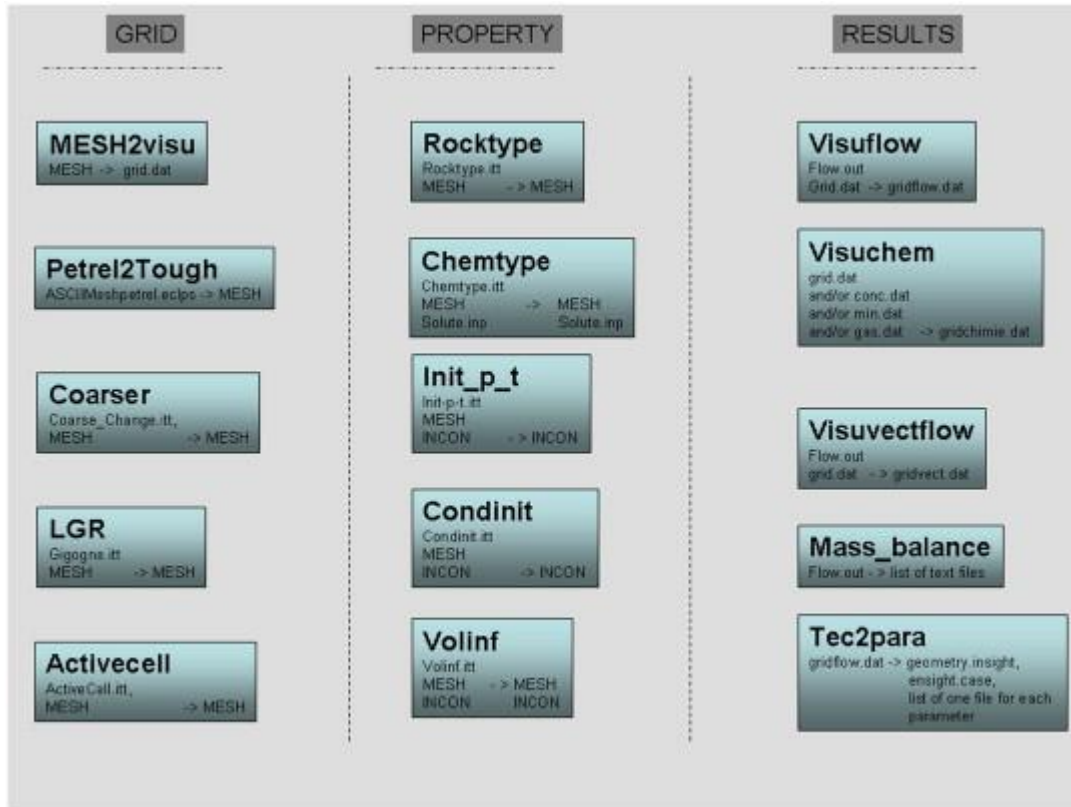
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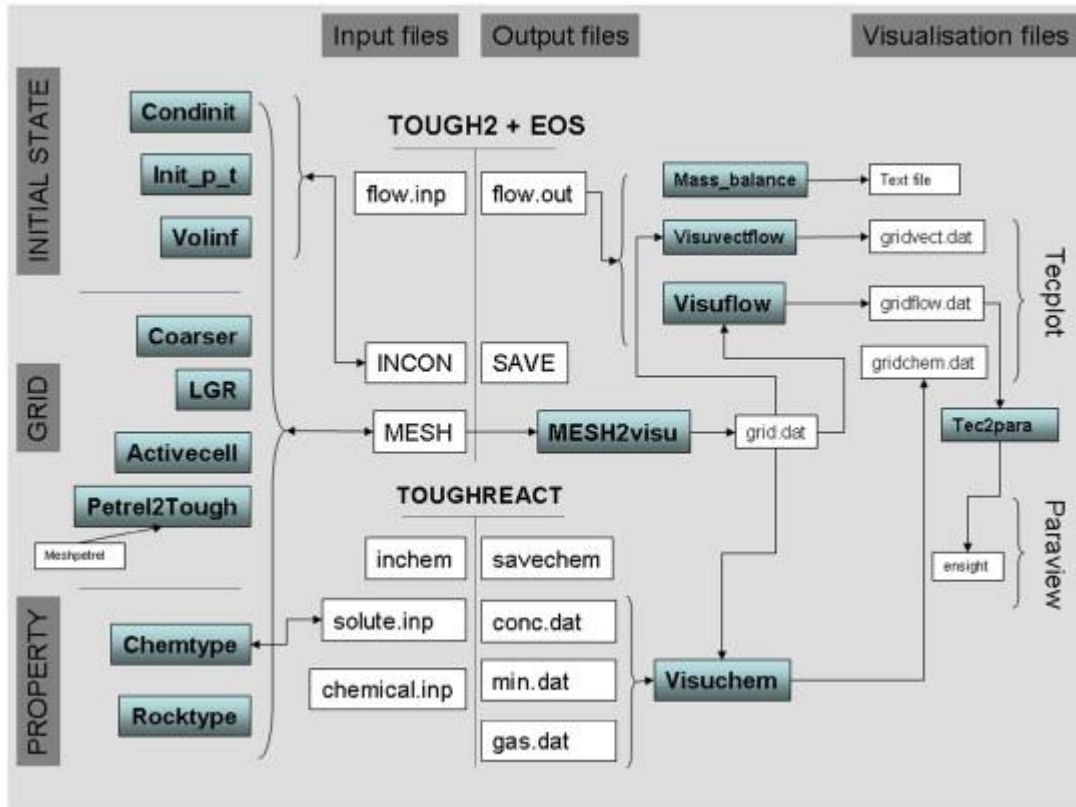


**Figure 1:** Input and output files for TOUGH2 and TOUGHREACT. Perm=permeability, Poro=porosity, P=Pressure, T=temperature, Sg=gas saturation, NaCl=salt mass concentration.

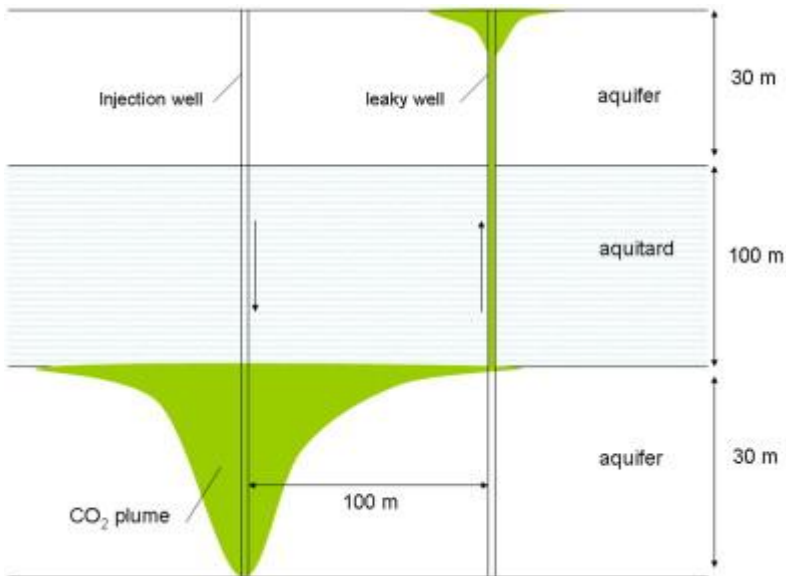


**Figure 2:** Modules developed for the workflow. Each module is a separate FORTRAN executable. Associated input and output files are listed under the module name.

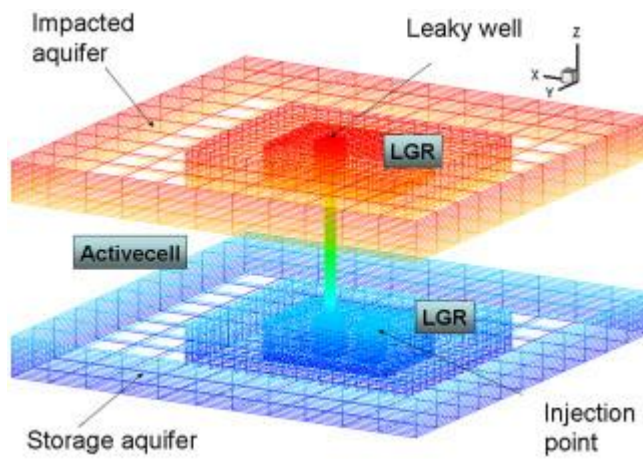




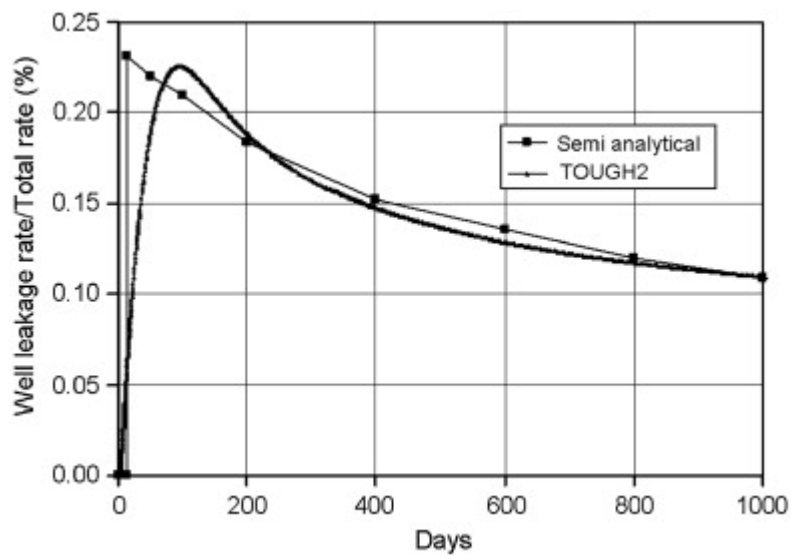
**Figure 3:** Workflow descriptive flow chart including modules and links with TOUGH2 and TOUGHREACT input and output files.



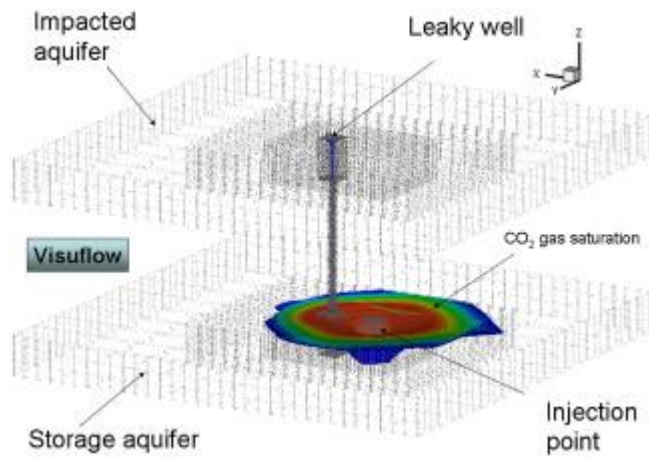
**Figure 4:** Schematic drawing of leakage scenario proposed for code benchmarking by Class *et al.* (2009).



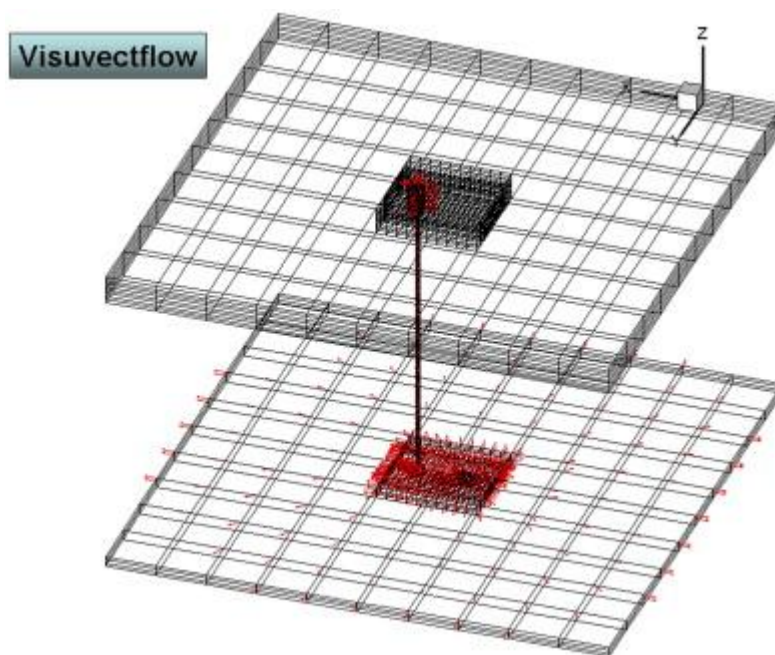
**Figure 5:** Mesh generation using “LGR” and “ActiveCell” modules applied to problem used for code benchmarking (Class *et al.*, 2009).



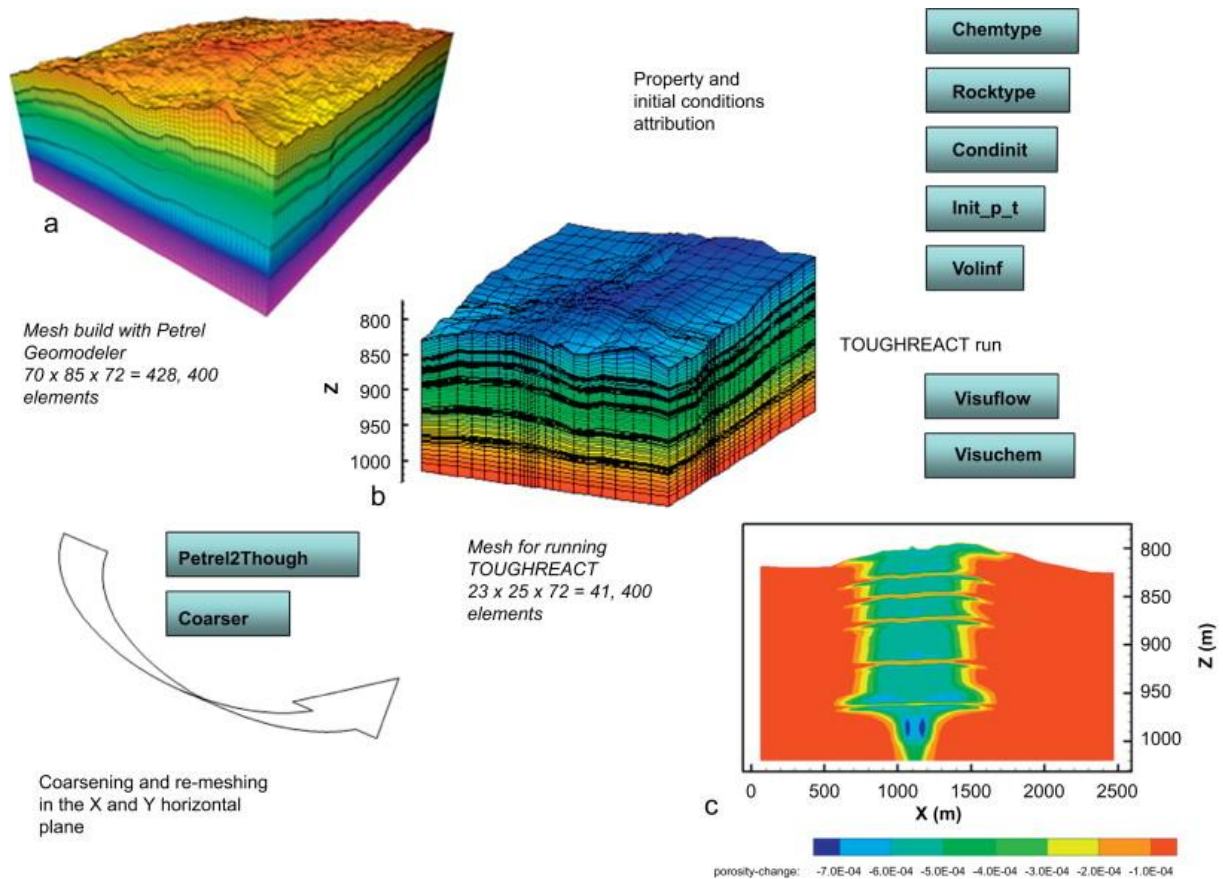
**Figure 6:** Results of code benchmarking (Class *et al.*, 2009) and comparison with semi-analytical solution.



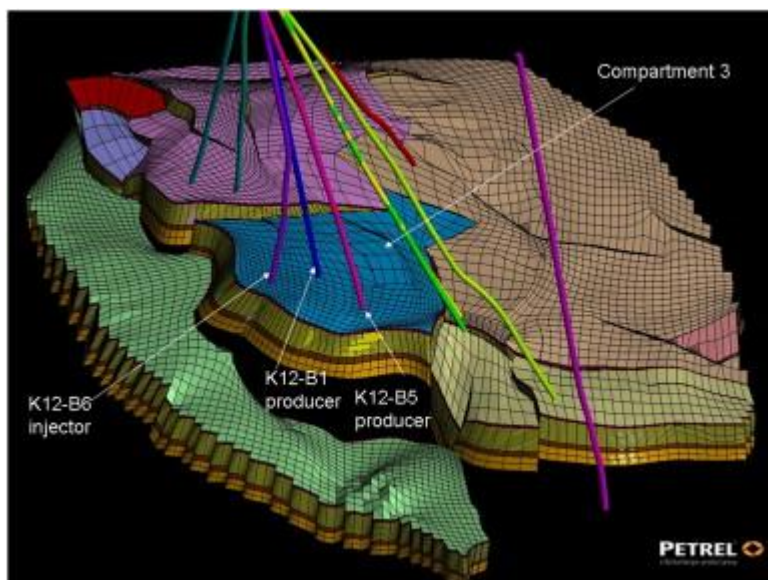
**Figure 7:** 3D visualization of gas bubble simulated with TOUGH2 for code benchmarking (Class *et al.*, 2009) using the “*Visuflow*” module.



**Figure 8:** 3D visualization of gas flow vector field simulated with TOUGH2 for code benchmarking (Class *et al.*, 2009) using the “*Visuvectflow*” module.

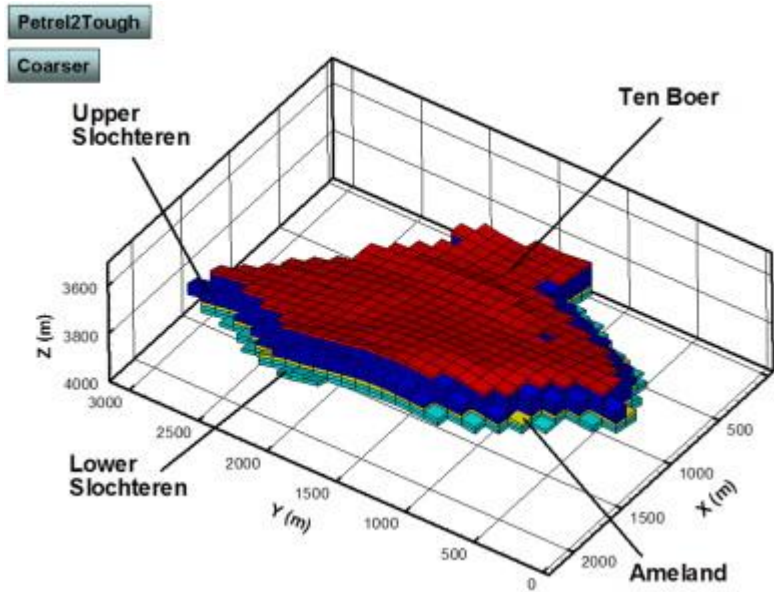


**Figure 9:** (a) Petrel mesh of the Utsira geological formation, (b) converted to a TOUGH2 mesh, and (c) reactive transport simulation with TOUGHREACT using mesh from (b)

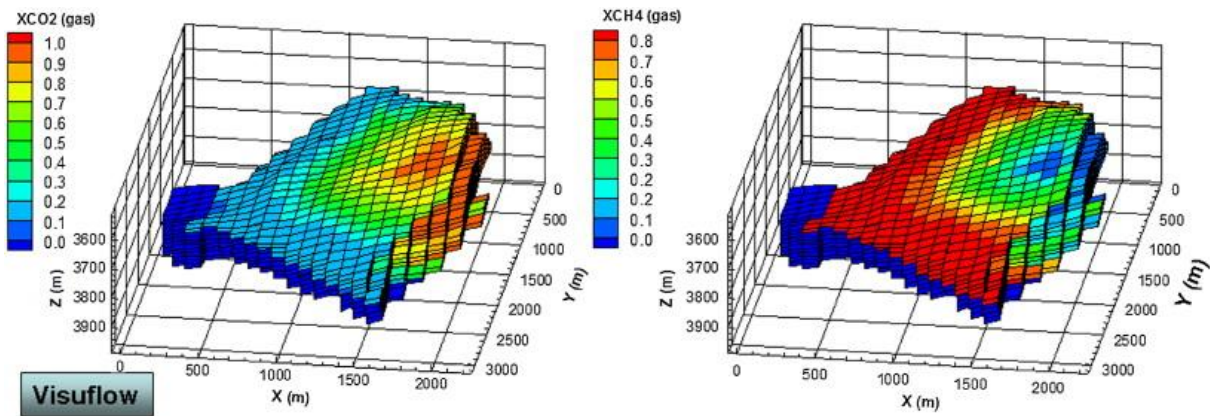


**Figure 10:** K12B-field model built with Petrel geo-modeler by SINTEF Institute (Geel *et al.*, 2006). CO<sub>2</sub> injection and CH<sub>4</sub> production is simulated in compartment 3 of the field.

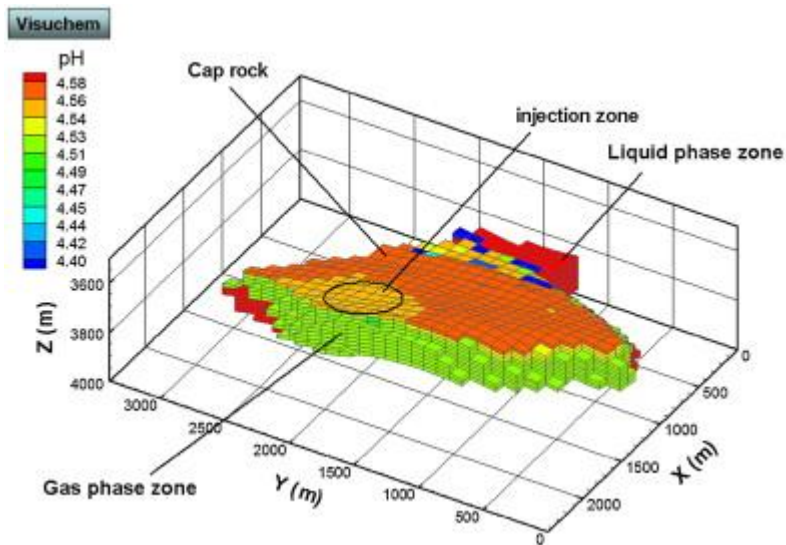




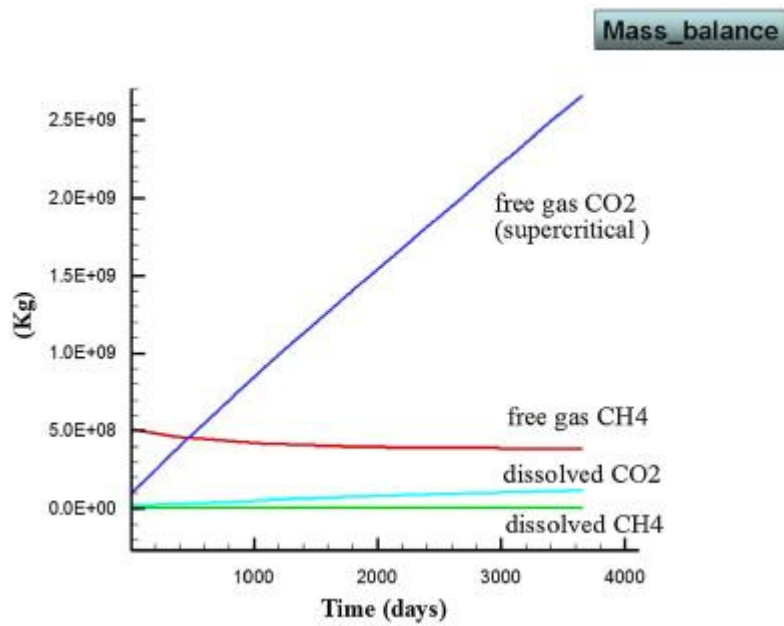
**Figure 11:** TOUGH2 mesh of compartment 3 for the K12-B gas field using “Petrel2Tough” and “Coarser” modules.



**Figure 12:** 3D visualization of multiphase flow simulation of Enhanced Methane production injecting carbon dioxide on the K12-B field using the TOUGH2-EOS7C simulator and the “Visuflow” module. “XCO2” and “XCH4” are the mass fraction of CO<sub>2</sub> and CH<sub>4</sub> in the gas phase, respectively.



**Figure 13:** 3D visualization of reactive flow simulation of CO<sub>2</sub> injection in the K12-B field using the TOUGHREACT simulator and the “VisuChem” module.



**Figure 14:** Mass balance between injected CO<sub>2</sub> and produced CH<sub>4</sub> simulated at the K12-B gas field using the “Massbalance” module.