

## Numerical modeling of geological storage



**Jonathan Ennis-King**  
Cooperative Research Centre  
for Greenhouse Gas  
Technologies (CO<sub>2</sub>CRC)/CSIRO  
Earth Science and Resource  
Engineering

China-Australia Geological Storage of  
CO<sub>2</sub>  
School, May 2014

© CO<sub>2</sub>CRC  
All rights reserved



## Outline

- **Why do numerical modelling?**
- **Physics of simulation**
- **Philosophy of model building**
- **Practical limits to simulation**
- **Upscaling**
- **Recent developments**

## Why do numerical modeling?

- **Data is expensive to collect, which justifies considerable effort to extract the best value from it.**
- **Data is scarce and limited in resolution and scale, so it needs to be “extended”**
- **Projects are expensive and risky, so numerical modelling is needed to explore uncertainty and reduce risk.**

3



## The dangers of simulation

**“If you do it too much, you come to believe that it’s the real thing”**

- **Simpler techniques may be sufficient to address the objectives.**
- **Complicated is often equated to better, especially in a multi-disciplinary workflow.**
- **Pictures are a great communication tool, so simulations based on inadequate data and poor methodology still look good!**

4



## The physics of simulation

The key governing equations are:

- Mass and energy conservation
- Transport law (e.g. multi-phase Darcy's law)
- Fluid equations of state: CO<sub>2</sub>, brine, other gases

These have to be supplemented by initial conditions, boundary conditions and source terms (wells).

5



## What physics is missing?

The software will not include all the physics e.g.

- Darcy's law starts to break down at high flow rates, as can occur in some gas wells. An additional term is then needed in the flow equations
- Hydrodynamic dispersion (along and normal to the direction of flow) is often neglected This is usually much larger than molecular diffusion.
- Wellbore storage effects may be absent unless a well model is included in the simulation.

6



## Philosophy of model building

### Define your objectives first!

- What questions are you trying to answer with the simulation?
- How accurate an answer do you need?
- What limits are there to time/resources for the simulation study?
- How much data is there to base a model on?

7



## First kind of objective

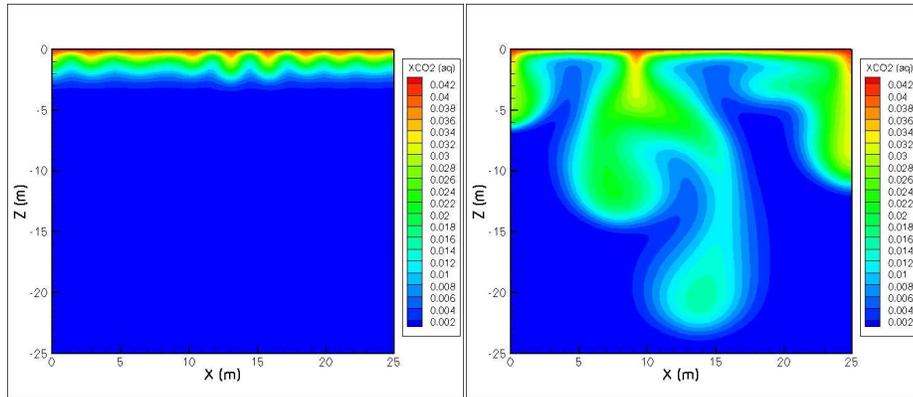
Research questions e.g. How does the hydrodynamic gradient affect CO<sub>2</sub> migration?

- These are often based on relatively small amounts of representative data.
- Realism is not important, so significant simplifications can be made.
- There may be a way to compare to another theoretical treatment

8



## Example of a research question: convection of dissolved CO<sub>2</sub>



27 years

90 years

 $k_h=100$  mD,  $k_v=50$  mD

9



## Second kind of objective

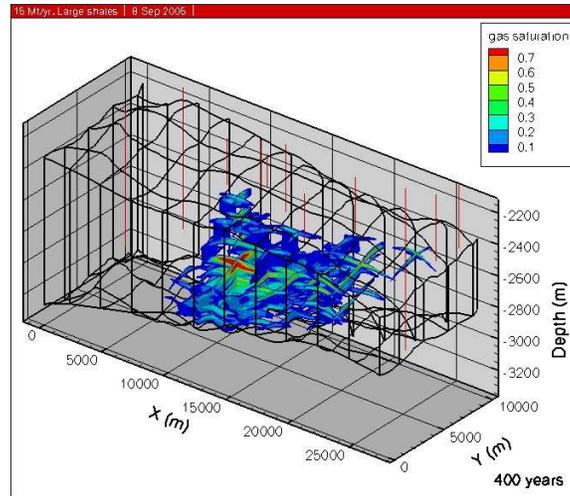
**Make technical prediction in a site-specific context to support decisions e.g.**

- **How much CO<sub>2</sub> can be stored? How should it be monitored? What are the risks?**
- **Data may be sparse (high-level site assessment) or relatively abundant (commercial prospect or depleted field).**
- **Small models may be adequate, but will likely lead to full-field 3D as data becomes available.**

10



## Example: Timing of vertical migration of CO<sub>2</sub>



## Seek understanding!

“The purpose of computing is insight, not numbers”  
Richard Hamming.

- Simulations can produce vast quantities of data, and beautiful pictures.
- **You should NEVER rely on results you don't understand**
- The hardest part of simulation is to develop an intuition for the physical processes. You need a good understanding of reservoir engineering and the physics of multiphase flow in porous media.



## Small is beautiful?

**Models should be fit-for-purpose:**

- Resist the “one big model” temptation.
- Multi-disciplinary workflows encourage big models if you can’t easily iterate.
- Early models should be small so you can run a lot of them, and investigate sensitivities.
- Mature models (with field data) should be bigger, but still allow for a suite of models.

13



## Practical limitations

**To solve the governing equations requires:**

- discretization in space – splitting the domain up into gridblocks
- discretization in time – advancing in finite timesteps.

**This has a series of consequences**

- limitations on size
- numerical artifacts
- upscaling and resolution of data

14



## Size limits

Call the number of equations  $n$  (= number of gridblocks times number of mass components)

- The memory requirements are proportional to  $n$
- The CPU time scales between  $n^{1.5}$  and  $n^2$ . Single CPU allows  $\sim 10^5$  blocks. Parallelism helps but still limited to millions of blocks.
- Field-scale models are coarse: 10-50m blocks width is common.

15



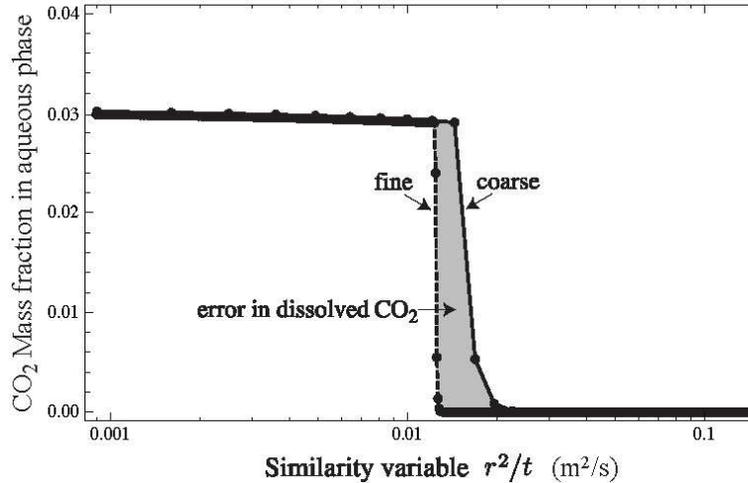
## Numerical Artifacts

- Orientation effects e.g. fluid flow is easier along grid axes rather than diagonally across them
- Numerical diffusion is proportional to  $v \Delta t$  where  $v$  is the flow velocity. This can be more significant than real physical diffusion or dispersion.
- Local equilibrium assumed in each gridblock. Thus during the injection phase, the amount of dissolved  $\text{CO}_2$  will be overestimated. This can be corrected for: Green and Ennis-King, (2012) *Comput. Geosci.* 16: 1153-1161

16



## Effect of grid refinement on CO<sub>2</sub> dissolution

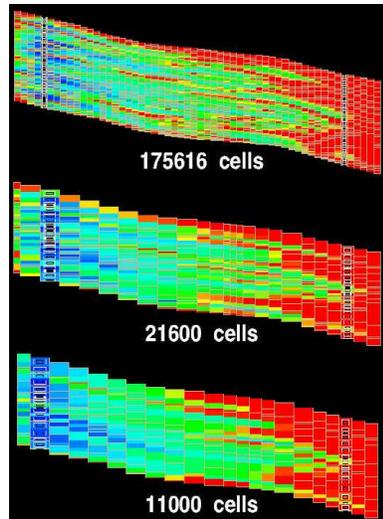


## Upscaling of data

Each grid block only has one value for porosity, permeability, saturation, composition etc. This has two important consequences:

- we cannot resolve anything in the results below the size of a grid block.
- geological data measured on different scales e.g. core data, has to “upscaled” or averaged in an intelligent way.

## Example of permeability upscaling



Issue is what to preserve with the upscaling:

- average migration speed?
- breakthrough time?
- plume shape?

19



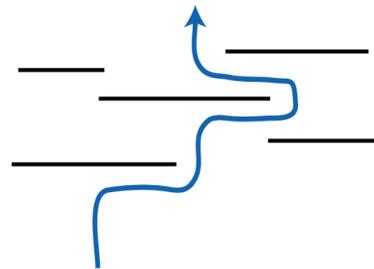
## Vertical permeability

- Due to the density difference between CO<sub>2</sub> and water, vertical migration is important except in thin reservoir or for short times.
- Deep injection schemes rely on tortuosity of migration paths – two phase model can use object modelling of barriers.
- It's common to characterize through the ratio  $k_v/k_h$  where  $k_v$  is vertical perm and  $k_h$  is horizontal perm. “Default” often  $k_v/k_h = 0.1$

20



## Vertical permeability



$$K_v / K_h \ll 1$$

21



## Upscaling of relative permeability

**Core-measured properties aren't always appropriate for grid blocks thicker than the capillary transition zone.**

**A variety of schemes exist to make this upscaling correction:**

- **analytic (vertical equilibrium) – tend to straighten the rel. perms.**
- **“dynamic” – rely on matching fine scale cross-section simulations to coarser ones.**

22



## Geostatistics

- **Fine scale data (e.g. porosity and permeability) is only available at wells.**
- **Geostatistics fills in everything else, based on estimates of correlations (variograms).**
- **Don't put too much faith in nice pictures**
- **Don't trust a single realisation**
- **Gridding should follow geological features**

23



## Be nice to geologists on your team

- **The building of the geological model requires significant time and effort, even for simple models.**
- **Good communication requires understanding of geological terms and their implications e.g. depositional environments.**
- **It's very desirable to be able to iterate!**
- **Simulation efficiency must be balanced against faithfulness to geology.**

24



## Software for simulation

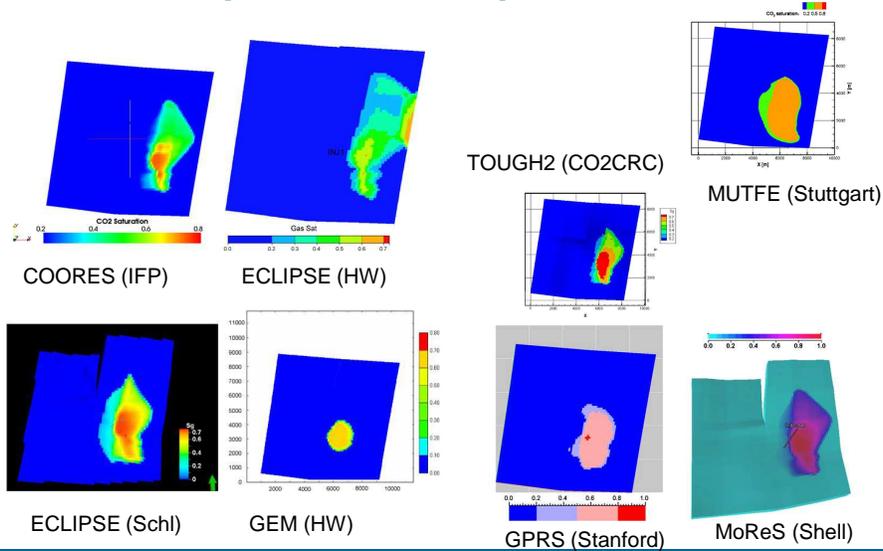
### Large variety of choices

- Commercial codes: Eclipse, GEM, Tempest, MoReS etc
- Research codes: TOUGH (LBNL), GPRS (Stanford), PFLOTRAN (LANL), STOMP (PNNL), VESA (Princeton), NUFT (LLNL), etc
- Open source codes: DUMUX, OPM

See Class et al. (2009). A benchmark study on problems related to CO<sub>2</sub> storage in geologic formations. *Comput. Geosci.*, 13(11), 409-434.



## Example: Code comparison results



## Directions in numerical simulation

### Focus on more coupled problems and additional physics

- Chemical reactions coupled to multiphase flow (e.g. TOUGHREACT, NUFT)
- Geomechanics coupled to multiphase flow (e.g. TOUGH/FLAC)
- Wellbore coupling issues (e.g. T2well)
- Tracers

### Focus on field projects and monitoring

- Interpreting monitoring data (e.g. P/T gauges)
- Designing monitoring e.g. seismic forward modeling



## CO2CRC Participants



Supporting Partners: The Global CCS Institute | The University of Queensland | Process Group | Lawrence Berkeley National Laboratory  
 CANSYD Australia | Government of South Australia | Charles Darwin University | Simon Fraser University

