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# **From geological models to reservoir simulation**

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**CAGS Technical Workshop**

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# Modelling

- **Modelling is used to:**
  - design injection (location and number of wells, monitoring);
  - forecast the migration of injected carbon dioxide.
- **Modelling can include:**
  - coupled geochemistry;
  - coupled geomechanics;
  - tracer migration.
- **Most modelling uses computer models;**
  - Although analytical models are being developed.

# Computer models

- **Computer models usually:**
  - **solve the multiphase equations for fluid flow in porous media;**
  - **use finite-difference techniques for solving the flow equations;**
  - **require the simulated region to be broken up into grid blocks;**
  - **are based on techniques and code developed in the petroleum industry over several decades.**

## Darcy's law for fluid flow

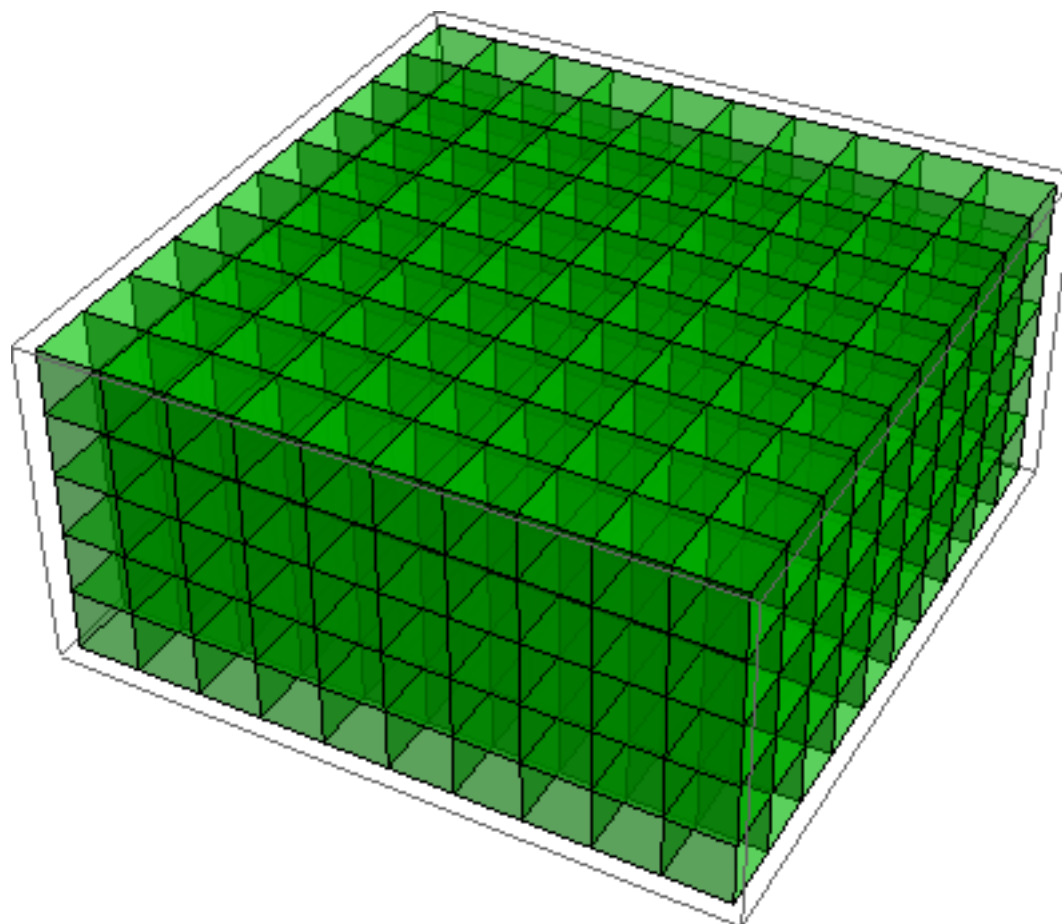
$$\mathbf{q} = -\frac{k}{\mu}(\nabla p - \rho \mathbf{g})$$

$$\nabla p = \frac{\partial p}{\partial x} + \frac{\partial p}{\partial y} + \frac{\partial p}{\partial z}$$

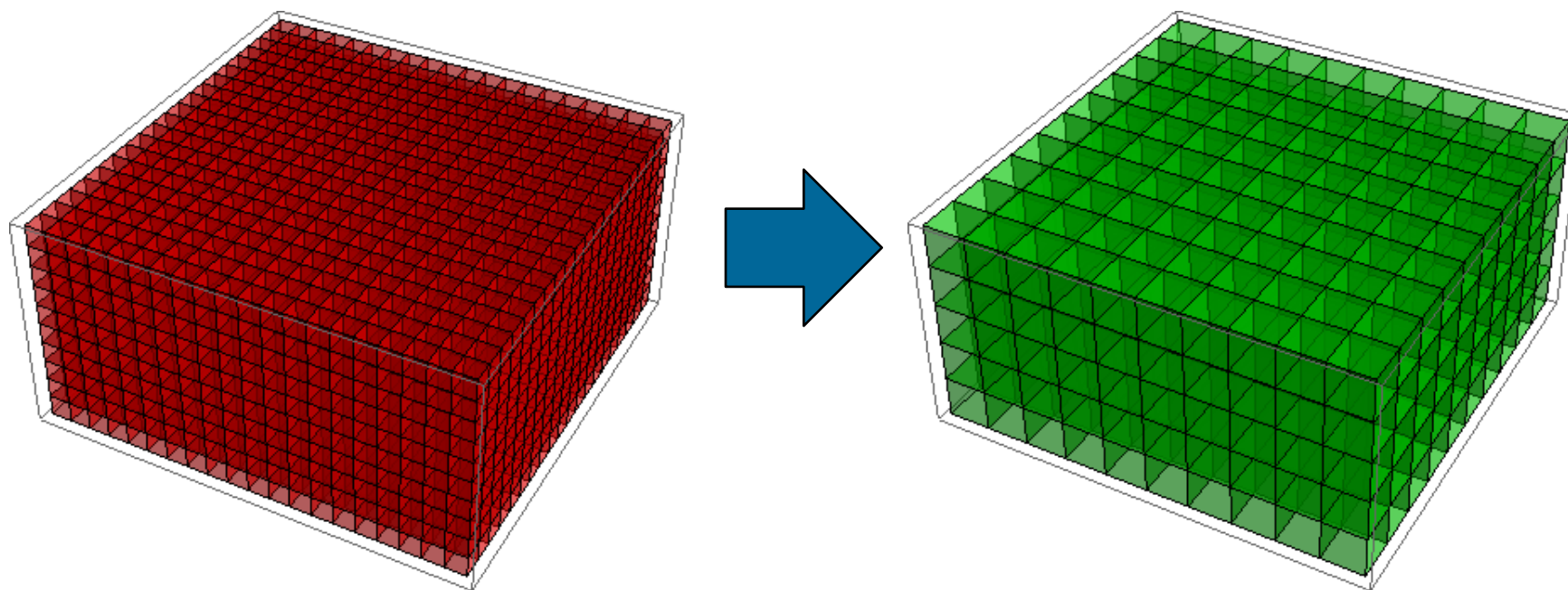
## Finite-difference approximation

$$\frac{\partial p}{\partial x} \longrightarrow \frac{\Delta p}{\Delta x} = \frac{p_{i+1} - p_i}{x_{i+1} - x_i}$$

# Simulation grid

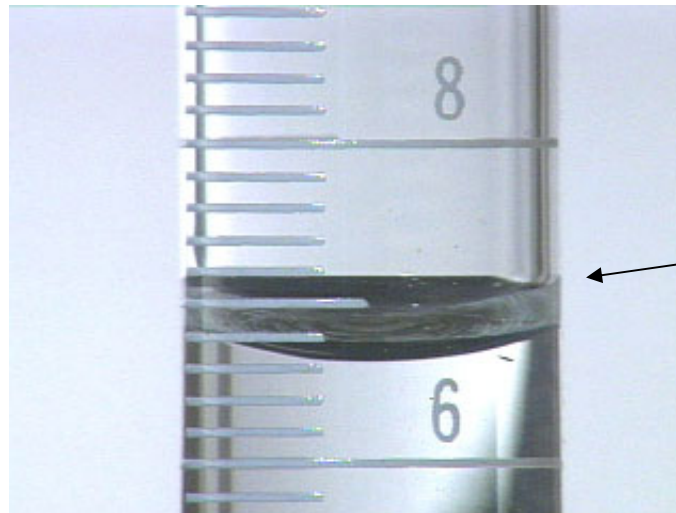


# Upscaling



## Two-phase immiscible flow terminology

- **Drainage** – two-phase flow with  $\text{CO}_2$  displacing brine where the brine preferentially contacts (wets) the rock surfaces.
- **Imbibition** – two-phase flow with brine displacing  $\text{CO}_2$  where the brine preferentially contacts the rock surfaces.
- **Relative permeability** – in two-phase flow, the reduction in effective permeability due to the presence of the other fluid.



Water wetting glass



## Multiphase flow equations

$$\mathbf{q}_w = -\frac{k k_{rw}}{\mu_w} (\nabla p_w - \rho_w \mathbf{g})$$

$$\mathbf{q}_{nw} = -\frac{k k_{rnw}}{\mu_{nw}} (\nabla p_{nw} - \rho_{nw} \mathbf{g})$$

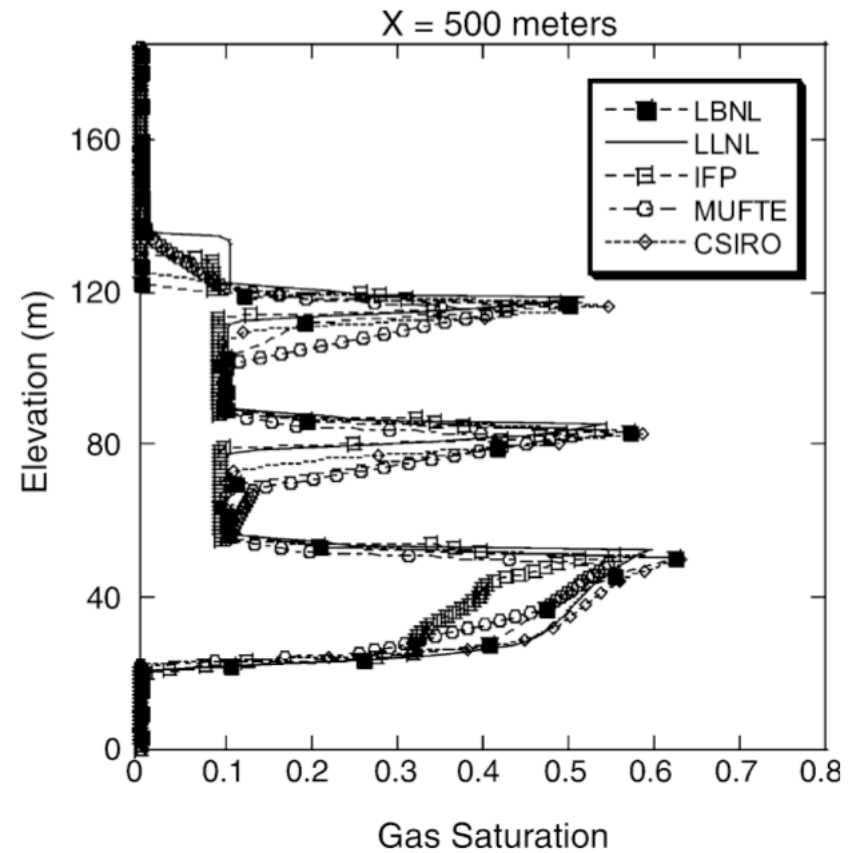
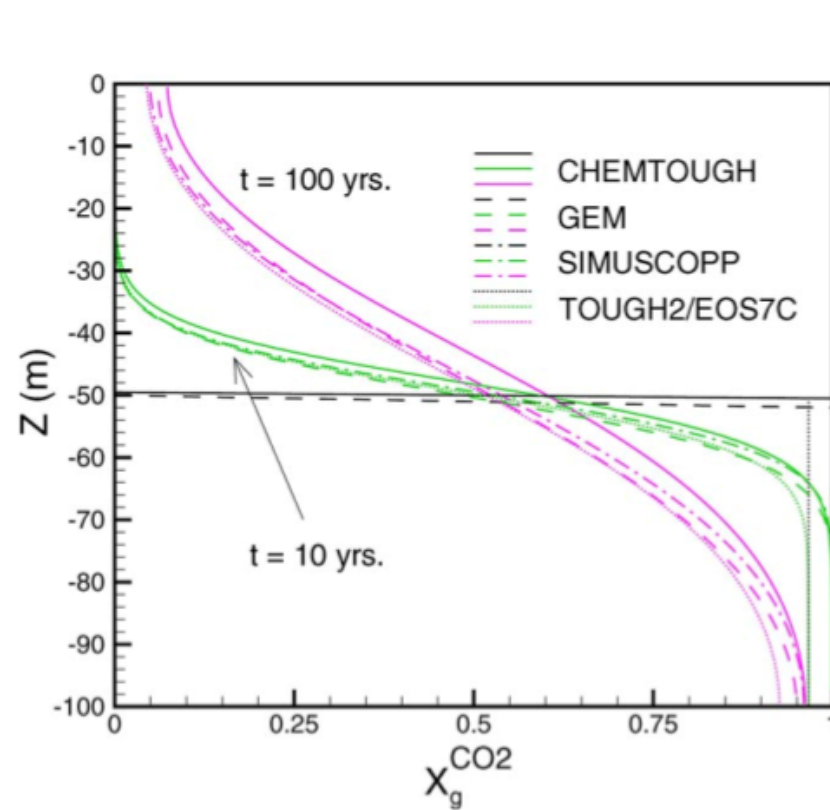
$$\phi \frac{\partial S_w}{\partial t} + \nabla \mathbf{q}_w = 0$$

$$S_w + S_{nw} = 1$$

$$\phi \frac{\partial S_{nw}}{\partial t} + \nabla \mathbf{q}_{nw} = 0$$

$$p_c = p_{nw} - p_w$$

# Code comparison

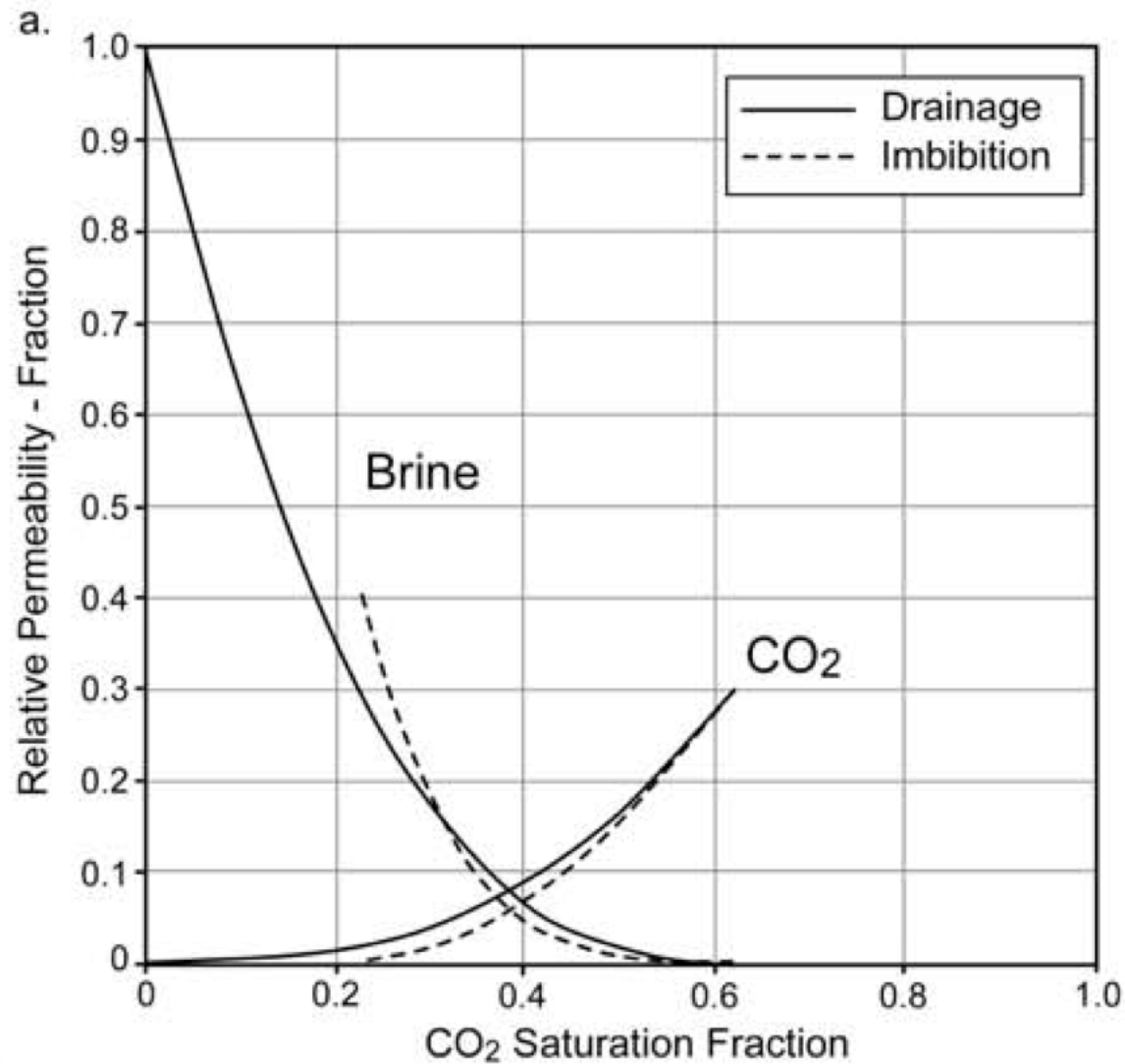


Pruess et al. 2004 Energy

# Models used in Class et al. 2009 comparison

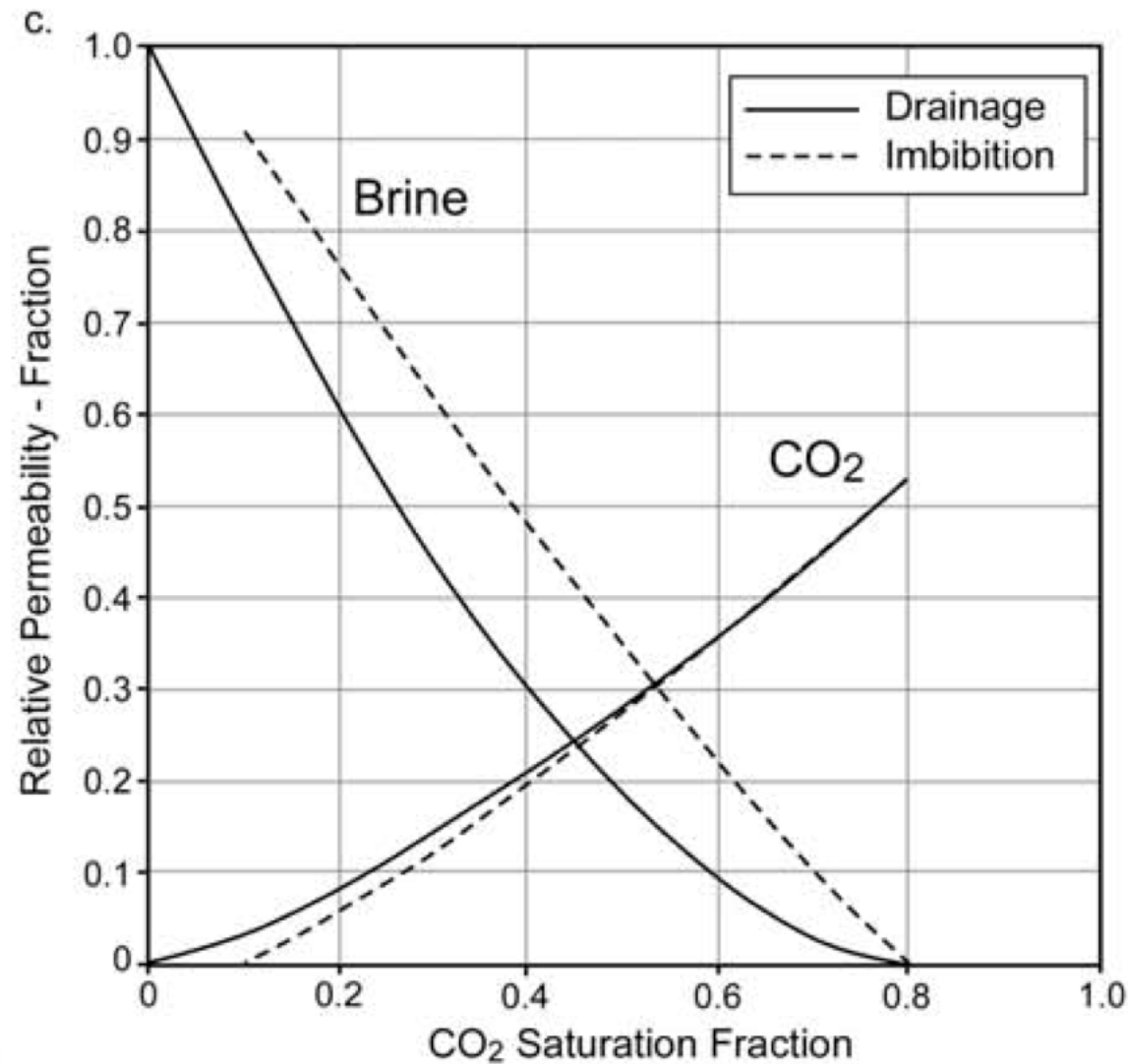
Name of code/model	Applying institution	Participation in problem(s)	Discretisation	
			In space	In time
COORES	IFP	1.1, 1.2, 2.1, 2.2, 3.1	FV	Implicit
DuMux	Uni. Stuttgart	1.1	BOX	Implicit
ECLIPSE	Schlumberger, Heriot-Watt Uni.	1.1, 1.2, 2.1, 2.2, 3.1, 3.2	IFDM	Implicit
FEHM	LANL	1.1, 1.2	CVFE	Implicit
GEM	Heriot-Watt Uni.	3.1, 3.2	IFDM	Implicit
GPRS	Stanford Uni.	3.1, 3.2	FV	Implicit
IPARS-CO2	CSM Uni. Texas	1.1, 2.1, 2.2, 3.1	Mix. FEM	Impl. pressure expl. conc.
MoReS	Shell	3.1, 3.2	IFDM	Implicit
MUFTE	Uni. Stuttgart	1.1, 1.2, 2.1, 2.2, 3.1	BOX	Implicit
ROCKFLOW	BGR	1.1, 1.2	FE	Implicit
RTAFF2	BRGM	1.2	FEM	Implicit
ELSA	Uni. Bergen/Princeton	1.1		
TOUGH2	CSIRO, BRGM, RWTH Aachen	1.1, 2.1, 2.2, 3.1	IFDM	Implicit
VESA	Princeton Uni.	1.1, 3.1, 3.2	FD, vertic. averaged	Impl. pressure expl. interface

# Relative permeability



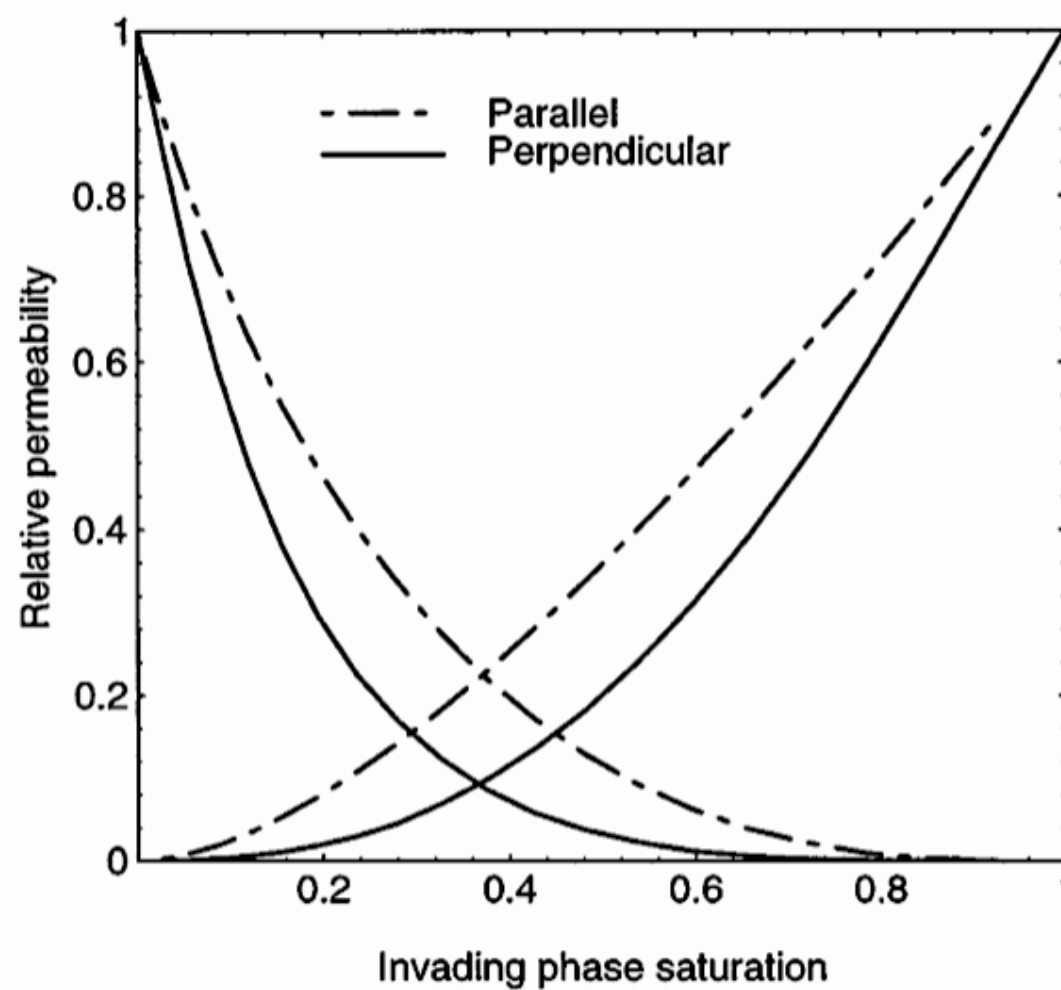
Bennion and Bachu (2006)  
SPE 102138

# Relative permeability



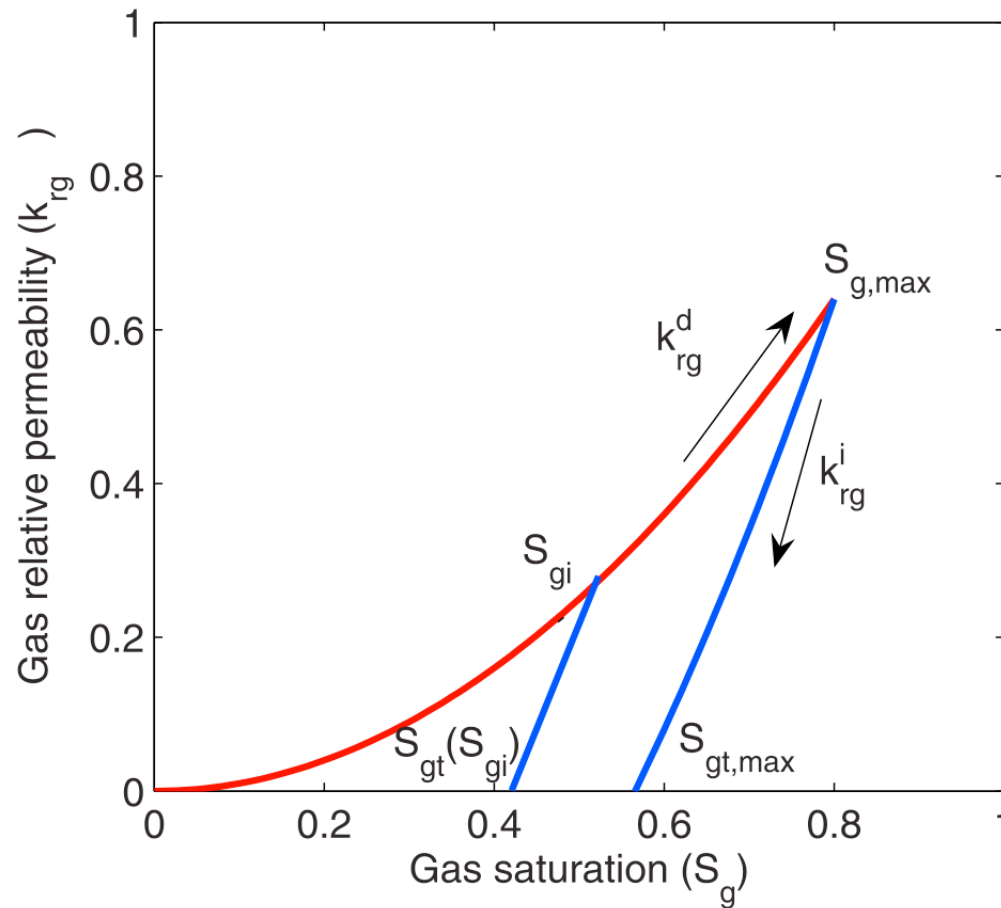
Bennion and Bachu (2006)  
SPE 102138

## Relative permeability can depend on direction



Paterson et al. (1998)  
SPE 50938

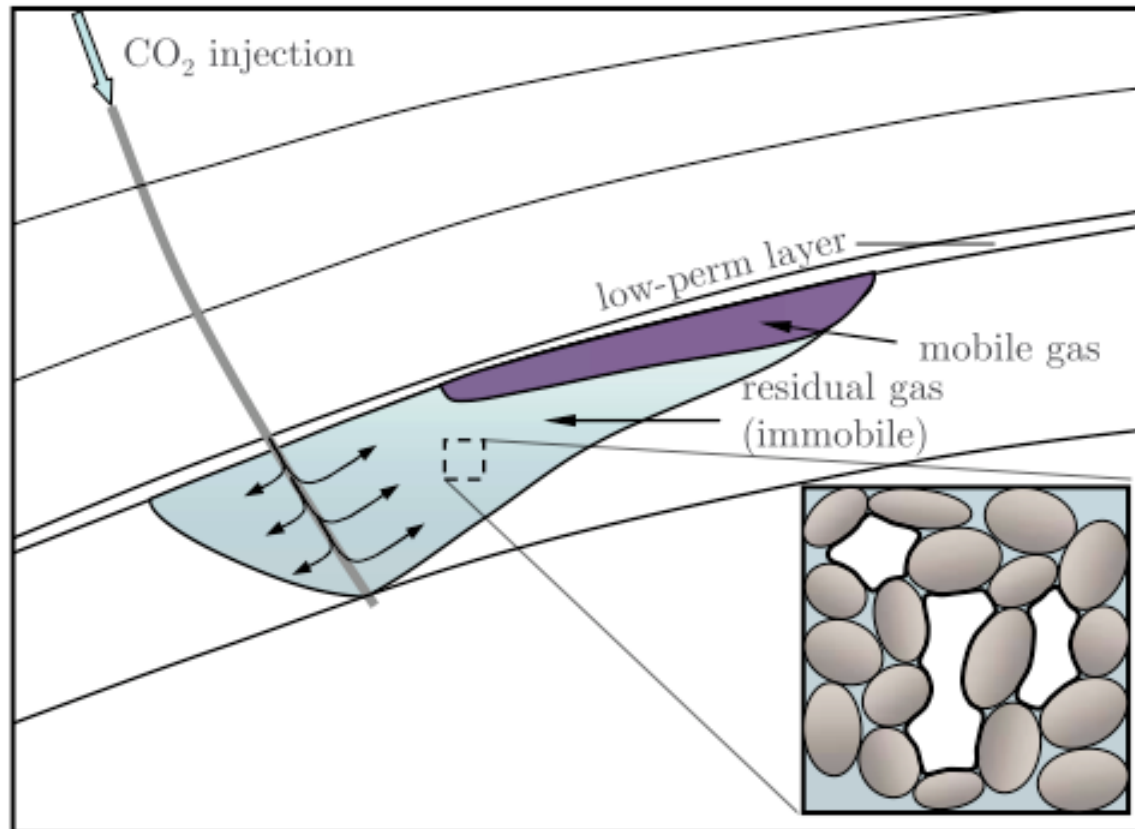
# Relative permeability hysteresis



Juanes et al. (2006) WRR



# Residual capillary trapping



**Figure 1.** Schematic of the trail of residual CO<sub>2</sub> that is left behind because of snap-off as the plume migrates upward during the postinjection period.

Juanes et al. (2006) WRR



# Permeability and porosity

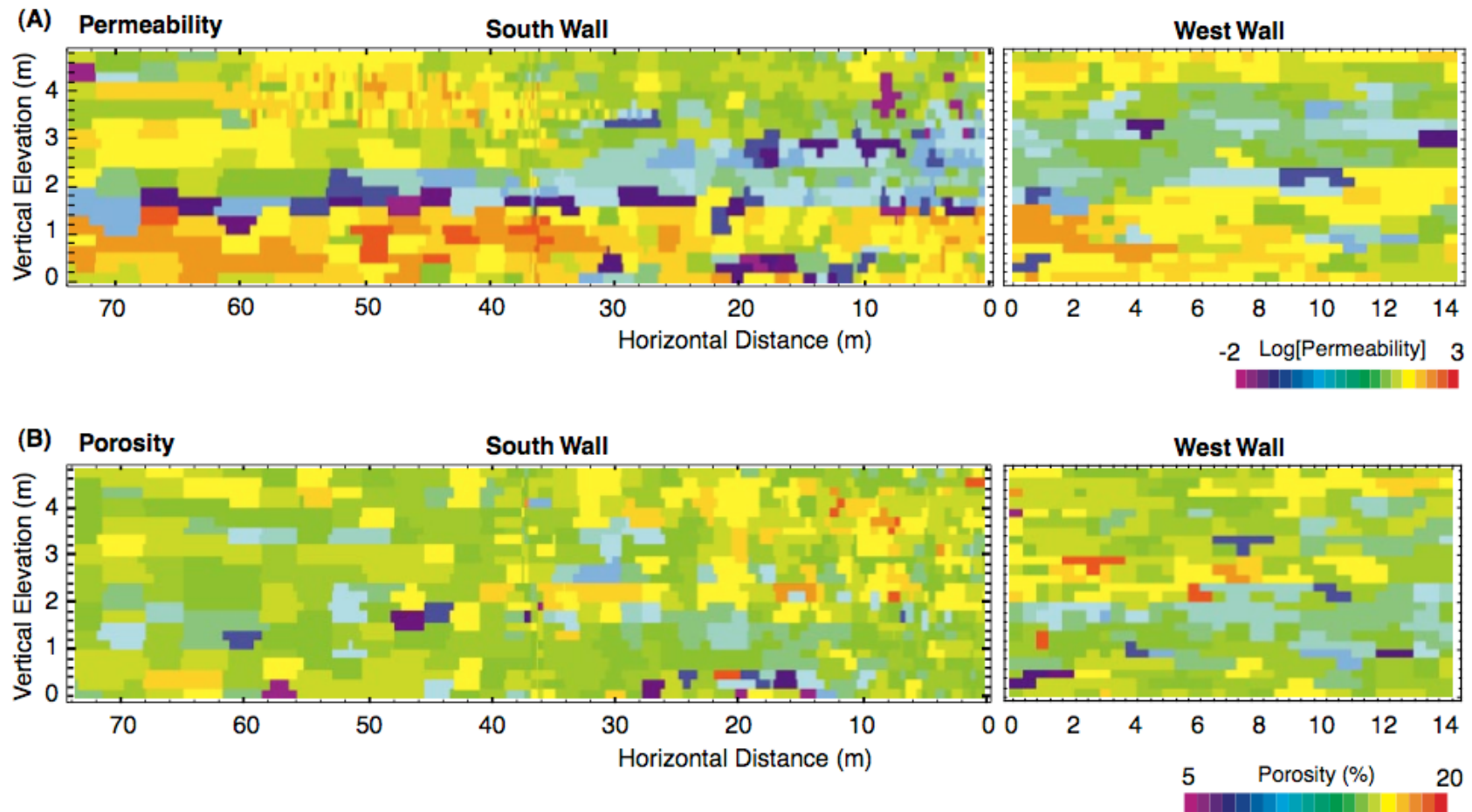
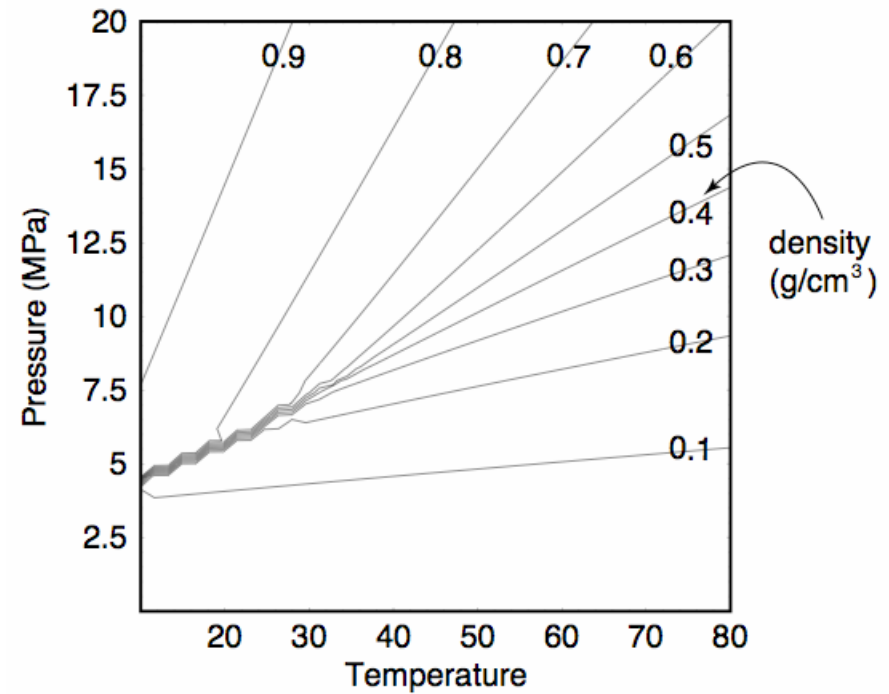
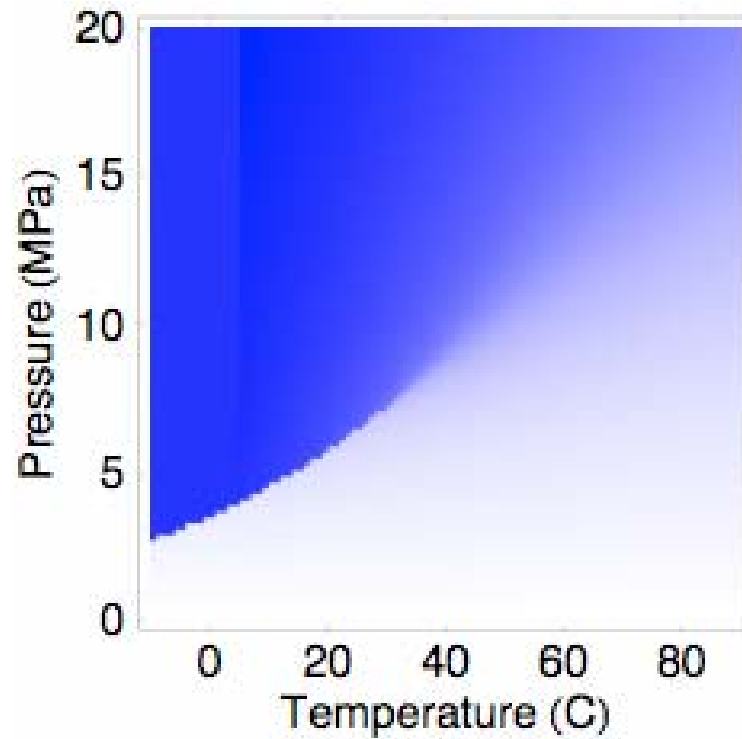


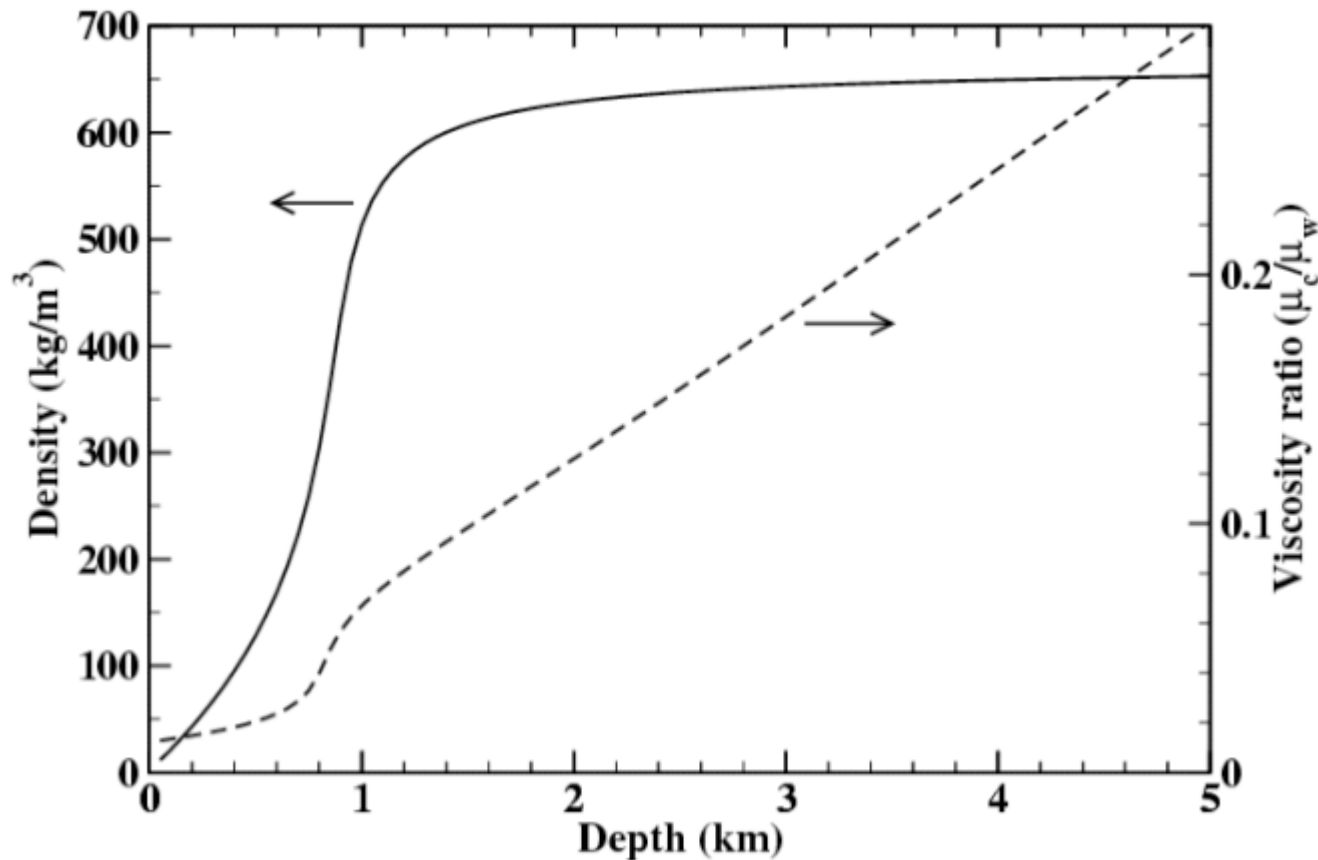
Figure 4—(A) Permeability and (B) porosity distribution within the study outcrop. Note the horizontal scales for the south and west walls are different.

Liu et al. 1996 AAPG

# Carbon dioxide density



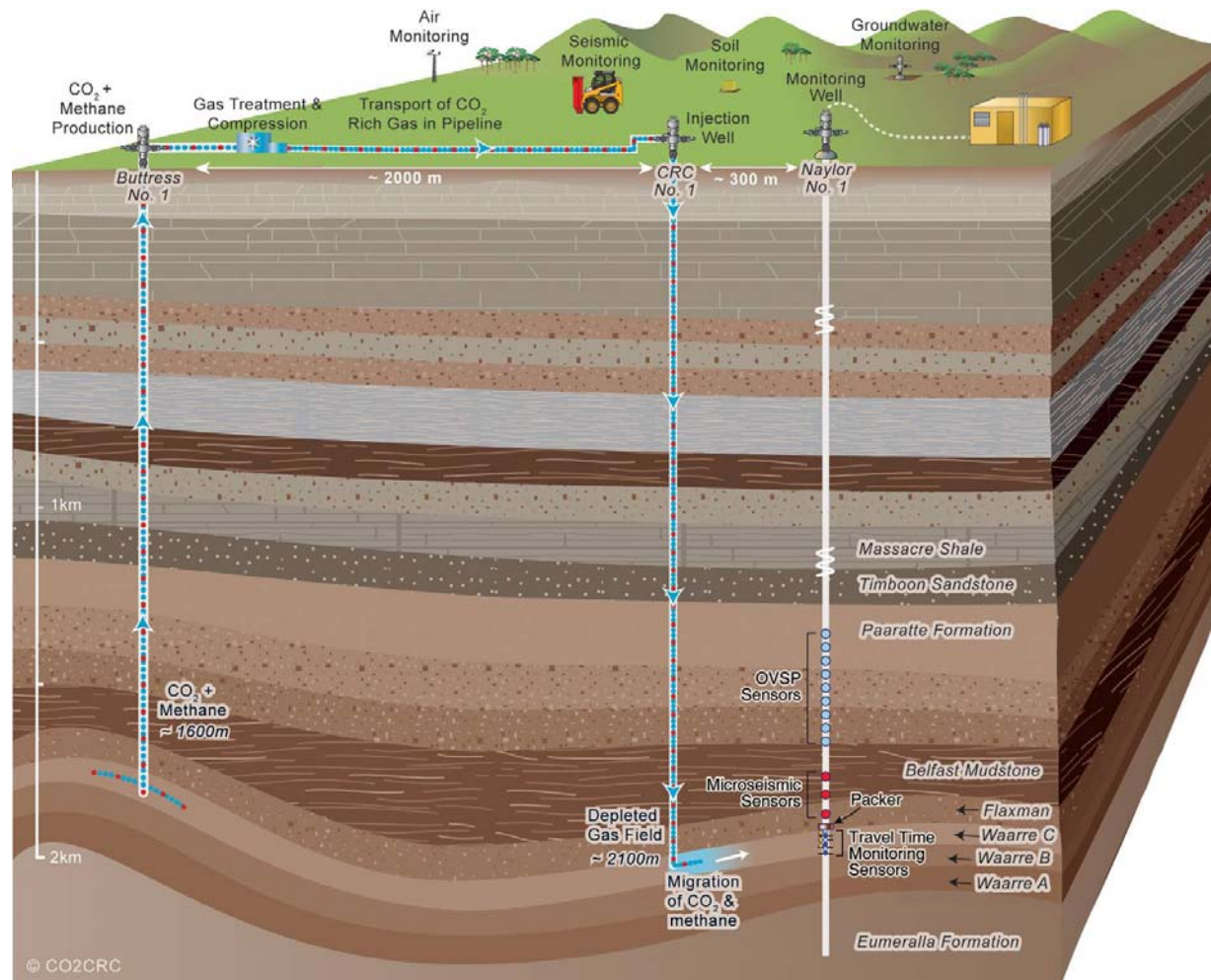
# Viscosity



**Figure 2: CO<sub>2</sub> density and viscosity at subsurface conditions, surface temp. 15 C, 30 C/km and 10 MPa/km.**

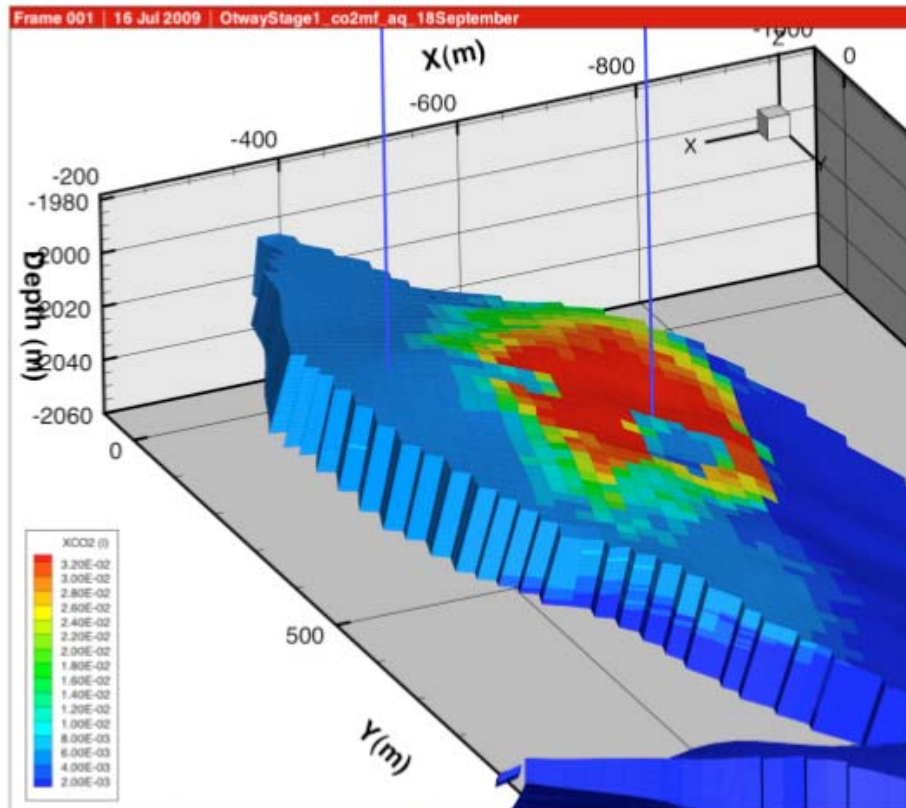
Ennis-King & Paterson 2002 SPE 77809

# CO2CRC Otway Project

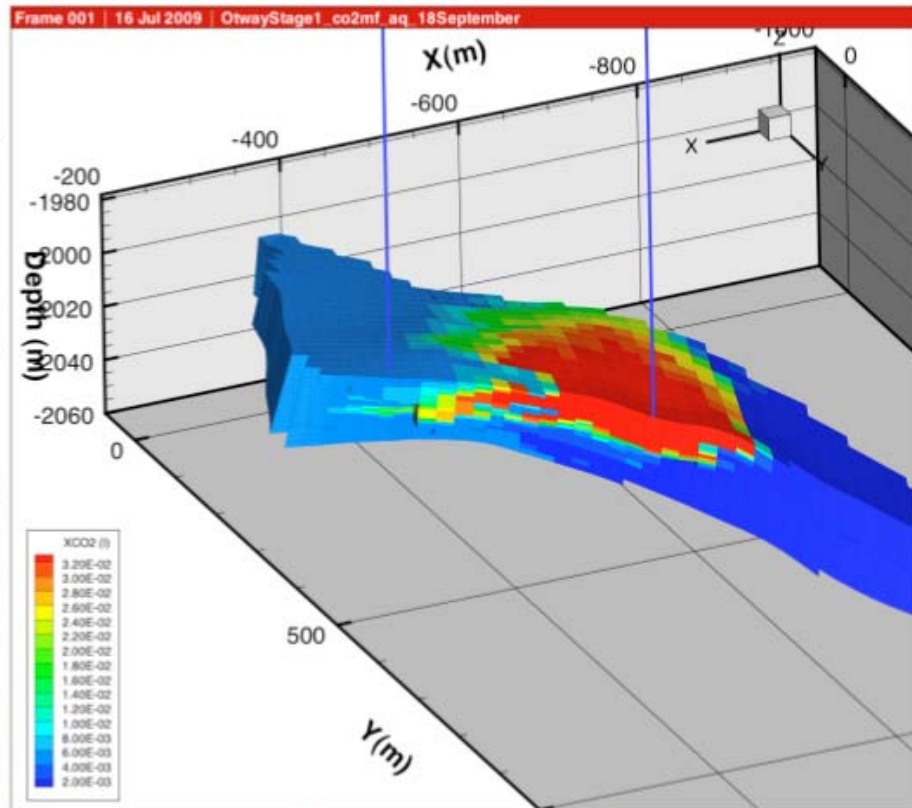




# CO2CRC Otway project: CO<sub>2</sub> mass fraction



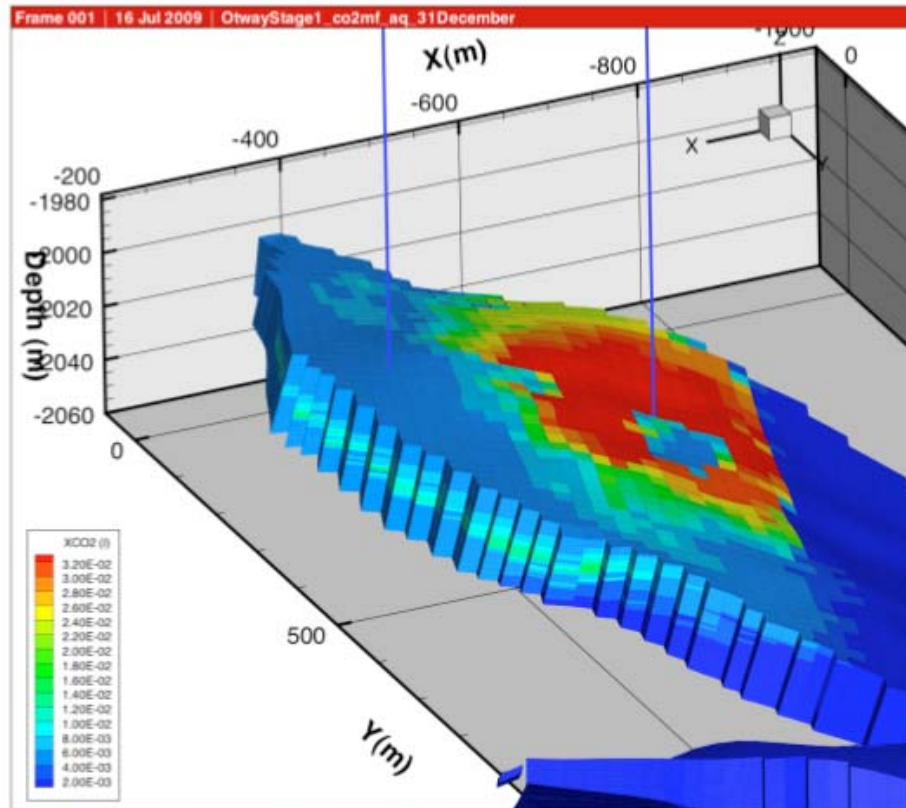
(a) Carbon dioxide mass fraction 18 Sept: no cutaway.



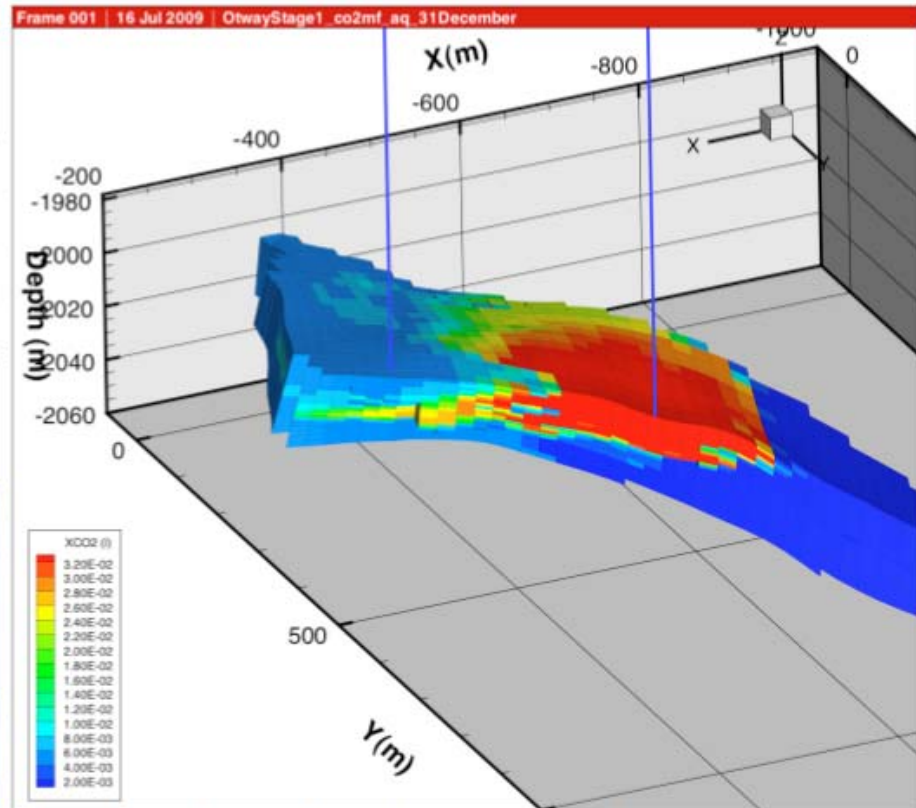
(b) Carbon dioxide mass fraction 18 Sept: cutaway.

J. Ennis-King

# CO2CRC Otway project: CO<sub>2</sub> mass fraction



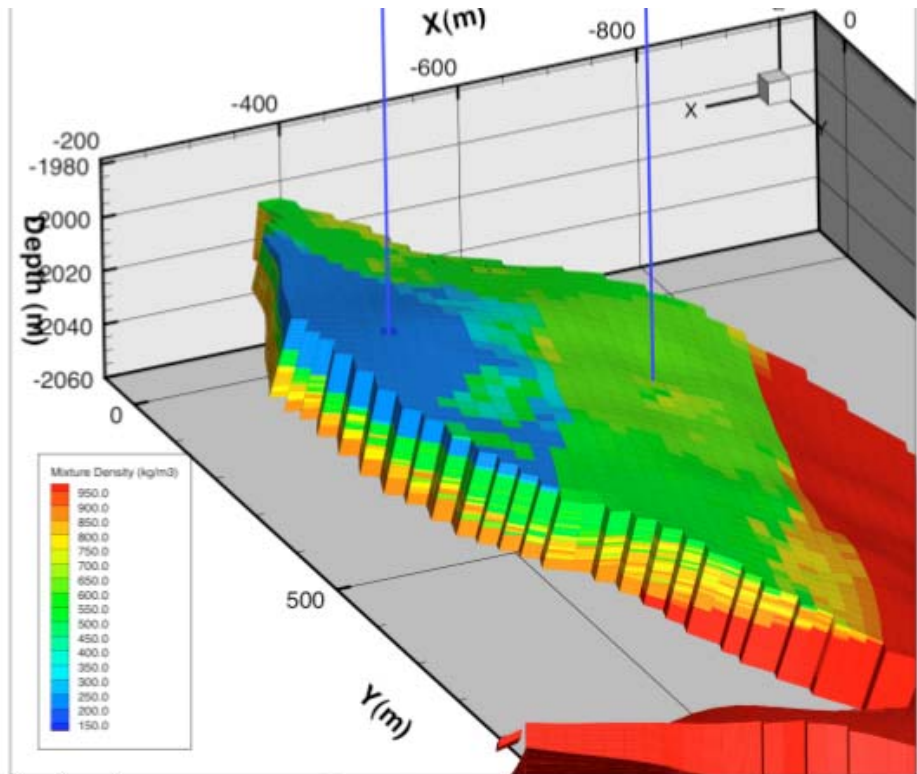
(a) Carbon dioxide mass fraction 31 Dec: no cutaway.



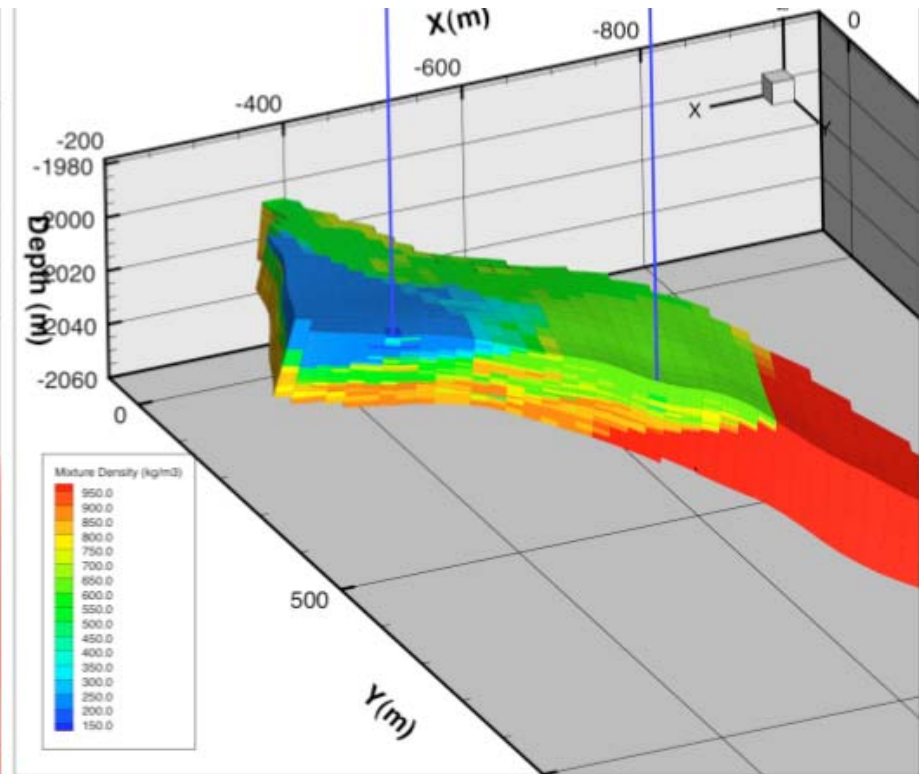
(b) Carbon dioxide mass fraction 31 Dec: cutaway.

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# CO2CRC Otway project: total fluid density



(a) Average fluid density: no cut-away.

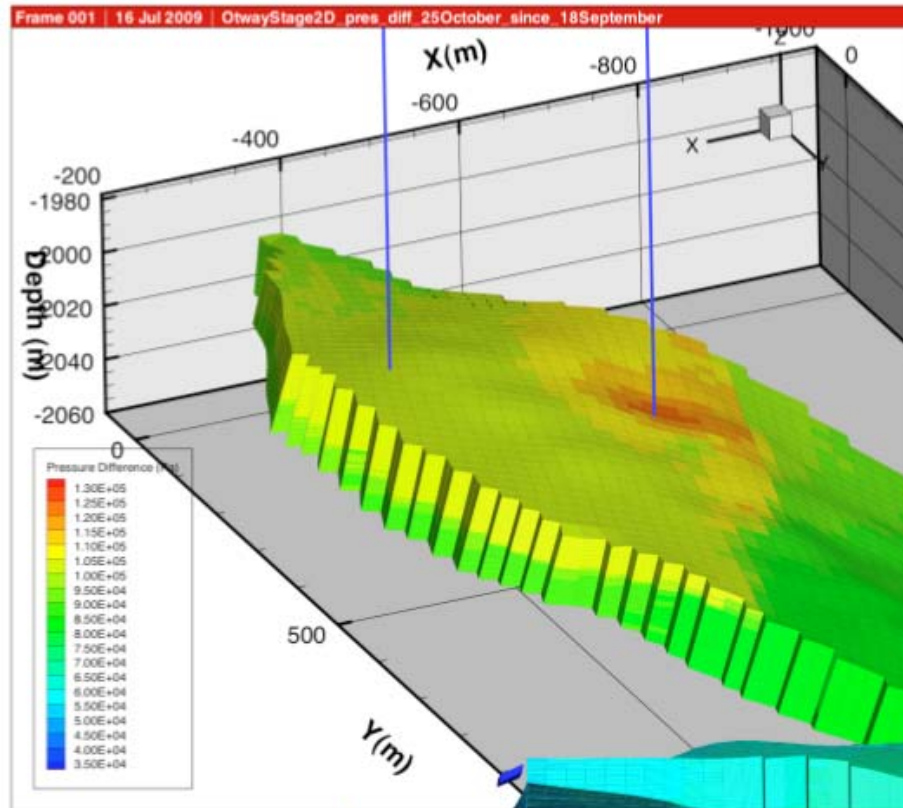


(b) Average fluid density: Cutaway.

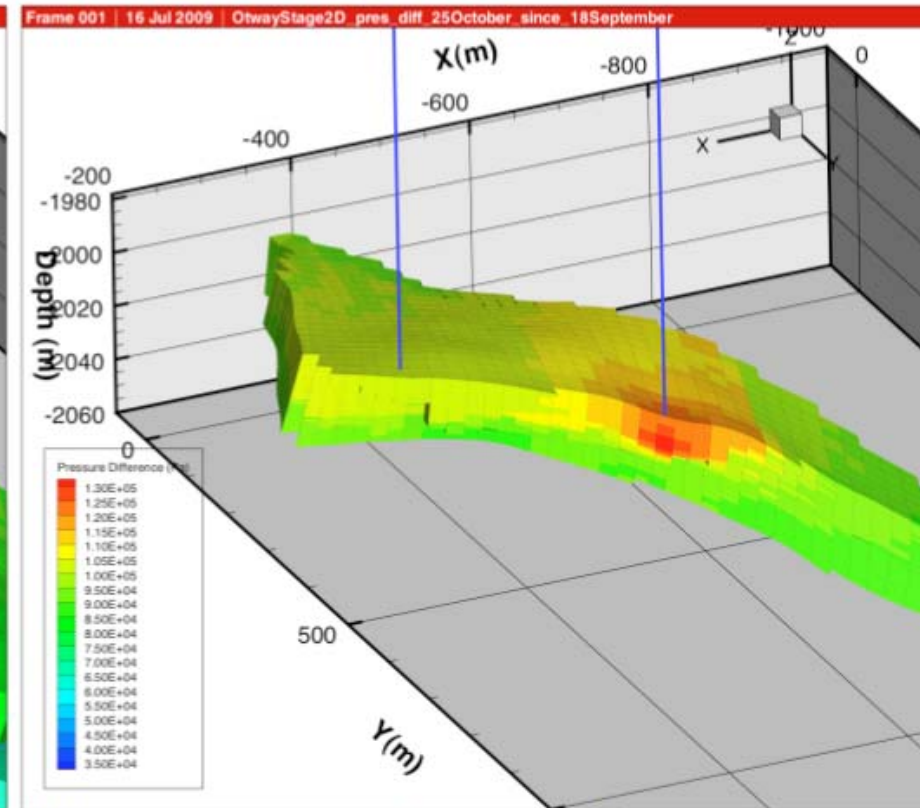
J. Ennis-King



# CO2CRC Otway project: pressure difference



(a) Pressure difference between 18 Sept and 25 Oct: no cutaway.

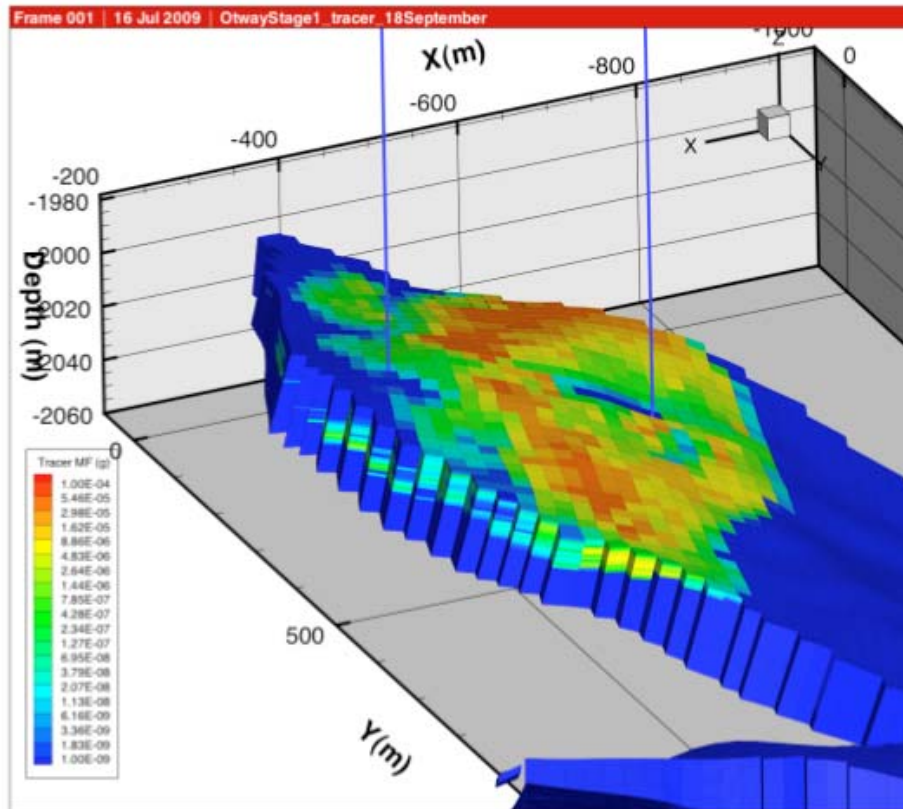


(b) Pressure difference between 18 Sept and 25 Oct: cutaway.

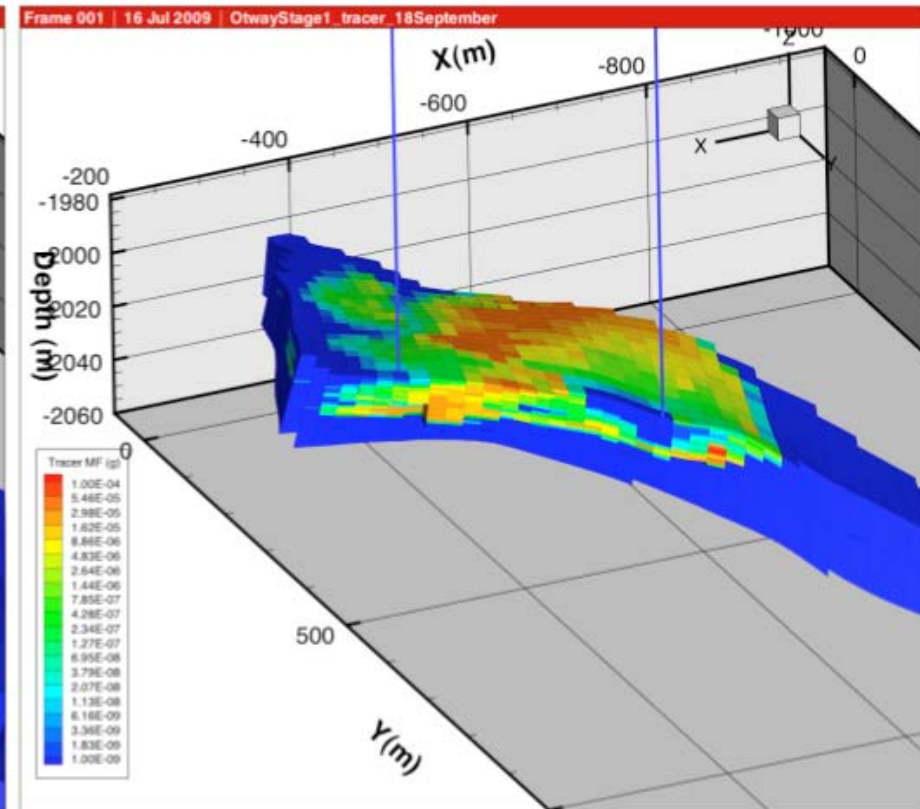
J. Ennis-King



# CO2CRC Otway project: tracers



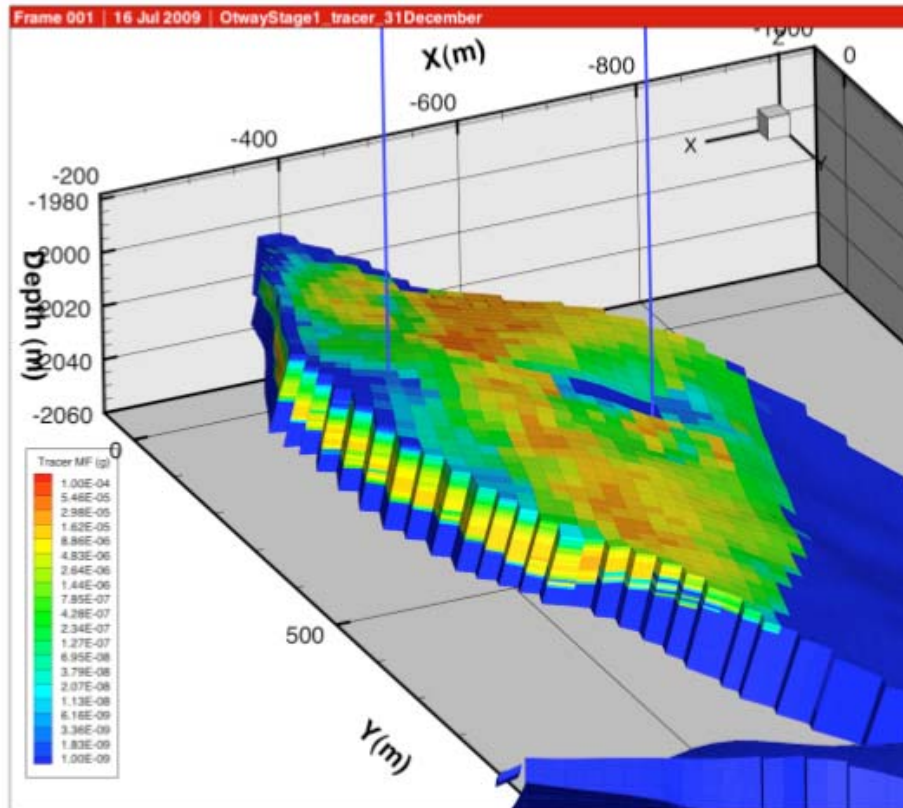
(a) Tracers 18 Sept: no cutaway.



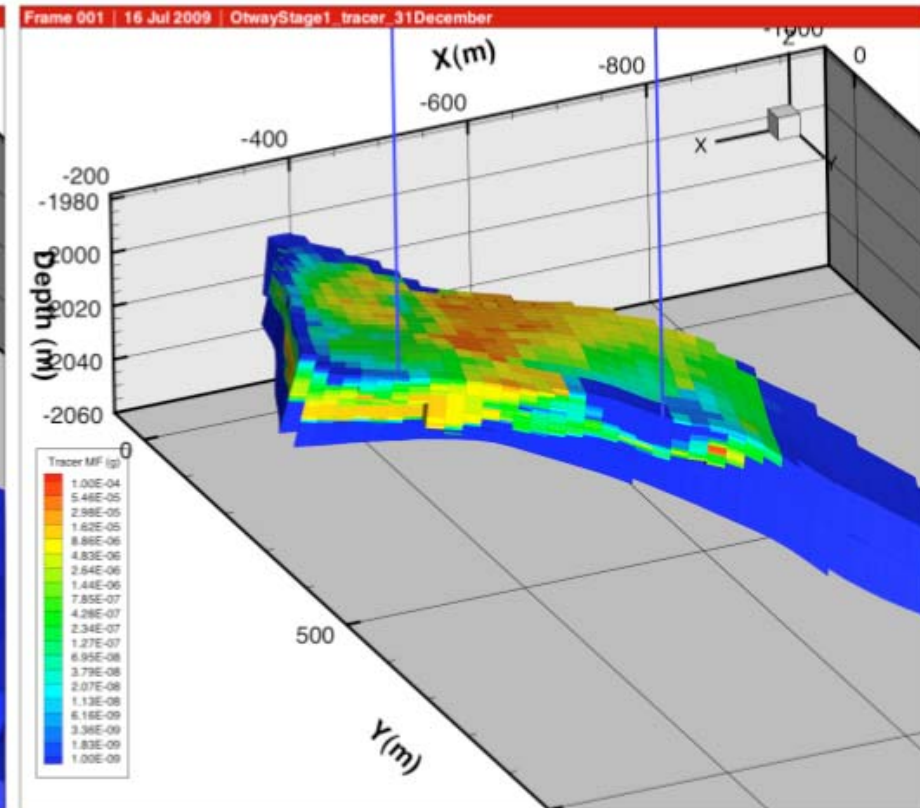
(b) Tracers 18 Sept: cutaway.

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# CO2CRC Otway project: tracers



(a) Tracers 31 Dec: no cutaway.



(b) Tracers 31 Dec: cutaway.

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# Simulation input and output

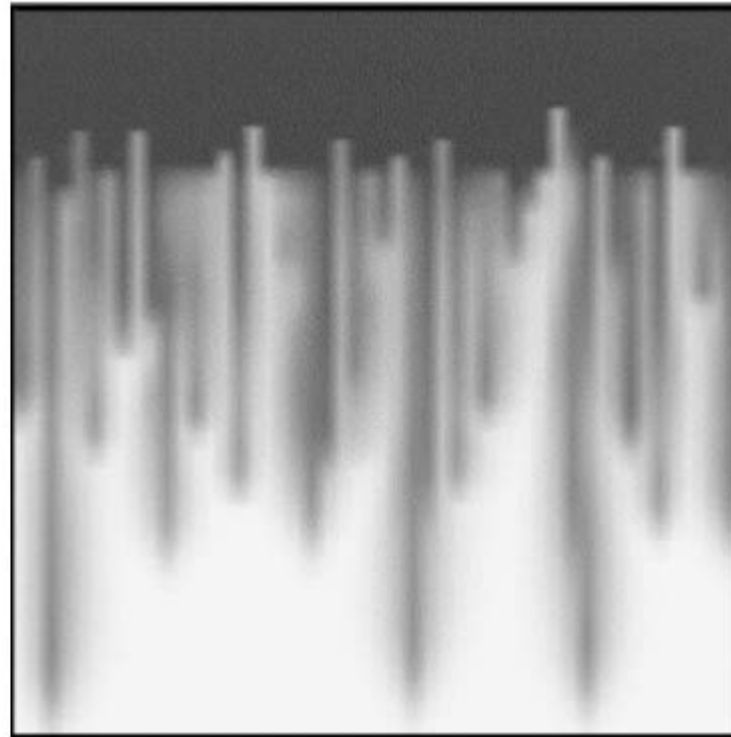
- **Input:**

- Static model (permeability, porosity, fault boundaries...)
- Dynamic properties (relative permeability, capillary pressure)
- Initial conditions (pressure, temperature,...)
- Boundary conditions (aquifer drive, ...)
- Flow rates at wells

- **Output:**

- Maps of pressure, fluid saturation, ....
- Tracer concentration (if implemented)
- Dissolved components (if implemented)
- Chemical reaction products (if implemented)
- Stress and strain (if implemented in a geomechanical model)

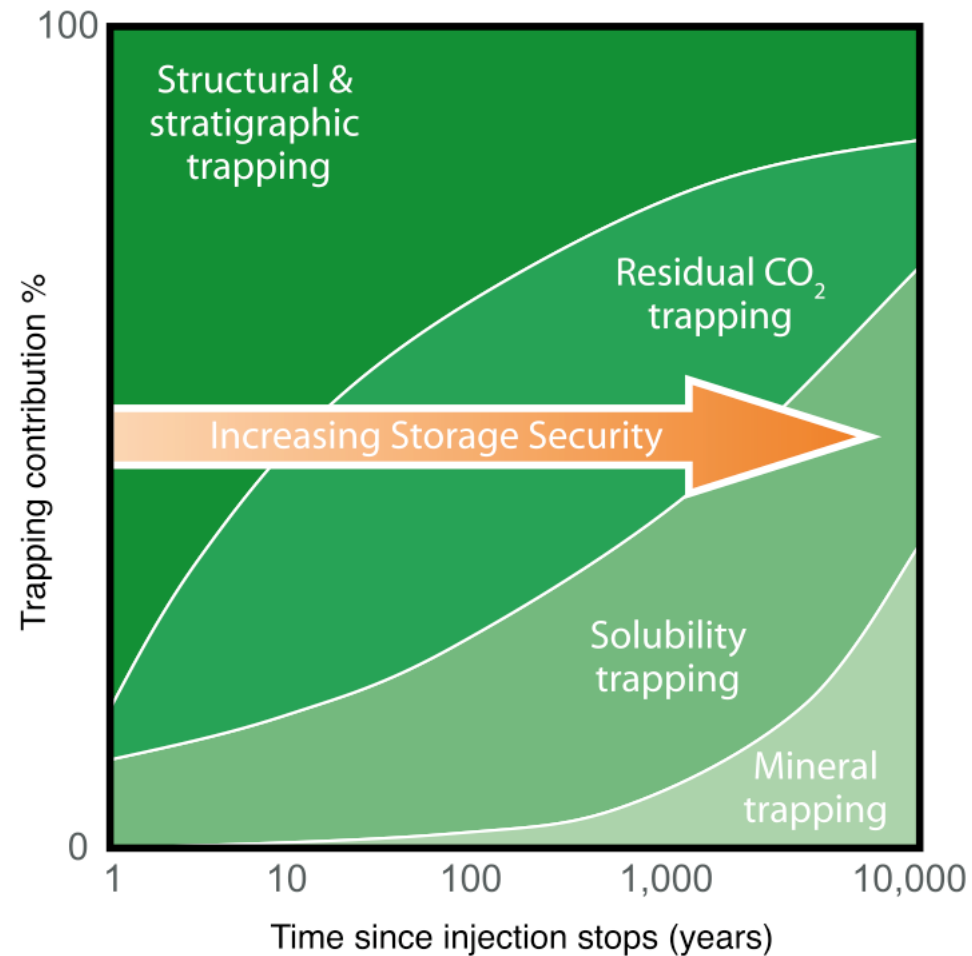
## Dissolution and convection



**Fig. 5—Distribution of dissolved CO<sub>2</sub> for  $k_v/k_h=0.1$  after 2,100 years. The width of simulation cell is 500 m. The full width is shown in this figure, but only the top 80 m vertically.**

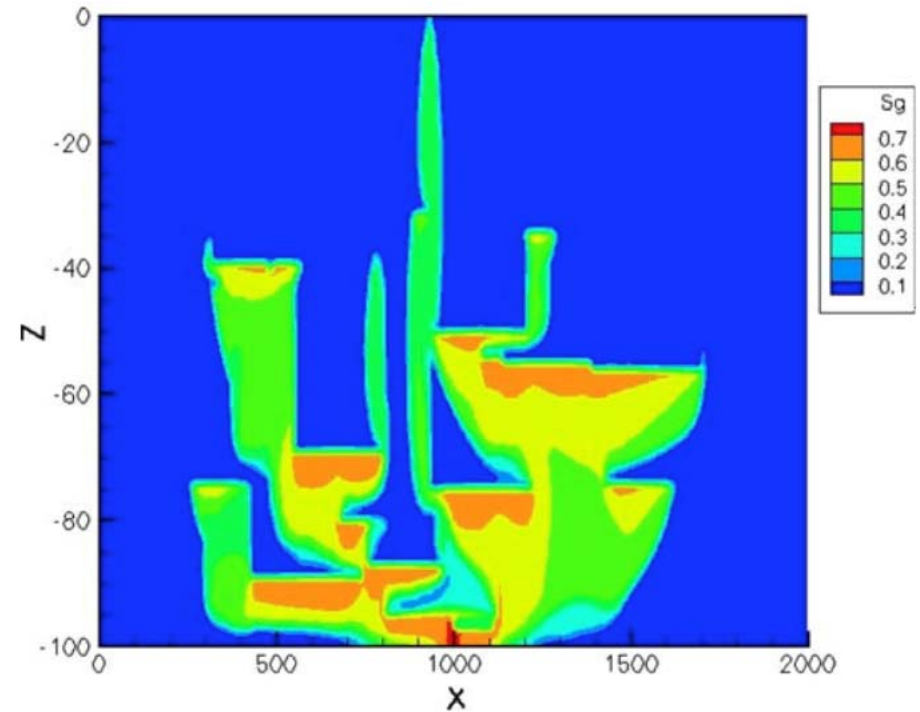
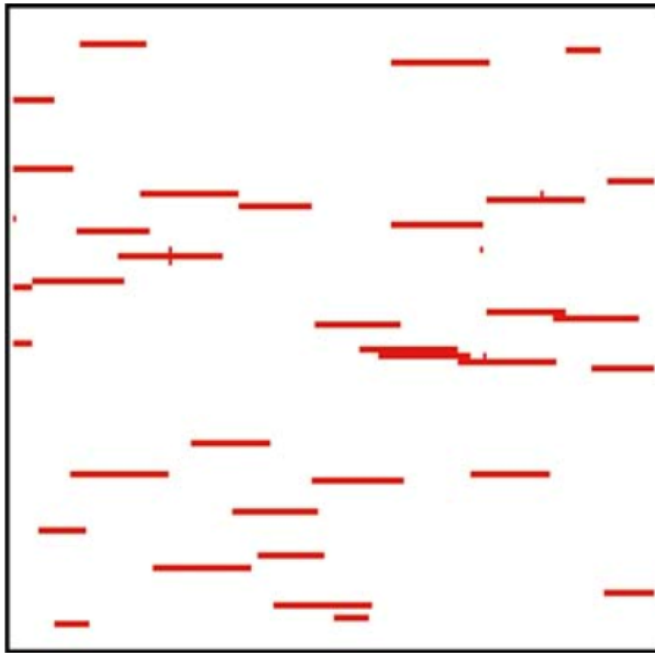
Ennis-King & Paterson 2005 SPE J

# Trapping mechanisms over time





# Upscaling vertical permeability



Green & Ennis-King, TiPM, 2009

# Conclusions

- **Modelling is a useful tool in the design of carbon dioxide storage projects.**
- **Modelling depends on the quality of the data and the skill of the user (old saying: garbage in, garbage out).**
- **In the right hands with correct questions it can provide powerful answers.**

# CO2CRC Participants



NZ Resource Consortium



SOLID ENERGY  
Coals of New Zealand



Government of Western Australia  
Department of Mines and Petroleum



Supporting participants: Department of Resources, Energy and Tourism | CANSYD | Meiji University  
Process Group | University of Queensland | Newcastle University | U.S. Department of Energy | URS



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