COMPUTER MODELLING GROUP LTD.

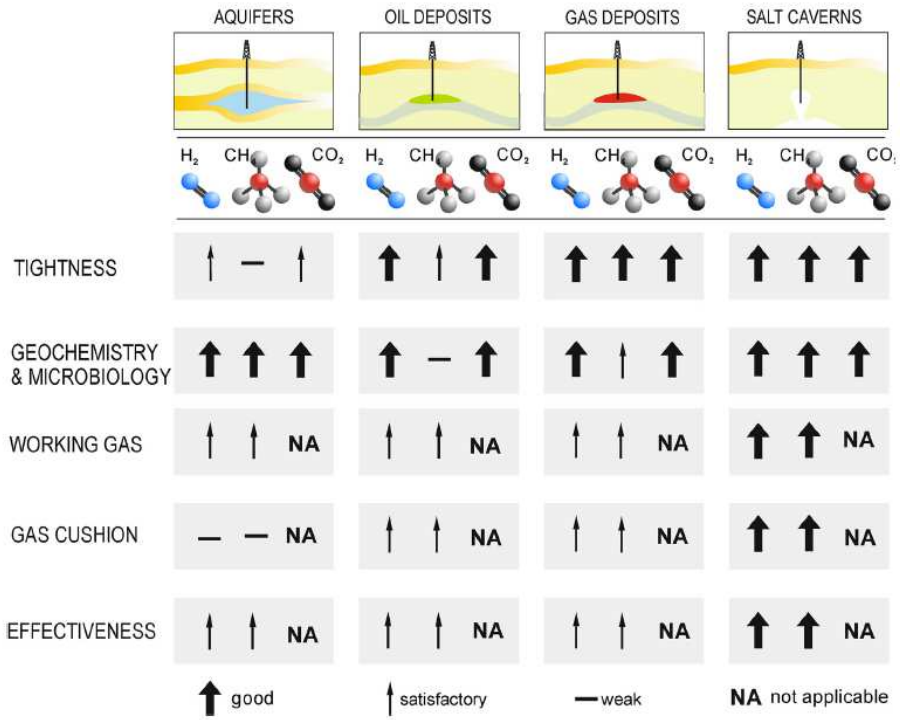
Underground Hydrogen Storage Simulation Using CMG

Faraj Zarei

Energi Simulation Summit Oct 1st, 2021

#FutureOfSimulation

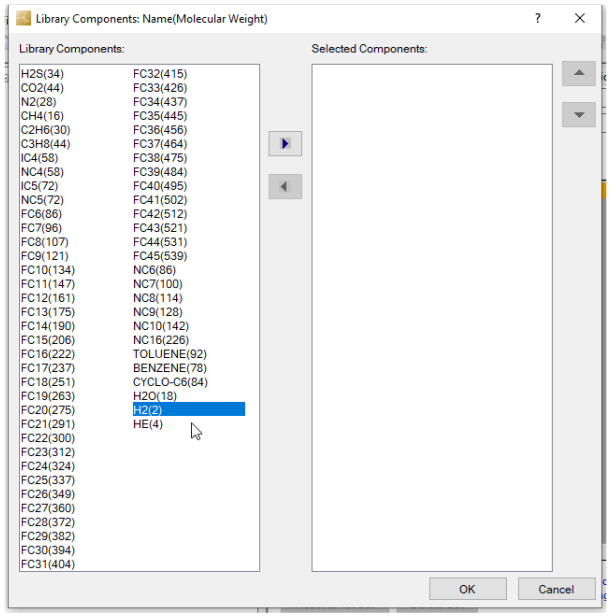
Major Differences Between H_2, CO_2 and CH_4



Assessment of the suitability of individual types of geological structures for underground storage of hydrogen, methane, and carbon dioxide. (from Tarkowski, R. et al. (2021))

WinProp

WinProp is CMG's compositional equation-of-state based software for phase behavior and properties calculation. Its capabilities include:



- Fluid characterization

PR(1978)	Peng-Robinson equation of state with 1978 expression for constant "a".
PR(1976)	Peng-Robinson equation of state with 1976 expression for constant "a". This is the original equation of state.
SRK(G&D)	Soave-Redlich-Kwong equation of state with the constant "a" proposed by Grabowski and Daubert[1].
SRK	Original Soave-Redlich-Kwong equation of state.

- Matching the fluids' model with laboratory data
- Multiple-contact miscibility calculations
- Solubility of light gases in water or brine
- Generating fluid model for IMEX, GEM, and STARS

GEM

GEM is an equation-of-state (EoS) compositional simulator which can simulate most of the important mechanisms involved in the underground hydrogen storage processes.

Relative permeability hysteresis

- Gas phase trapping

Gas solubility in aqueous phase

- Henry's law based
- K-Value based (future GEM releases)

Diffusion

H_2O Vaporization

- During gas injection

Reactions

- Chemical equilibrium
- Arrhenius
- Mineral dissolution and precipitation

Geomechanics

- Change in porosity and permeability
- Cap rock integrity

Thermal Option

- Reservoir temperature could change with time

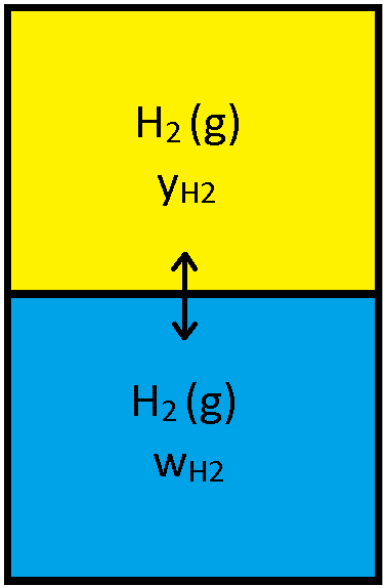
Hysteresis

Relative permeability of gas phase (usually non-wetting) could be a function of saturation histories.

- Gas injection into the reservoir results in an increase in the gas saturation.
- The flow calculations of the gas phase initially follows the input liquid-gas relative permeability drainage curve.
- At the production stage, water invades the gas zone.
- Hysteresis of the gas relative permeability takes place.
- This would result in trapping the gas in the porous media.

Gas Solubility in Aqueous Phase

- Ideal (simplified Henry's law)
- Henry (general Henry's law)
- K-Value based (future GEM releases)



The dissolution rate is very fast. The gas and aqueous phases are assumed to be in thermodynamic equilibrium, and the equation for thermodynamic equilibrium is the equality of water and gas phase fugacities. The dissolution process is reversible.

$$f_{ig} = f_{iw}$$

f_{ig} fugacity of component i in the gas phase → from EoS

f_{iw} fugacity of component i in the aqueous phase → from Henry's Law

Gas Solubility in Aqueous Phase

Gas solubility from general Henry's law: $f_{H2\ (gas)} = f_{H2\ (aqueous)} = W_{H2} * \text{Henry-Const}_{H2}$

W_{H2} : H_2 mole fraction in the aqueous phase

Henry constant for H_2 is function of pressure at the moment.

- HENRYC reference Henry's constant [kPa / PSI]
- VINFINITY partial molar volume in water at infinite dilution [litre/mol]
- REFPH reference pressure for Henry's constant [kPa / PSI]

} required inputs

Henry's constant for CO_2, CH_4, H_2S, N_2 can be a function of pressure, temperature and salinity.

Detailed information can be found in the **Solubility Data (Optional)** page in the **GEM User Guide**.

Aqueous Phase Density & Viscosity

Aqueous Phase Density will be calculated considering the dissolved gas or ions in solution:

- Linear: linear function of pressure
- Rowe-Chou

Aqueous Phase Viscosity:

- VISW: Constant
- KESTIN: Viscosity as a function of pressure, temperature and salinity
- POLYMER: Uses a mixing rule for the components present in the aqueous phase. Viscosity as a function of polymer concentration, temperature, pressure, salinity and shear effects.

Gas Phase Properties:

- Gas density: Peng-Robinson EOS
- Gas viscosity: Jossi, Stiel and Thodos correlation

H_2O Vaporization

Water vaporization can be modeled in GEM.

- This could happen while injecting gas into the reservoir.
- Having gaseous H_2O around the injector would affect the well injectivity.

$$g_{n_c} = f_{\mathrm{H_2O},\,g} - f_{\mathrm{H_2O},w} = 0$$

Detailed information about the H_2O fugacity calculations and how to activate this feature can be found in the following pages in the **GEM User Guide**:

- H2O Vaporization
- H2O Vaporization (Optional)

Reactions

Chemical reactions in GEM occur:

- Between components in the aqueous phase (chemical equilibrium or Arrhenius)
- Between minerals and aqueous components (mineral dissolution and precipitation)

The components in the aqueous phase include:

- Gaseous components that are soluble in the aqueous phase
- Components that exist only in the aqueous phase

Thermal Option

GEM supports use of thermal option where:

- The reservoir temperature cannot be assumed constant
- The injection takes place at a temperature different from the reservoir temperature

Solves energy equation → temperature distribution

- Convection (aqueous phase enthalpy: steam table look-up, oil and gas phase enthalpies: equation of state)
- Conduction (thermal conductivity of the rock and fluids)
- Heat loss to over-burden, under-burden, edge boundaries (analytical formulation)

Detailed information about formulations and how to activate the option can be found in the following pages in the **GEM User Guide**:

- Using the Thermal Option in GEM
- Thermal Option (Optional)
- Thermal Option in GEM (Appendix E)

Geomechanics

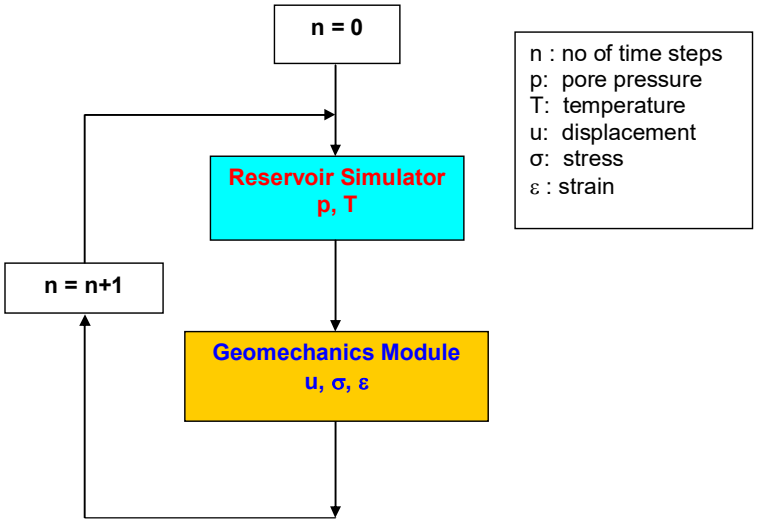
- Change in porosity and permeability
- Caprock integrity
  - During H_2 injection, if the pressure at the reservoir boundaries becomes sufficiently large, the seal provided by the caprock may be breached and flow across the breach/caprock may occur.
  - Caprock leakage capability in GEM allows modelling of the fluid lost to the reservoir surroundings when the caprock has been breached.

Coupling GEM & Geomechanics Module

One-way coupling:

Pressure and temperature are sent from the reservoir simulator to the geomechanics module.

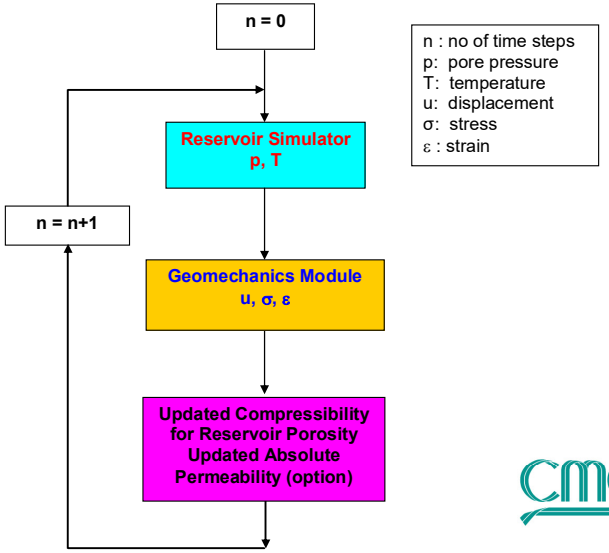
No information is sent from the geomechanics module to the simulator.



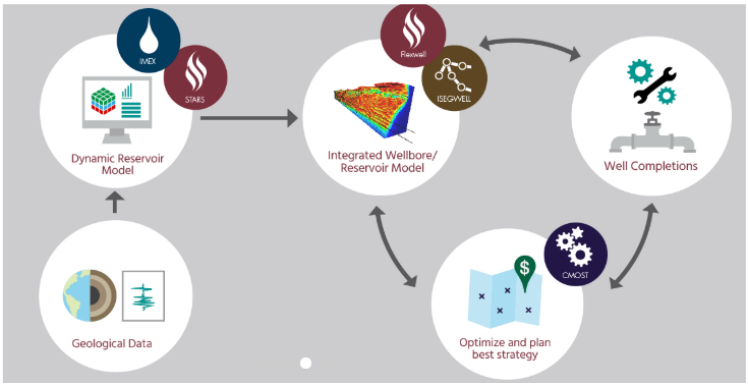
Two-way coupling:

Pressure and temperature are sent from the reservoir simulator to the geomechanics module.

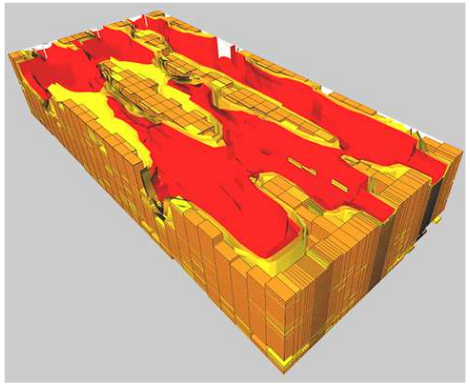
Stress and strain computed from the geomechanics module are used to determine new pore compressibility and absolute permeability.



STARS



- Industry leading three-phase multi-component thermal and steam additive simulator
- K-Value Based PVT
- Different gridding systems, naturally fractured and faulted reservoir systems
- Advanced well management options
- Stable adaptive implicit formulation, high performance, dynamic gridding
- Geomechanics, geochemistry



Source: cmgl.ca

COMPUTER MODELLING GROUP LTD.

GEM and STARS Features Relevant to H_2 Storage

	GEM	STARS
Gas mixtures (density, viscosity)	X	X
Diffusion	X	X
Chemical equilibrium reactions	X	X
Mineral prec./diss. reactions	X	X
Microbial effects, souring	X (with Arrhenius style reactions)	X
Aqueous solubility	X (Henry law based)	X (Kv based)
Thermal (and JT effect)	X	X
Geomechanics	X	X

- New K-Value solubility option in the future GEM releases
- GEM reactions need to be done in the aqueous phase. STARS can be used to model the reactions that have a gaseous or oleic reactant/product that is not soluble in the aqueous phase.
- STARS's reactions can have an additional parameter for reaction rate dependency on the concentrations of components (useful to model Monod bacterial growth).

Thank You

#FutureOfSimulation

cmgl.ca

CMG's Vision:

To be the leading developer and supplier of dynamic reservoir and production technologies in the WORLD