Simulation of Coupled Processes of Flow, Transport and Storage of CO_2 in Saline Aquifers

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DOE/EPA Collaborative Review

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Outline

- **Research project and team members**
- **Scope of work**
- **Physical and chemical processes of CO_2 geosequestartion**
- **Convective mixing**
- **Rock deformation**
- **Parallel simulation**
- **Future work**

Research Project and Team Members

DOE (NETL):

Area of Interest 2: Simulation

Duration: four year (2009-2013)

DOE Project Manager: Bruce Brown

Colorado School of Mines (CSM):

Yu-Shu Wu, Hossein Kazemi, Xiaolong Yin,
Jeffery Chen, Phil Winterfeld, and Ronglei Zhang

Lawrence Berkeley National Laboratory (LBNL):

Karsten Pruess (LBNL)

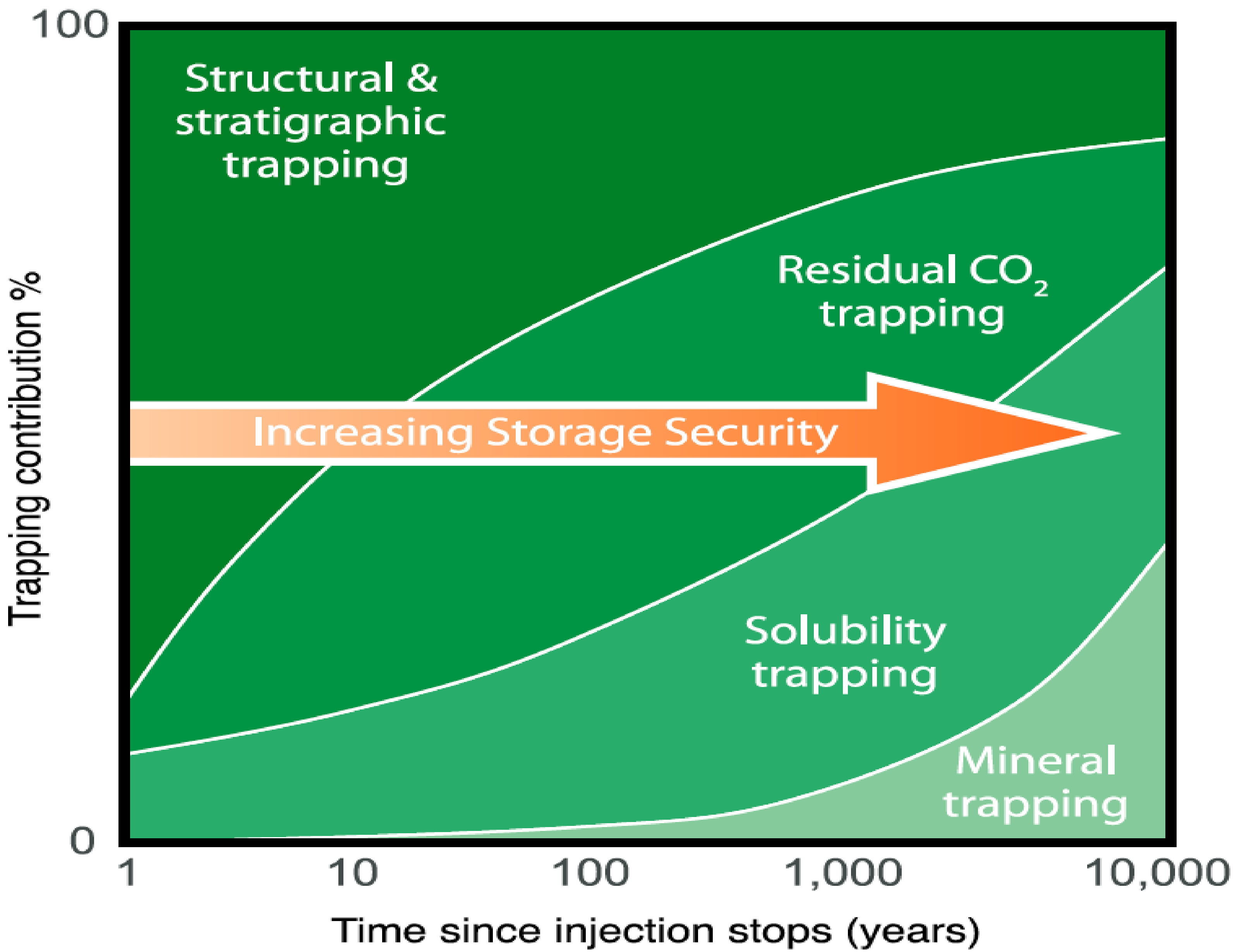
Computer Modeling Group (CMG):

Industry sponsor

SCOPE OF WORK

1. **Development of a three-phase, non-isothermal flow model to handle CO2-brine multiphase flow process (Pruess)**
2. **Coupling of pressure and rock mechanical deformation (Wu and Winterfeld)**
3. **Incorporation of representative geochemical reactions (Yin)**
4. **Characterization and modeling of the instability (Yin)**
5. **Implementation of parallel computing technologies (Chen)**
6. **Incorporation of general fracture conceptual models (Kazemi and Wu)**
7. **Model verification and application (All)**

Security of CO2 Storage vs. Time (IPCC Report 2005)



CO_2 Trapping Scenarios

Structural Trapping **(Trapping CO_2 as a mobile “gas”, a supercritical fluid, in reservoirs)**

Residual Gas Trapping **(Trapping CO_2 as an immobile “gas”)**

Solubility Trapping **(Trapping of CO_2 as a soluble component in brine)**

Mineral Trapping **(Conversion of CO_2 into carbonate minerals: Calcite, Dolomite, Siderite, etc.)**

CO2 Storage Capacity in North America

Formation Type	*10^9 Tons*	*%*
Saline Aquifers	3,297 - 12,618	91.8 - 97.5
Unmineable Coal Seams	157 - 178	4.4 - 1.4
Mature Oil & Gas Reservoirs	138	3.8 - 1.1
Total Capacity	3,592 - 12,934	100.0

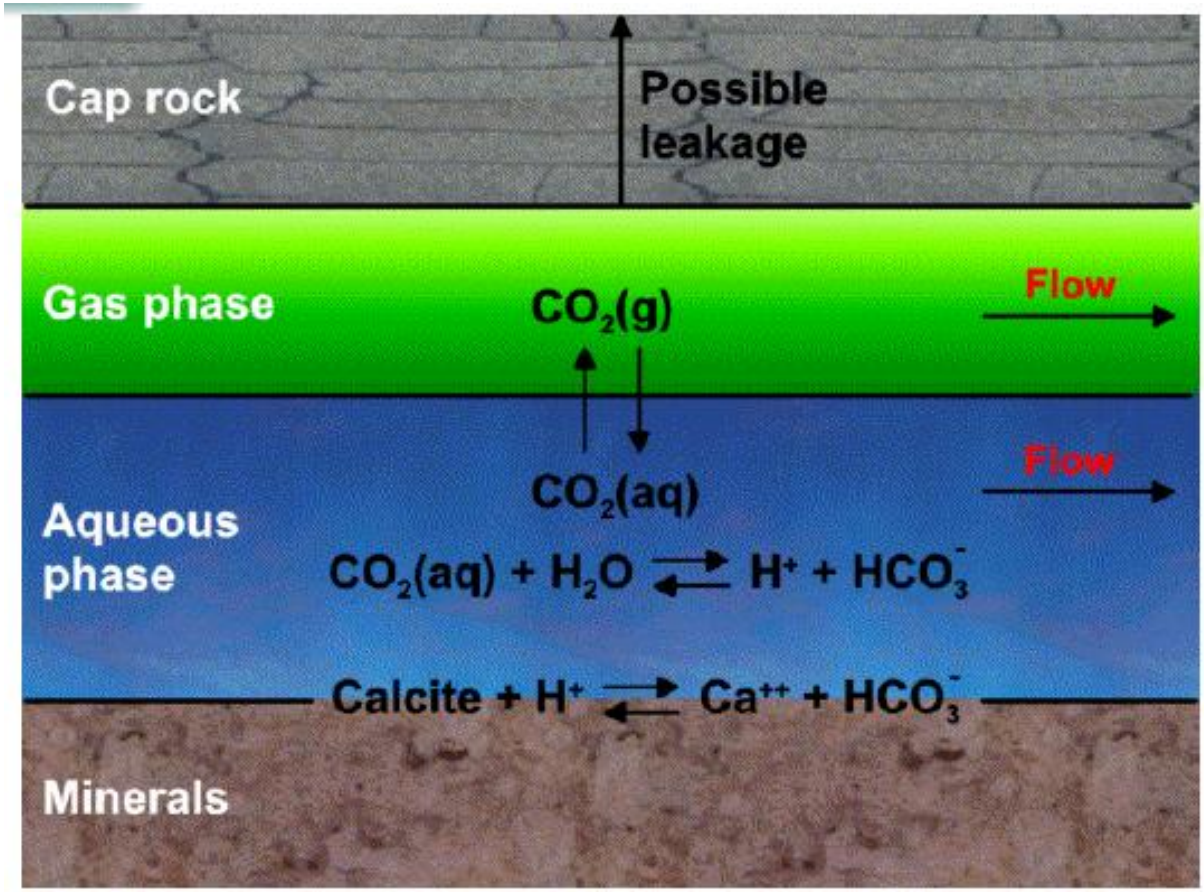
Source: DOE & NETL,"Carbon Sequestration Atlas of the United States and Canada", 2008

Physical / Chemical Processes

Structural Integrity – Elevated pressure and effects on existing fractures / faults

Dissolution – Mass transfer between CO2 and formation brine

Geochemistry – Reactions induced by dissolved CO2 with aquifer rock (mineralization)

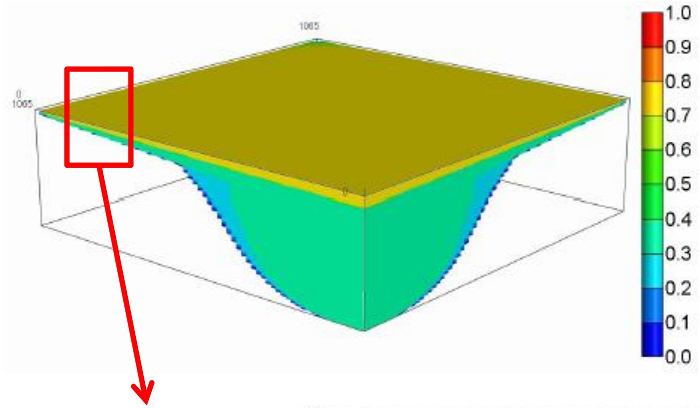


CMG)

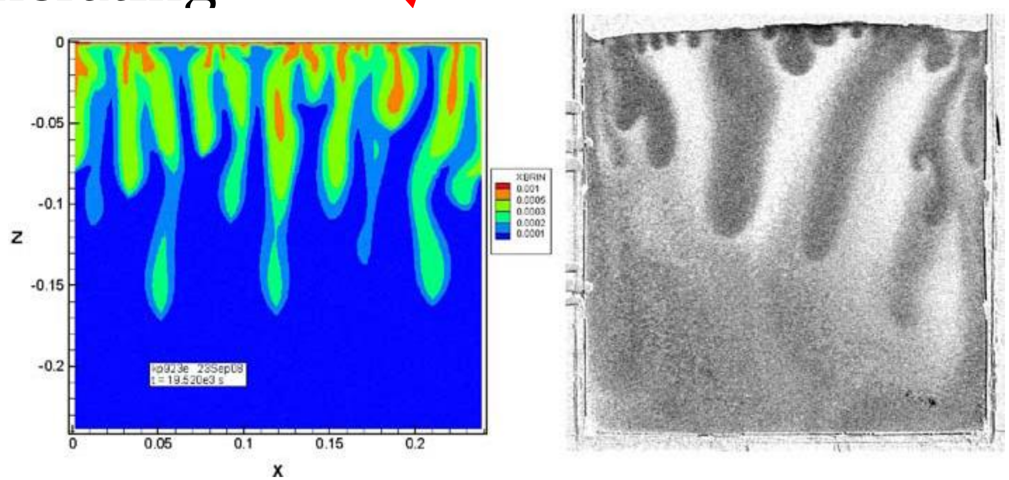
Convective Mixing

- Convective mixing is **an instability**
  1. CO_2 plume will migrate to above the brine due to buoyancy
  2. Dissolved CO_2 increases the density of brine below
  3. The heavier brine sinks into the lighter brine below, generating a convection
  4. Convection enhances mixing and solubility trapping

(Adapted from data provided by CMG)



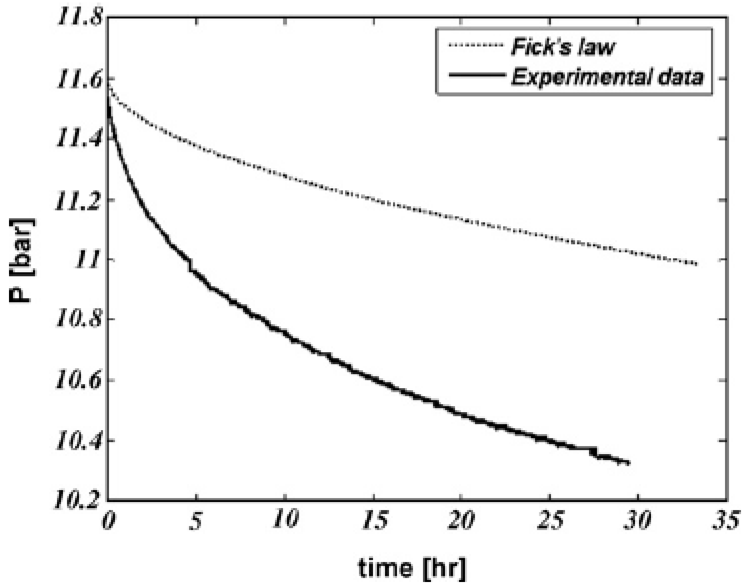
(Ennis-King & Paterson, 2005)



Kneafsey & Pruess, 2010 (Simulation & Experiment)

Significance of Convective Mixing

- Convective mixing leads to **significant increase** in dissolution rate
  - Lower risk of leakage
  - Potentially higher rate of mineralization
- The effect of convective mixing must be properly incorporated into CO_2 sequestration simulators



Farajzadeh et al. 2007 – Pressure reduction measured in experiment vs. calculation based on Fick's diffusion

Integral Properties and Modeling

- Fick's law of diffusion

$$\mathbf{q}_c = -\underline{\underline{\mathbf{D}}}\nabla c$$

- Enhanced diffusion due to convective mixing

$$\mathbf{q}_c^* = -\underline{\underline{\mathbf{D}}}\nabla c - D_{cm}\frac{\partial c}{\partial z}\mathbf{e}_z$$

We will use 2D and 3D simulations to characterize D_{cm} as a function of permeability, anisotropy, heterogeneity, and concentration gradient

Mechanical Coupling:

Effect of Pressure and Temperature on Rock Deformation

Poroelasticity and effective stress:

$$\varepsilon_b = \frac{1}{K}\left(P_c - \alpha P_p\right) = \frac{1}{K}\sigma'$$

(ε_b is bulk volumetric strain, P_c is confining pressure,

σ' is effective stress)

Modification of porosity, permeability and capillary pressure due to rock deformation

Effective Stress Dependence

- Mckee et al. (1988) – porosity depends on bulk rock compressibility (c_m) and effective stress, Carman-Kozeny equation for permeability:

$$d\phi = -c_m (1-\phi)\, d\sigma', \qquad k \propto \frac{\phi^3}{(1-\phi)^2}$$

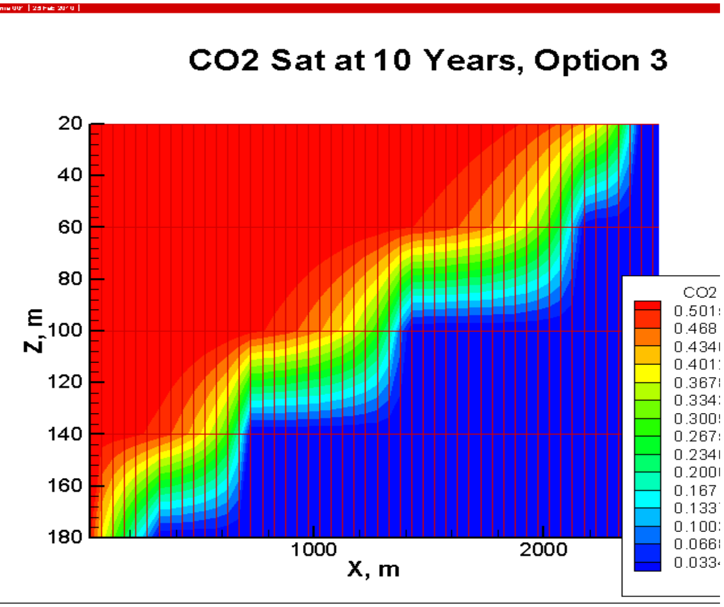
- Ostensen (1986) – permeability correlation for tight gas sands:

$$k^{0.44} = C \ln\left[1 + \left(\frac{\sigma^*}{\sigma'}\right)^2\right]$$

Simulation Example

- Modified example from Rutqvist et al. (2002)
- Brine formation (200 m thick)
- 2D system, large x-direction length and constant pore and confining pressure gradients
- CO_2 injection at one end, formation bottom, of 100x5 x-z grid for ten years
- Permeabilities and porosity calculated using fractured rock correlations (Rutqvist et al. 2002)
- Pc scaling using J-function

Comparison with Rutqvist et al. Gas Saturations



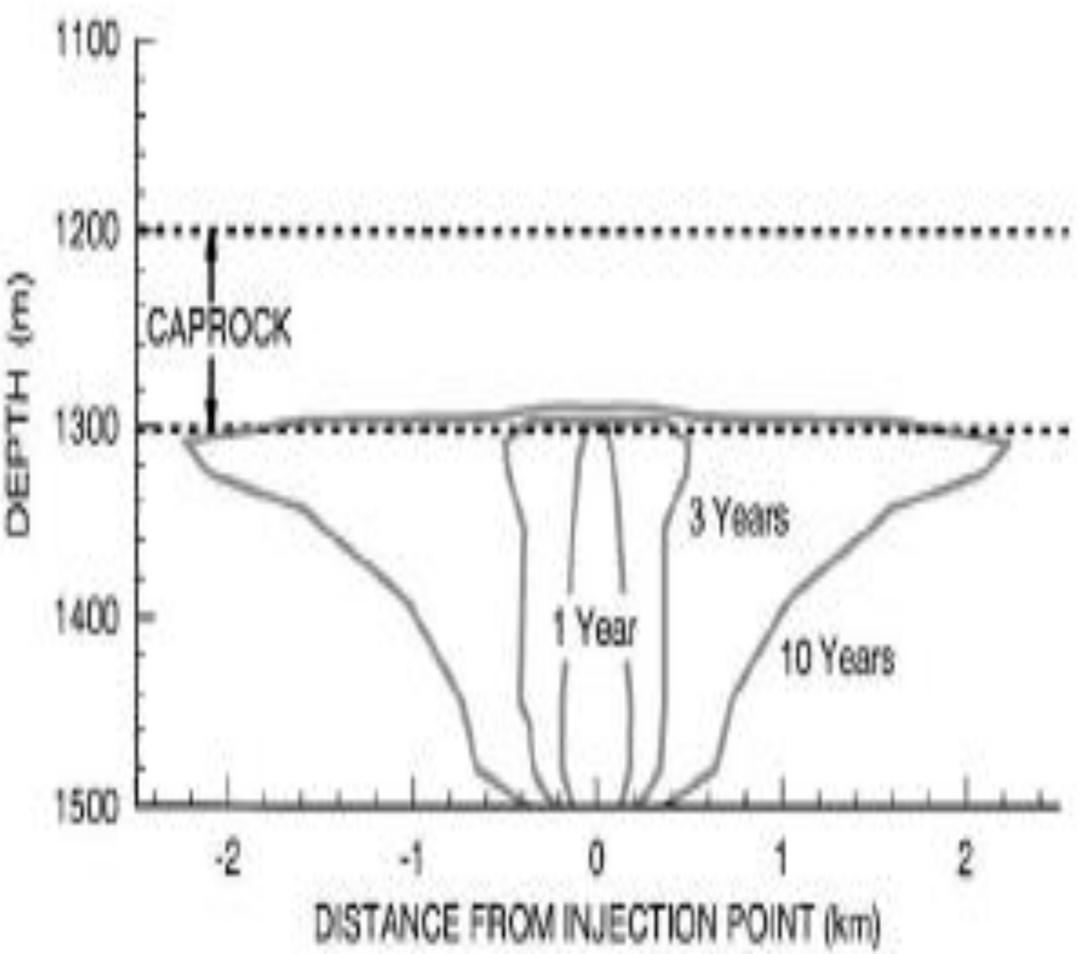
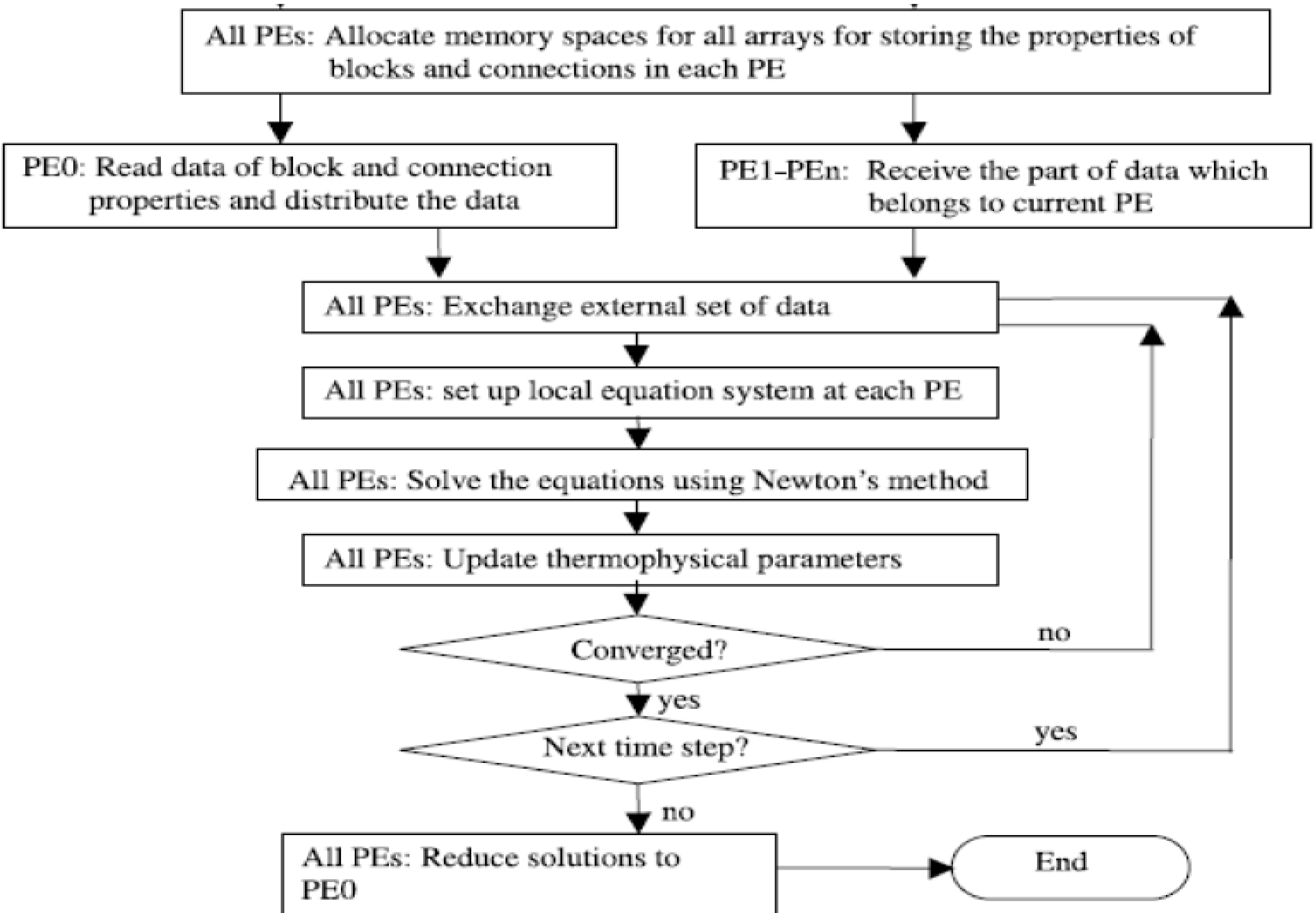


Fig. 6. Spread of the supercritical CO_2 fluid within the brine formation.

Parallel Simulation



Future Work

1. Develop and implement a three-phase flow module
2. Coupling of pressure and temperature effect on rock mechanical deformation
2. Integration of kinetic modeling of mineral dissolution and precipitation and non-aqueous reactions into models
3. Characterization and modeling of the instability
4. Improvement of parallel computing technologies
5. Development and incorporation of fracture conceptual models

Thanks!