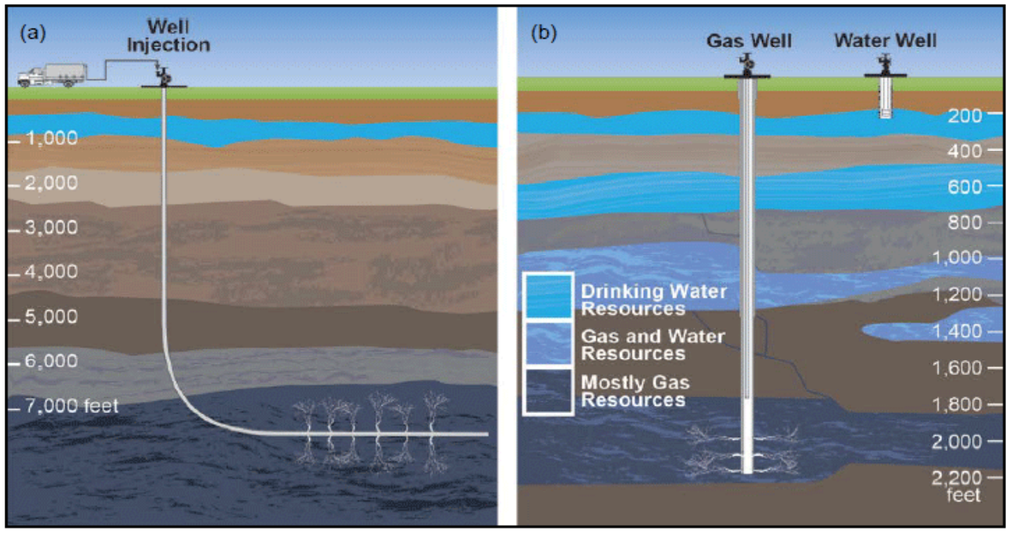
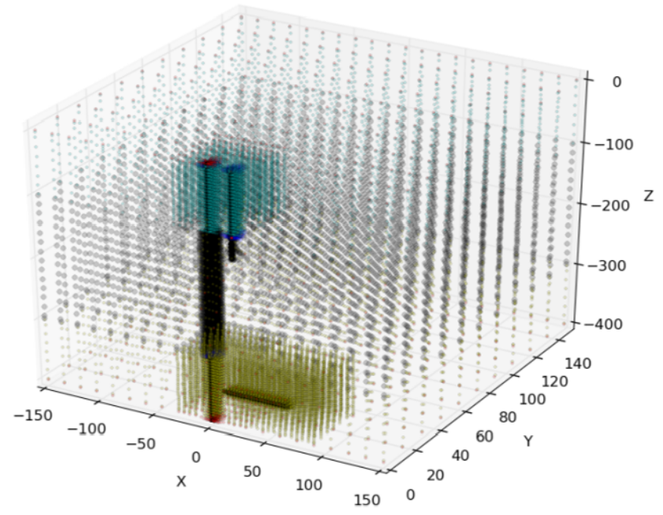
BERKELEY LAB
LAWRENCE BERKELEY NATIONAL LABORATORY

# Modeling Subsurface Scenarios: How Do We Do This?

**Technical Workshop Series:**
**Technical Follow-up Discussion on Subsurface Modeling**

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June 3, 2013

# OUTLINE

- **Overall Approach**
  - Geomechanical question
  - Flow and contaminant transport question
- **Modeling of Fluid Flow and Contaminant Transport**
  - The **TOUGH+RealGasH2O** code
  - The **TOUGH+RealGasH2OCont** code
- **Modeling of Coupled Flow-Thermal-Geomechanical Processes**
  - Coupling with the **FLAC3D** code
  - Coupling with the **ROCMECH** code

# OVERALL APPROACH

- **Are the geomechanical failure (and fracture propagation) scenarios physically possible?**
- **If a fast transport pathway between the shale and the groundwater aquifer does exist, what is contaminant transport affected by and what are the corrresponding time frames?**

# OUTLINE

- **Background**
- **Code Description**
  - Fundamental equations
  - Capabilities
- **Validation Examples**
- **Applications Examples**

# SIMULATION CODES

## TOUGH+ Core Code with Options

- **Member of the TOUGH family of codes:**
  - Used by 400+ organizations in 65+ countries
  - Qualified code, Yucca Mountain project: flow, contaminant transport
- **FORTRAN 95/2003**
- **Object-Oriented Programming Structure**
- **Modular structure, ease of expansion, maximum traceability, UNICODE**

# TOUGH+RealGasH2O (in review, C&G)

- 3D, non-isothermal
- Compositional (3 to 13 components): real gas mixture + H2O
- Darcy and non-Darcy flow, Knudsen diffusion, binary diffusion, sorption
- Fractured/unfractured media

# TOUGH+RGasH2OCont (in preparation)

- 3D, non-isothermal
- Compositional, 4 to 17 components: real gas mixture, oil, H2O, salt + solutes
- Halite precipitation

# NEEDED CAPABILITIES

- Darcy and non-Darcy flow through the matrix and fractures
- Inertial and turbulent effects (Klinkenberg effects)
- Real (as opposed to ideal) gas behavior
- Multi-phase flow (gas, aqueous, **organic phases** of fluids involved in hydraulic-fracturing); **variable viscosity (gels)**
- **Solute transport and density-driven flows (convection cells)**
- Mechanical dispersion, in addition to advection and molecular diffusion

**Blue: RGasH2OCont**

# NEEDED CAPABILITIES (cont.)

- Gas sorption: three possible sorption models (linear, Langmuir or Freundlich), equilibrium or kinetic conditions
- **Sorption (primary and secondary) of contaminants (organic and solutes)** expected in fracturing processes: three possible sorption models (linear, Langmuir or Freundlich), equilibrium or kinetic conditions
- Coupled flow and thermal effects
- **Halite formation**: salt precipitation in brines caused by lower P and T; can significantly affect fracture and matrix permeability, and contaminant transport

**Blue: RGasH2OCont**

# CODE DESCRIPTION

## Fundamental Equations

$$\frac{d}{dt}\int_{V_n} M^{\kappa}\,dV = \int_{\Gamma_n} \mathbf{F}^{\kappa}\cdot\mathbf{n}\,dA + \int_{V_n} q^{\kappa}\,dV$$

**Mass/heat balance**

**Mass accumulation**

$$M^{\kappa} = \sum_{\beta\equiv A,G} \phi\, S_{\beta}\rho_{\beta}X^{\kappa}_{\beta} + \quad \delta_S(1-\phi)\rho_R\Psi^{i}, \quad \kappa = \mathrm{w}, g^{i}\ (i=1,\ldots,N_G)$$

# CODE DESCRIPTION

## Fundamental Equations

**Gas Sorption**
**Langmuir isotherm**
**Equilibrium and Kinetic**

$$\begin{cases} \Psi^i = \dfrac{p_{dG} m_L}{p_{dG} + p_L} & \text{for ELaS} \\ \dfrac{d\Psi^i}{dt} = k_L \left( \dfrac{p_{dG} m_L}{p_{dG} + p_L} - \Psi^i \right) & \text{for KLaS} \end{cases}$$

**Multi-component**

$$\begin{cases} \Psi^i = \dfrac{p_{dG} B^i m^i{}_L \Upsilon^i}{1 + p_{dG} \sum_i B^i \Upsilon^i} & \text{for ELaS} \\ \dfrac{d\Psi^i}{dt} = k_L^i \left( \dfrac{p_{dG} B^i m^i{}_L \Upsilon^i}{1 + p_{dG} \sum_i B^i \Upsilon^i} - \Psi^{\,i} \right) & \text{for KLaS} \end{cases}$$

**Additionally: Linear and Freundlich**

# Fundamental equations

## Heat accumulation

$$M^{\theta} = (1-\varphi)\rho_R \int_{T_0}^{T} C_R(T)\, dT + \sum_{\beta=A,G} \varphi S_\beta \rho_\beta U_\beta + \delta_\Psi (1-\varphi)\rho_R \sum_{i=1}^{N_G} u^i Y^i$$

## Flow terms

$$\mathbf{F}^{\kappa} = \sum_{\kappa \equiv A,G} \mathbf{F}_\beta^{\kappa} \qquad \kappa \equiv w, g^i \ (i \geq 1)$$

$$\mathbf{F}_\beta = \rho_\beta \left[ -\frac{k\, k_{r\beta}}{\mu_\beta} \nabla\Phi_\beta \right] = \rho_\beta \mathbf{v}_\beta \ , \ \text{where} \ \nabla\Phi_\beta = \nabla P_\beta - \rho_\beta \mathbf{g}$$

# Fundamental equations

## Gas Flow: Inertial, slippage, diffusion effects

$$\mathbf{F}_G^{\kappa} = \left(1+\frac{b}{P_G}\right)\rho_G \mathbf{v}_G X_G^{\kappa} + \mathbf{J}_G^{\kappa}, \quad \kappa = \mathrm{w}, g_i \ (i \geq 1)$$

$$\mathbf{J}_G^{\kappa} = -\phi S_G\left(\phi^{1/3} S_G^{7/3}\right) D_G^{\kappa} \rho_G \nabla X_G^{\kappa} = -\phi S_G\left(\tau_G\right) D_G^{\kappa} \rho_G \nabla X_G^{\kappa}, \quad \kappa = \mathrm{w}, g^i \ (i \geq 1)$$

$$\frac{b}{P_G} = (1+\alpha K_n)\left(1+\frac{4K_n}{1+K_n}\right) - 1$$

## Knudsen diffusion

$$K_n = \frac{\bar{\lambda}}{r_{pore}} = \frac{\sqrt{\pi/2}\,\frac{1}{P_G}\mu_G\sqrt{\frac{RT}{M}}}{2.81708\sqrt{\frac{k}{\phi}}}$$

$$\alpha = \frac{128}{15\pi^2}\tan^{-1}\left[4\ K_n{}^{0.4}\right]$$

# Fundamental equations

## Dusty gas model (multi-component diffusion)

$$\sum_{j=1,\, j\neq i}^{N_G} \frac{Y^i N_D^j - Y^j N_D^i}{D_e^{ij}} - \frac{N_D^i}{D_K^i} = \frac{p^i \nabla Y^i}{ZRT} + \left(1 + \frac{kp}{\mu_G D_K^i}\right) \frac{Y^i \nabla p^i}{ZRT}$$

## Non-Darcy Flow Options: Forchheimer equation

$$\nabla \Phi_\beta = -\left( \frac{\mu_\beta}{k\, k_{r\beta}} \mathbf{v}_\beta + \beta_\beta \rho_\beta \mathbf{v}_\beta \left| \mathbf{v}_\beta \right| \right) \quad \Rightarrow \quad \mathbf{v}_\beta = \frac{2 \nabla \Phi_\beta}{\frac{\mu_\beta}{k\, k_{r\beta}} + \sqrt{\left( \frac{\mu_\beta}{k\, k_{r\beta}} \right)^2 + 4 \beta_\beta \rho_\beta \left| \nabla \Phi_\beta \right|}}$$

Additional Non-Darcy Option: Barree and Conway model (2007)

# Fundamental equations

**Heat Flow**

$$\mathbf{F}^{\theta} = -\bar{k}_{\theta}\nabla T + f_{\sigma}\sigma_{0}\nabla T^{4} + \sum_{\beta \equiv A,G} h_{\beta}\,\mathbf{F}_{\beta}$$

**Sources and Sinks**

$$\hat{q}^{\kappa} = \sum_{\beta \equiv A,G} X_{\beta}^{\kappa} q_{\beta}, \quad \kappa = \mathrm{w}, g^{i}\ (i = 1,\ldots,N_{G}); \quad \hat{q}^{\theta} = \sum_{\beta \equiv A,G} q_{\beta} h_{\beta}$$

**H2O Properties:** Steam tables (IFC, 1967; NIST, 2000)

**Real gas mixture properties:** Cubic equations of state (RK, SRK, PR), 11 component library (Moridis et al., 2008; WebGasEOS)

# TOUGH+ Modeling

- **Minimum of assumptions**
- **All known processes accounted for**

# VALIDATION EXAMPLES

## Problem V1: Real gas flow in a cylindrical reservoir

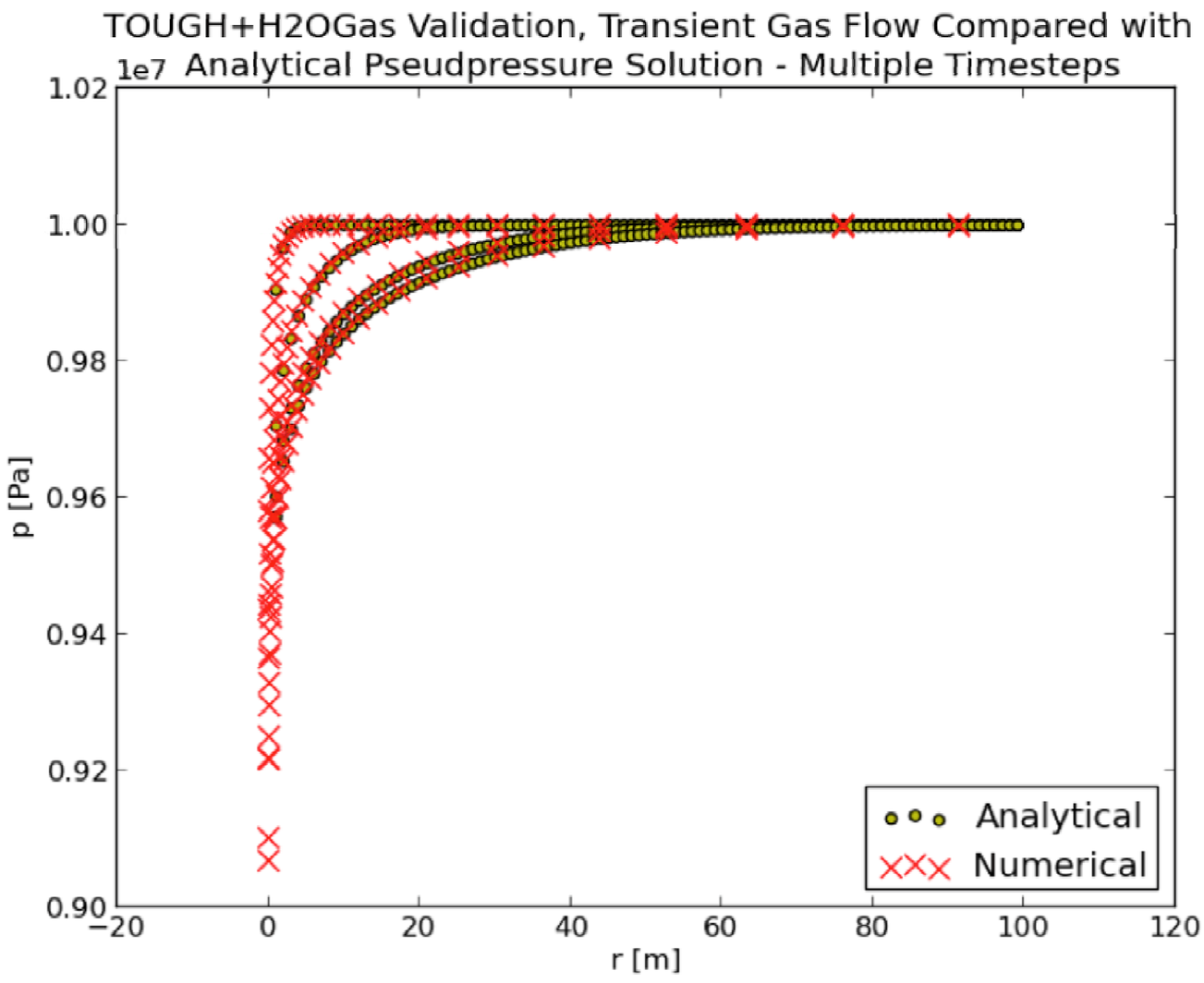
### SPECIFICS

| Data Type | Values |
|---|---|
| Matrix permeability $k$ | $3.04 \times 10^{-14}$ m$^2$ (30.4 mD) |
| Reservoir thickness $h$ | 10 m |
| Well radius $r_w$ | 0.059 m |
| Reservoir radius $r_e$ | 100 m |
| Reservoir pressure $p$ | 10 MPa |
| Reservoir temperature $T$ | 60 °C |
| Reservoir porosity $\phi$ | 0.30 |
| Rock compressibility | $2 \times 10^{-10}$ 1/Pa |
| Gas composition | 100% $CH_4$ |
| Gas EOS | Peng-Robinson |

**Analytical solution of Fraim & Wattenbarger (1986) using pseudo-pressure concept**

# VALIDATION EXAMPLES

## Problem V1: Real gas flow in a cylindrical reservoir



# VALIDATION EXAMPLES

## Problem V2: Water flow in a cylindrical reservoir

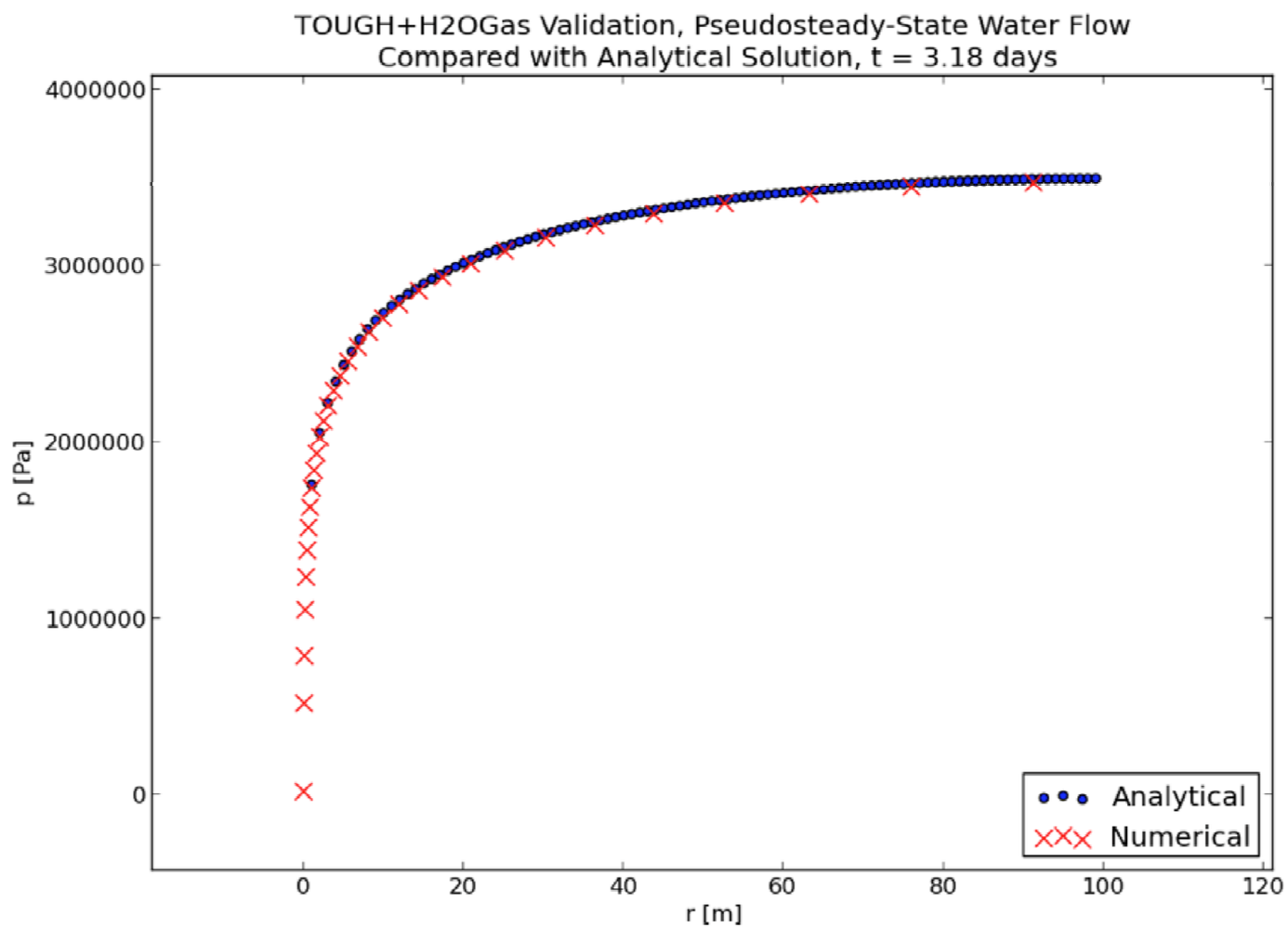
### SPECIFICS

| Data Type | Values |
|---|---|
| Matrix permeability $k$ | $3.04 \times 10^{-14}$ m$^2$ (30.4 mD) |
| Reservoir thickness $h$ | 10 m |
| Well radius $r_w$ | 0.059 m |
| Reservoir radius $r_e$ | 100 m |
| Reservoir pressure $p$ | 10 MPa |
| Reservoir temperature $T$ | 30 °C |
| Reservoir porosity $\phi$ | 0.30 |
| Total compressibility $c_t$ | $4.88 \times 10^{-10}$ 1/Pa |
| Gas EOS | Peng-Robinson |

**Analytical solution of Blasingame (1993) – pseudo-steady state**

# VALIDATION EXAMPLES

## Problem V2: Water flow in a cylindrical reservoir



# VALIDATION EXAMPLES

## Problem V3: Gas flow in a tight gas reservoir with vertical well intersecting a vertical fracture plane

### SPECIFICS

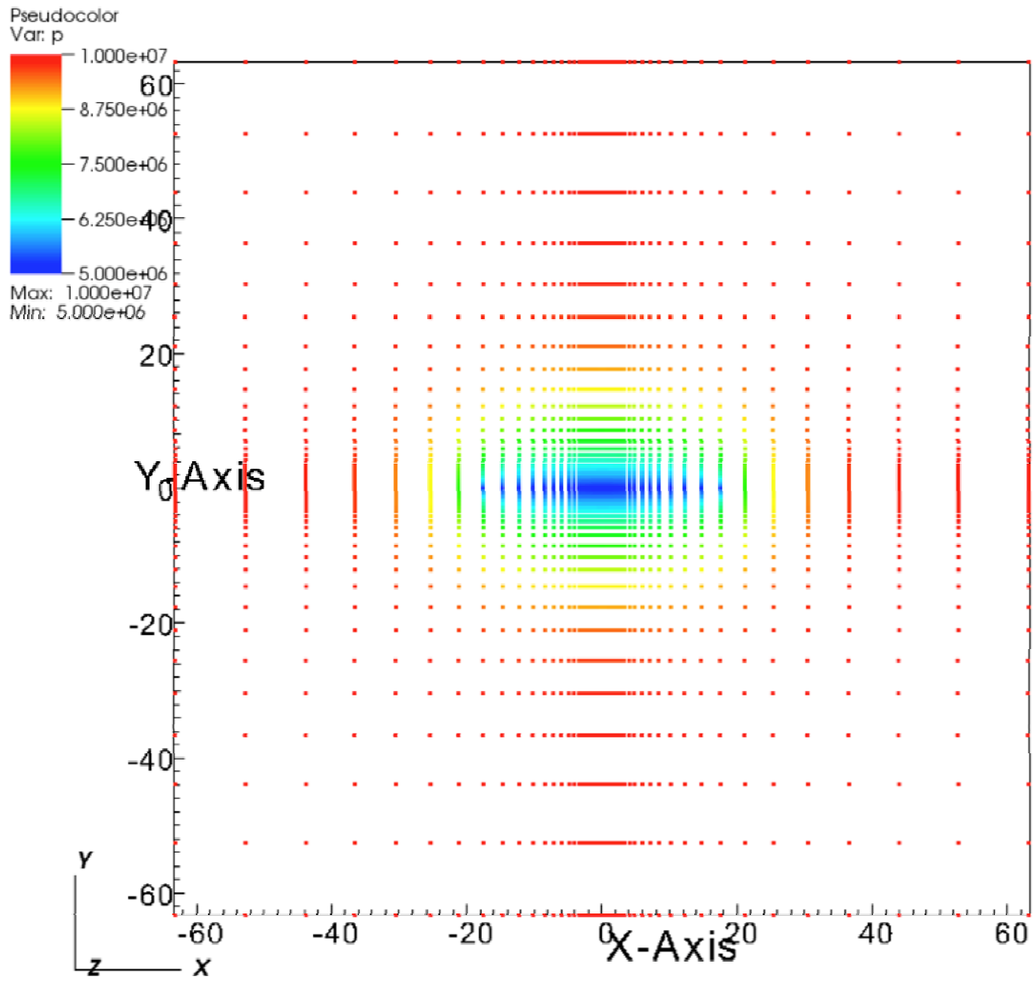
| Data Type | Values |
|---|---|
| Matrix permeability $k$ | $3.08 \times 10^{-19}$ m$^2$ (30.8 nD) |
| Fracture permeability $k_f$ | $6.68 \times 10^{-14}$ m$^2$ (0.668 D) |
| Fracture half-length | 20 m |
| Reservoir thickness $h$ | 10 m |
| Well radius $r_w$ | 0.05 m |
| Well pressure $p_w$ | 5 MPa |
| Reservoir pressure $p$ | 10 MPa |
| Reservoir temperature $T$ | 60 °C |
| Reservoir porosity $\phi$ | 0.10 |
| Rock compressibility | $2 \times 10^{-10}$ 1/Pa |
| Gas composition | 100% $CH_4$ |
| Gas EOS | Peng-Robinson |

**Analytical solutions of Cinco-Ley et al. (1978) and Cossio (2012)**

# VALIDATION EXAMPLES

## Problem V3: Gas flow in a tight gas reservoir with vertical well intersecting a vertical fracture plane

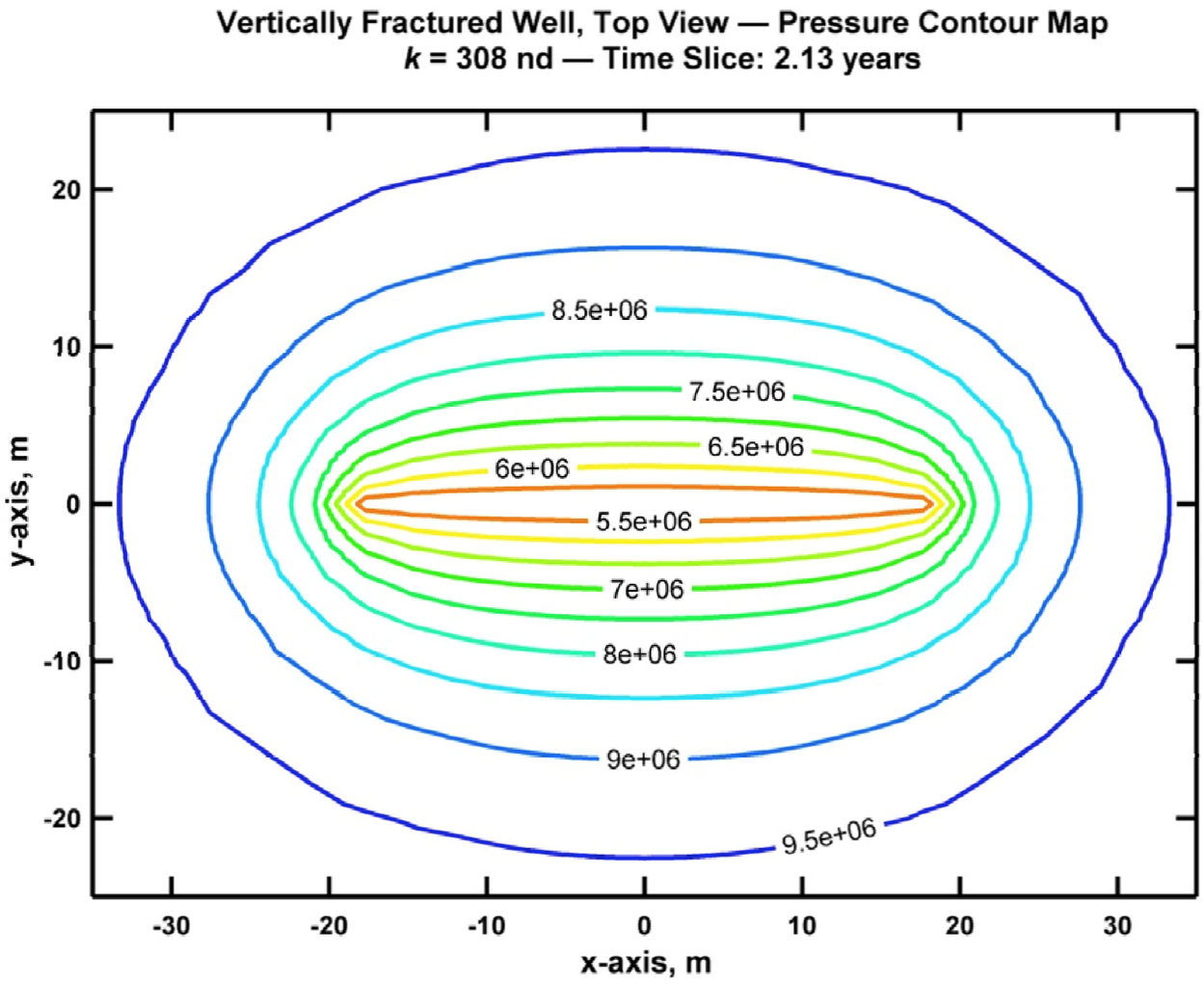
**Point cloud of pressure distribution**



# VALIDATION EXAMPLES

## Problem V3: Gas flow in a tight gas reservoir with vertical well intersecting a vertical fracture plane

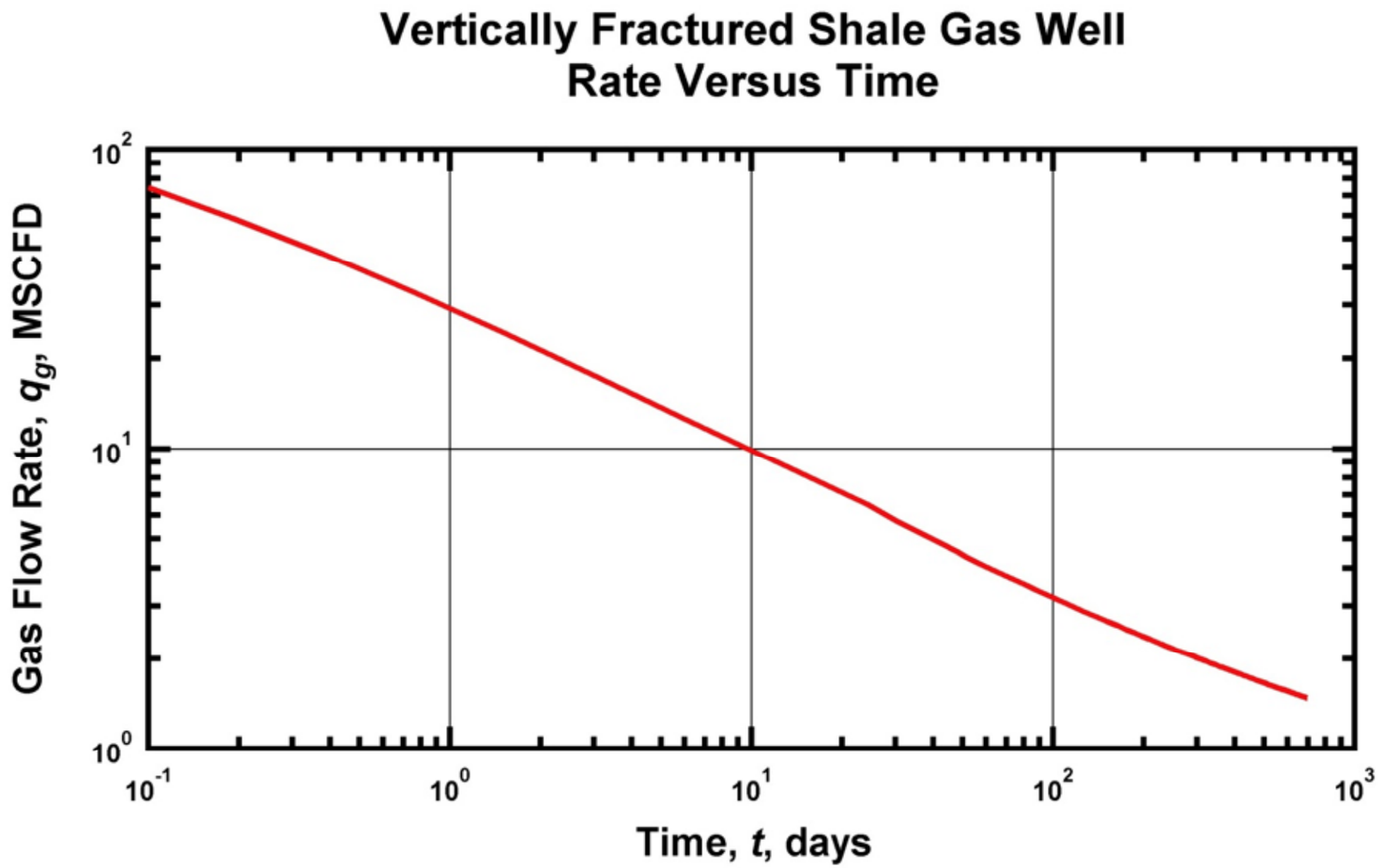
**Contour plot of pressure distribution**



# VALIDATION EXAMPLES

**Problem V3: Gas flow in a tight gas reservoir with vertical well intersecting a vertical fracture plane**

**Production rate predictions: identical results (2 curves)**



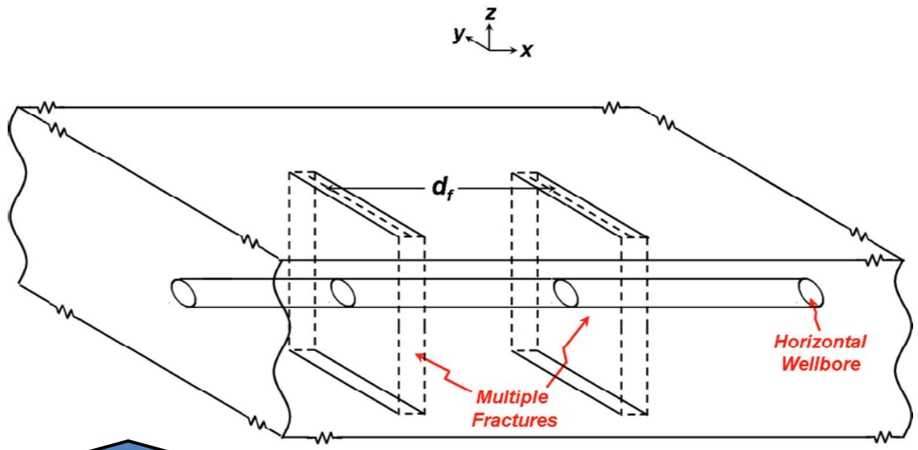
# APPLICATION EXAMPLES

## Problem A1: Gas production from a shale gas reservoir using a horizontal well

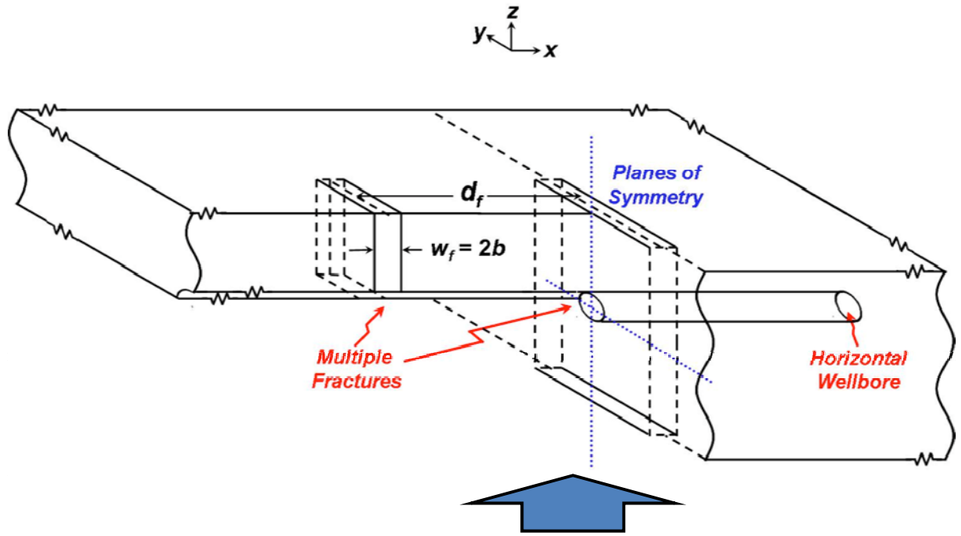
### System Subdomains

- **S-1**: The original (undisturbed) rock system
  - Matrix
  - Possibly naturally fractured: Native fractures (NF)

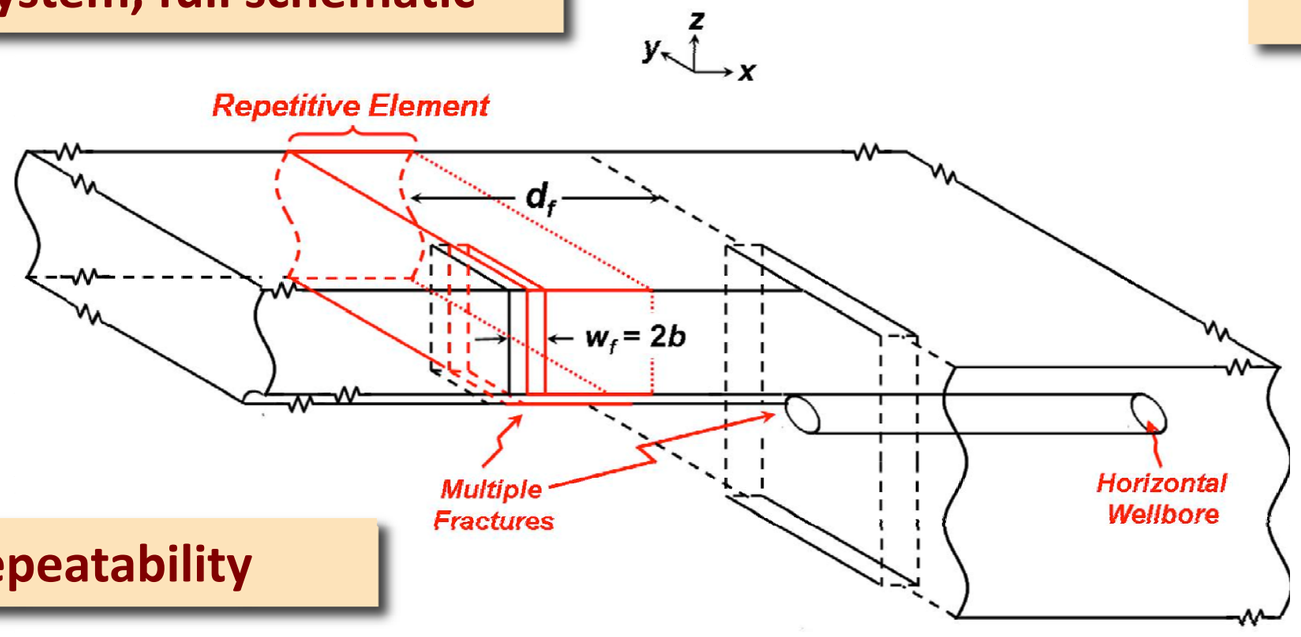
# APPLICATION EXAMPLES: Problem A1




**Well system, full schematic**




**Symmetry argument**




**Repeatability**

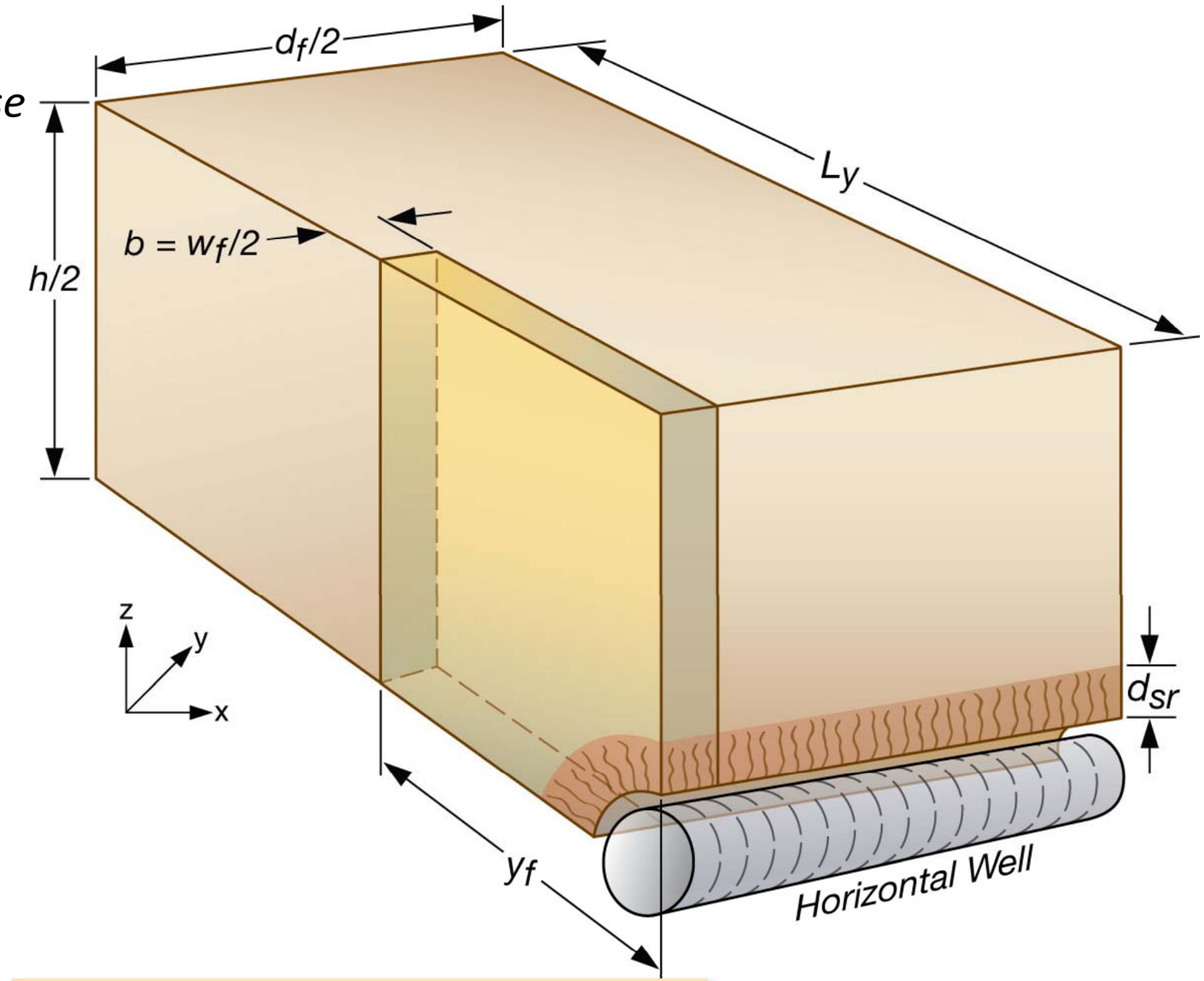
**Computational element: Symmetry and repeatability (Freeman et al., 2009)**

# APPLICATION EXAMPLES: Problem A1

Important parameters

- *$d_{sr}$: thickness of stress-release fractured zone around wellbore*
- *$d_f$: primary fracture spacing*
- *b: primary fracture aperture*
- *$y_f$: y-reach of the primary fractures*
- *$L_y$: reservoir width*
- *h: reservoir thickness*

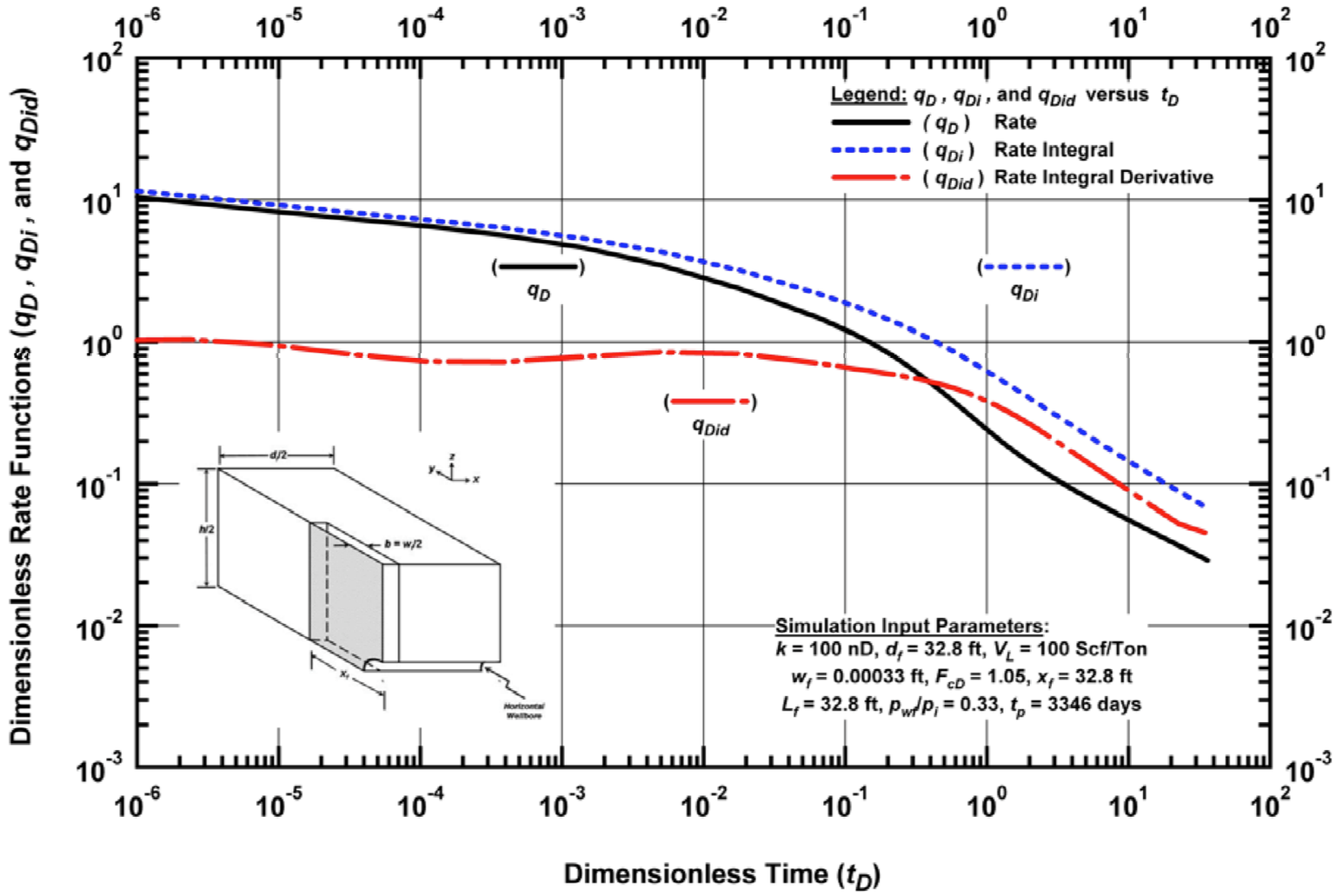
Similarly for vertical wells




**Type I: Reference**

# APPLICATION EXAMPLES: Problem A1

**Numerical simulation results: 800,000 elements (Freeman, 2010; Moridis et al., 2010)**



# APPLICATION EXAMPLES: Problem A1

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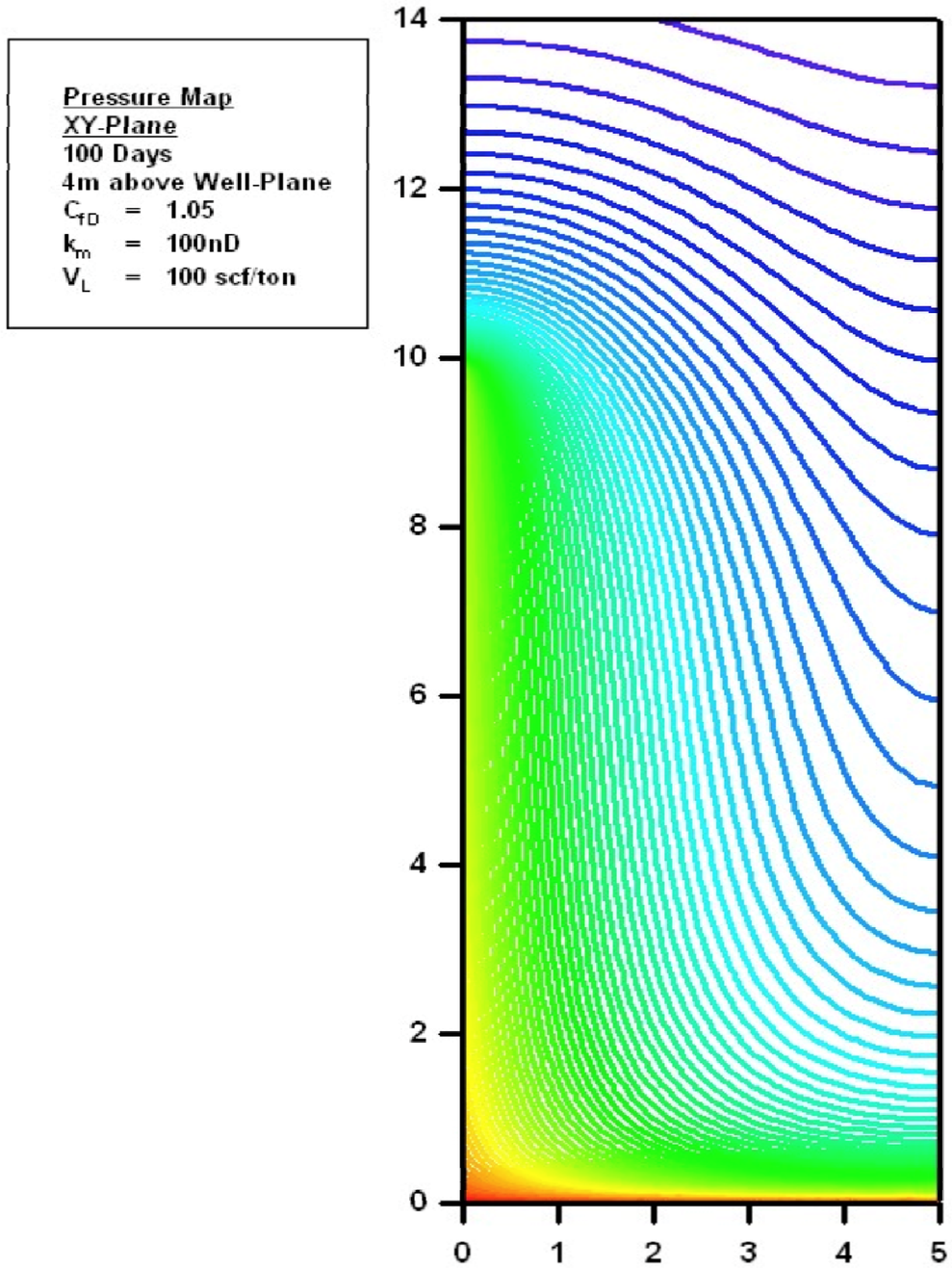
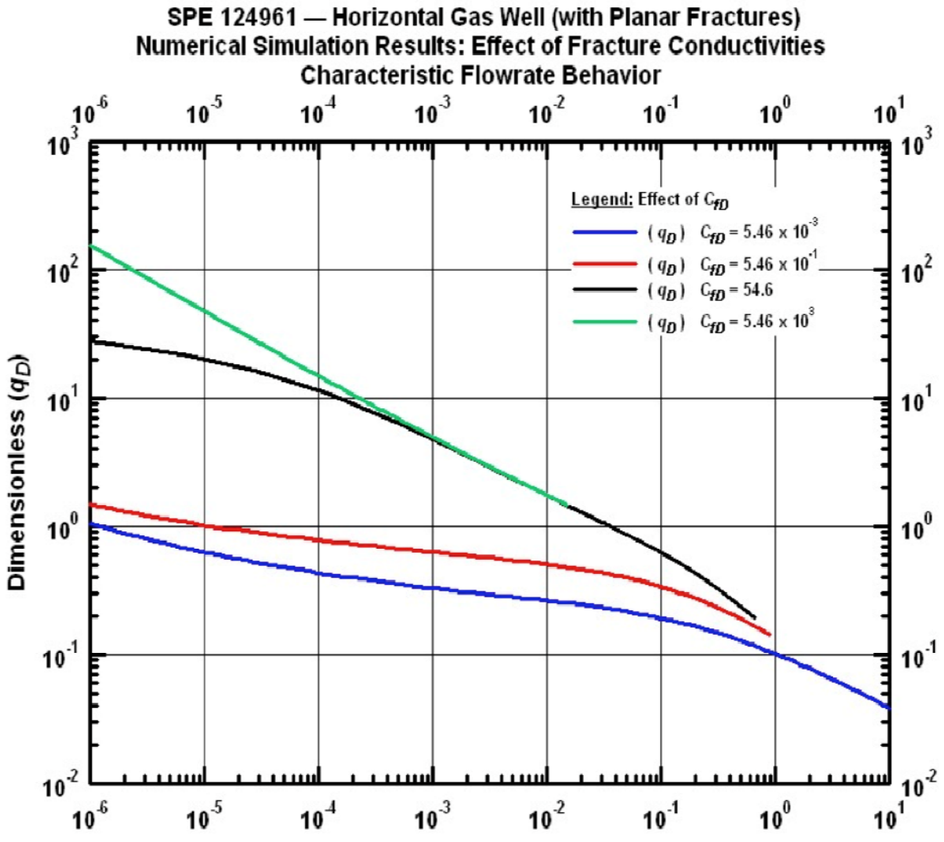
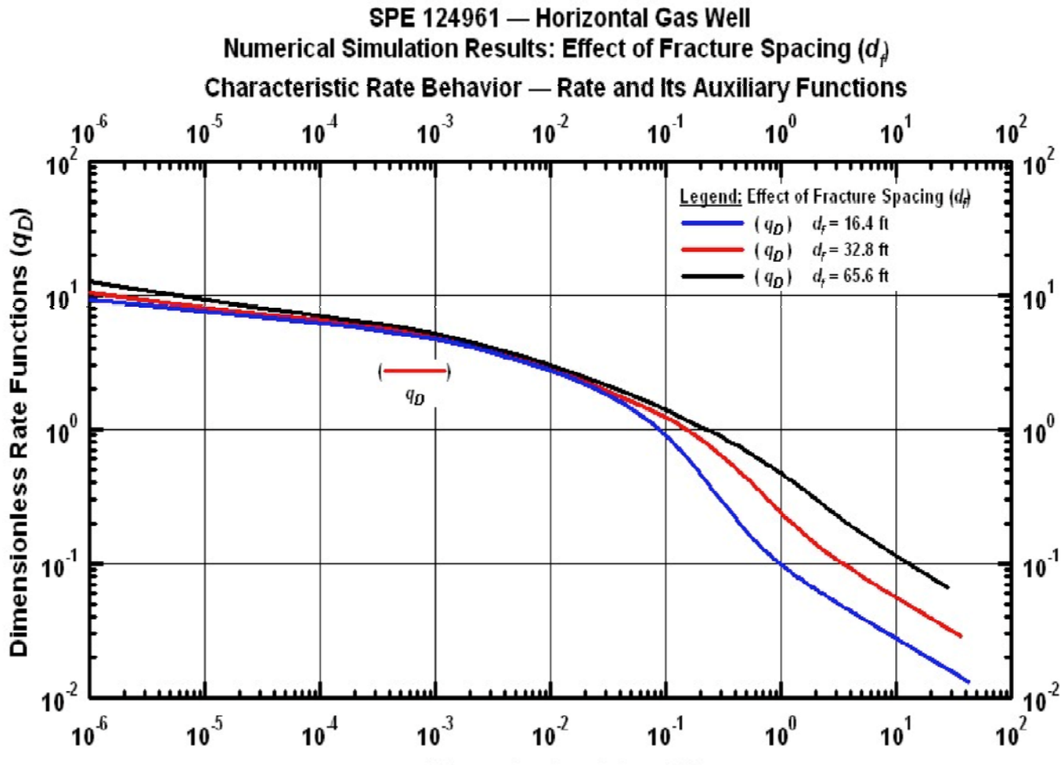


# APPLICATION EXAMPLES: Problem A1




**Sensitivity analyses (Freeman et al., 2011)**



# APPLICATION EXAMPLES

## Problem A2: Gas production from a shale gas reservoir with a complex fracture system using a horizontal well

### System Subdomains

- **S-1**: The original (undisturbed) rock system
  - Matrix
  - Possibly naturally fractured: Native fractures (NF)

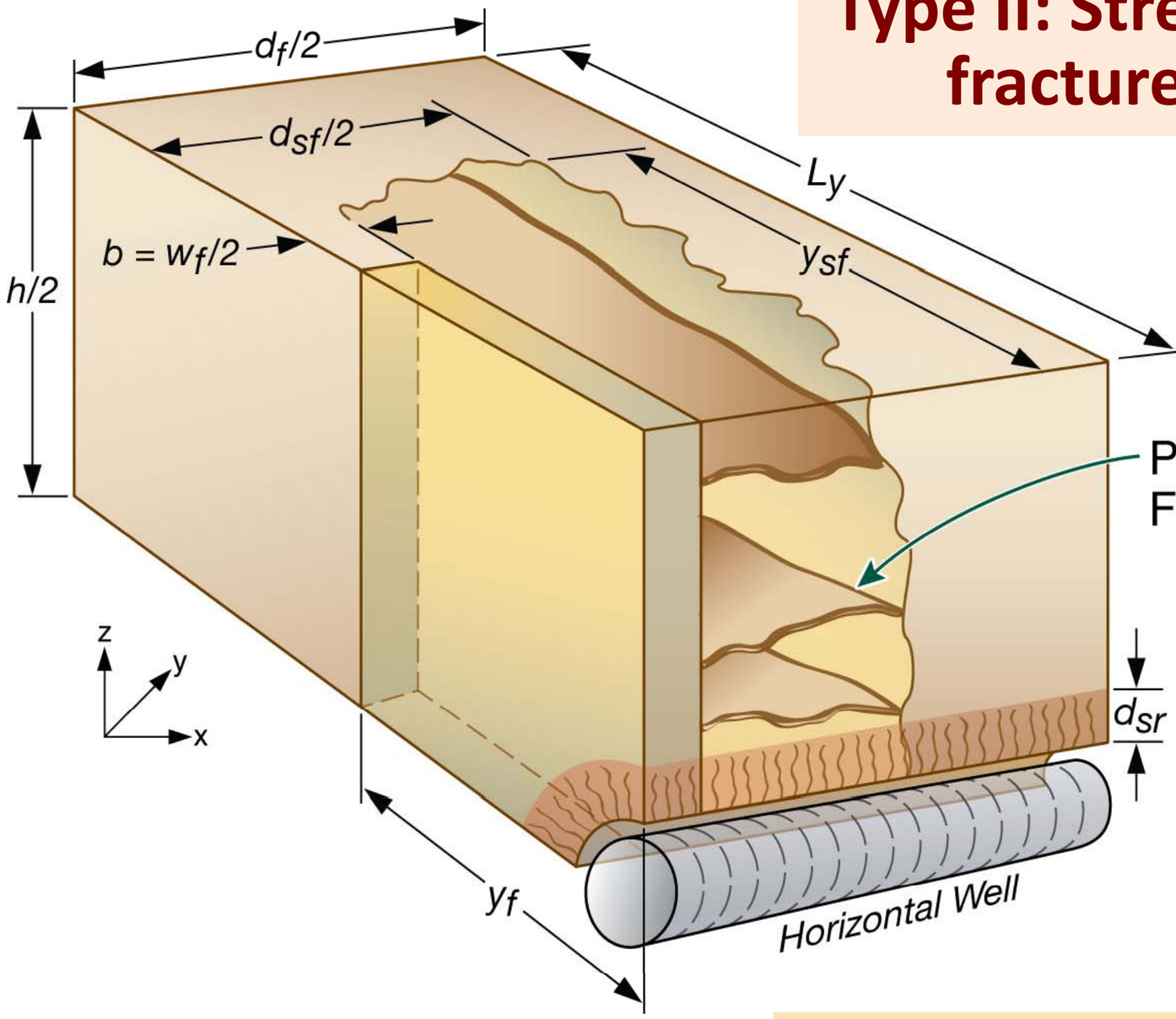
- **S-2**: Fractures induced during stimulation: Primary fractures (PF)
  - Dominant pathways of flow to well
  - May intercept the NF system

- **S-3**: Stress-release fractures related to PF: Secondary fractures (SF)
  - Usually perpendicular to PF
  - Penetrate S-1, connected to PF, may intercept NF

- **S-4**: Stress-release fractures related to well drilling: Radial/tertiary fractures (RF/TF)
  - Usually cylindrical shape centered around the well axis
  - Connected to S-1 and PF, may intercept NF and SF

# APPLICATION EXAMPLES: Problem A1

## Type II: Stress-release planar fractures (secondary)

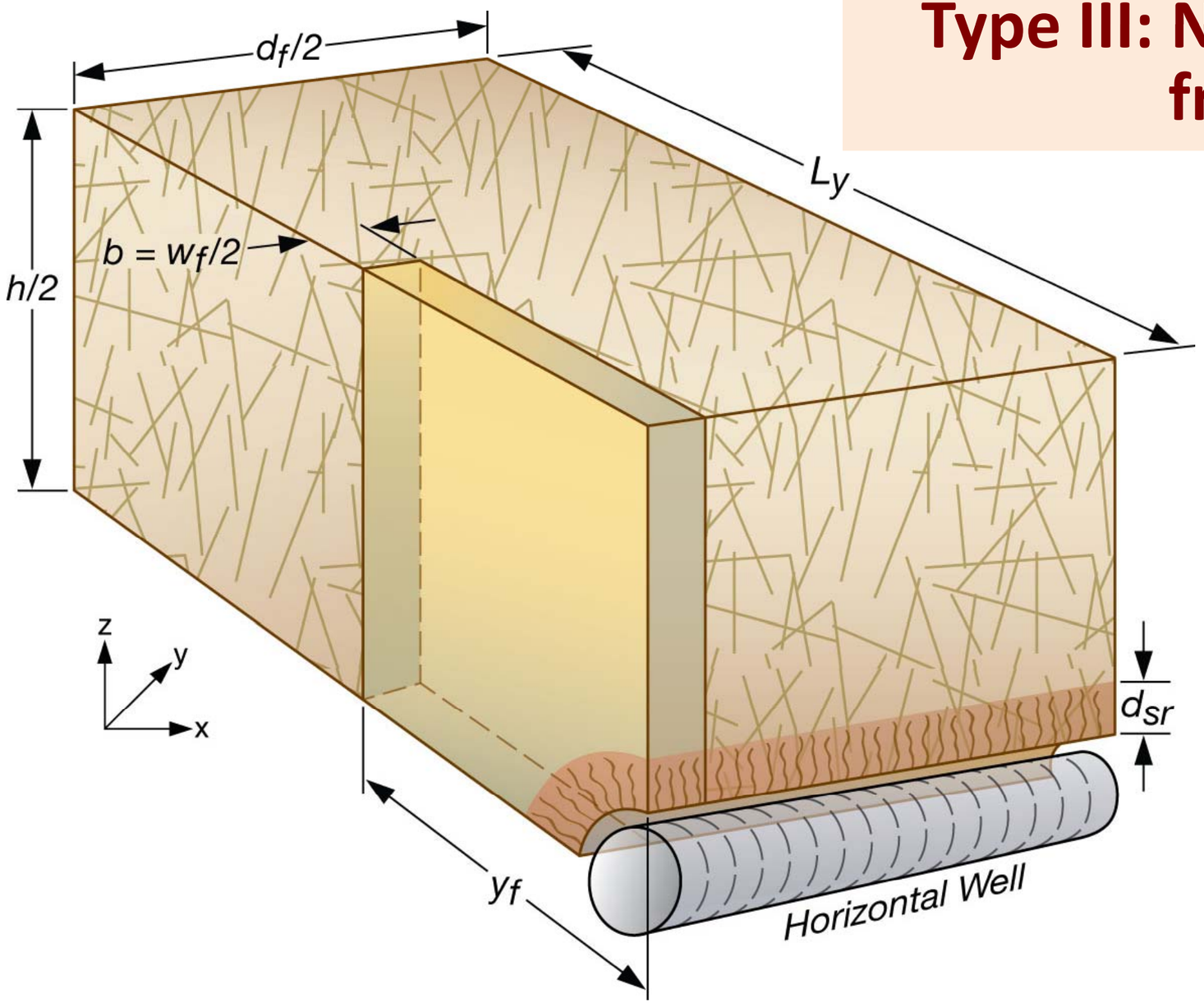



Important parameters

- $d_{sf}$: *x-reach of the secondary fractures*
- $y_{sf}$: *y-reach of the secondary fractures*

Similarly for vertical wells

# APPLICATION EXAMPLES: Problem A2




## Type III: Native & primary fractures

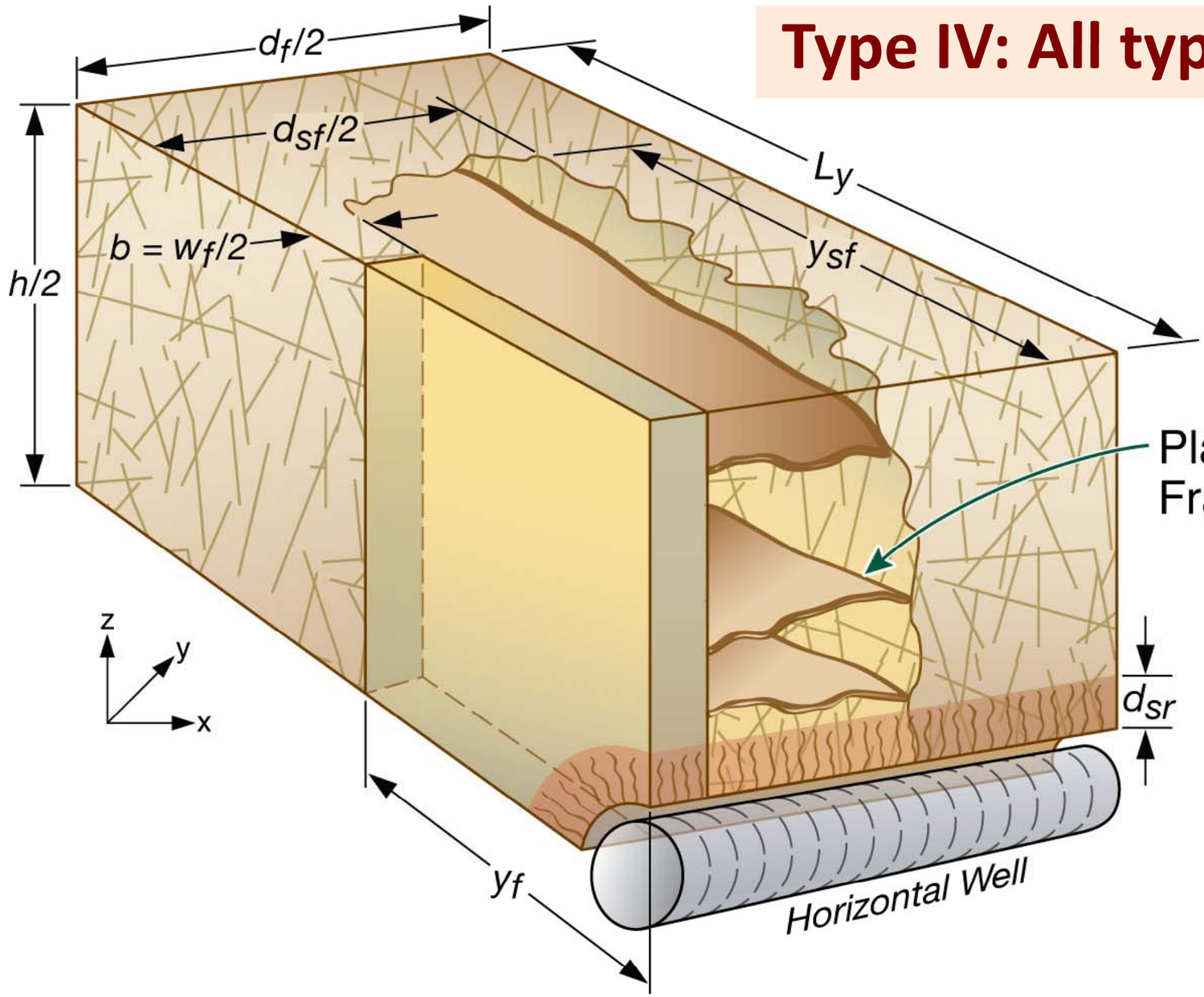
Similarly for vertical wells

Native fractures

- *Difficult to describe individually*

# APPLICATION EXAMPLES: Problem A2

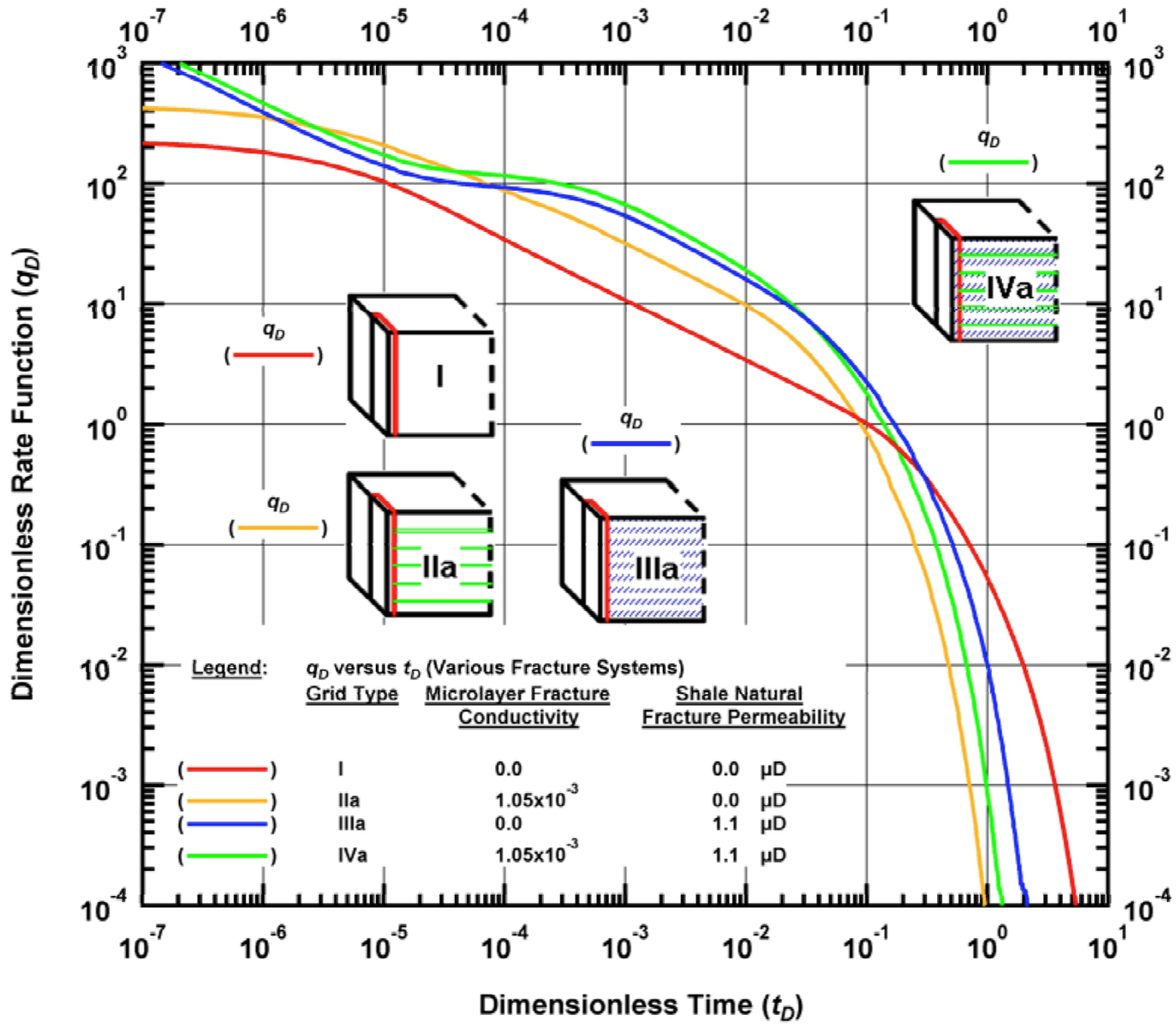
## Type IV: All types of fractures




Similarly for vertical wells

# APPLICATION EXAMPLES: Problem A2

**Numerical simulation results: up to 1,200,000 elements (Freeman, 2010; Moridis et al., 2010)**

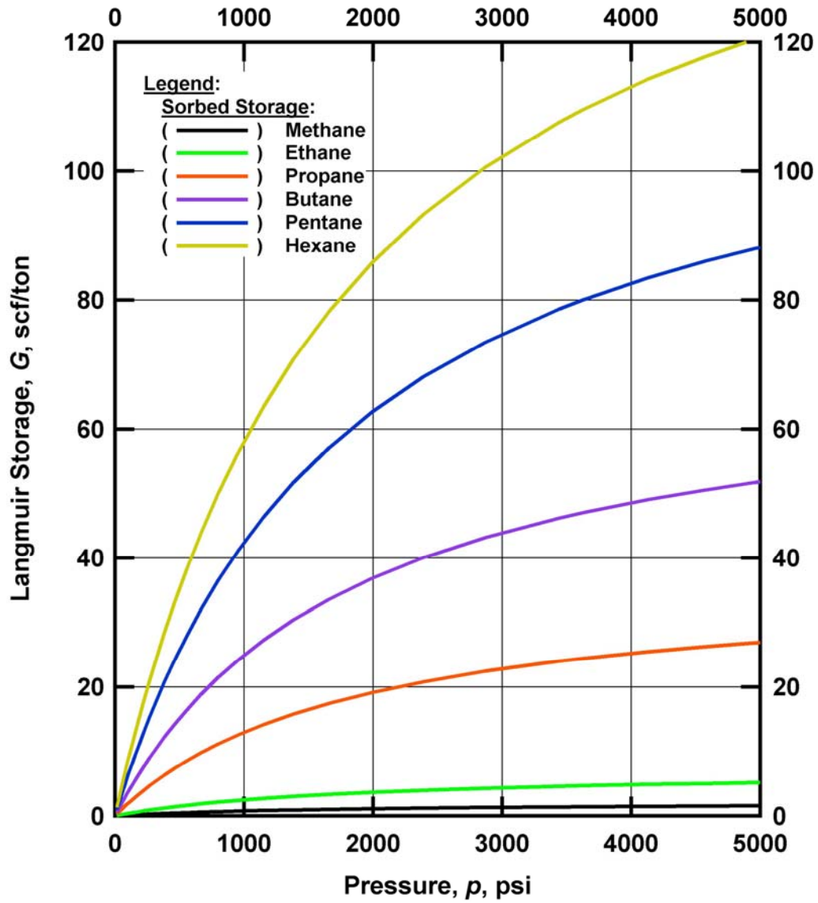


# APPLICATION EXAMPLES

## Problem A3: Flowing gas composition changes in shale gas wells

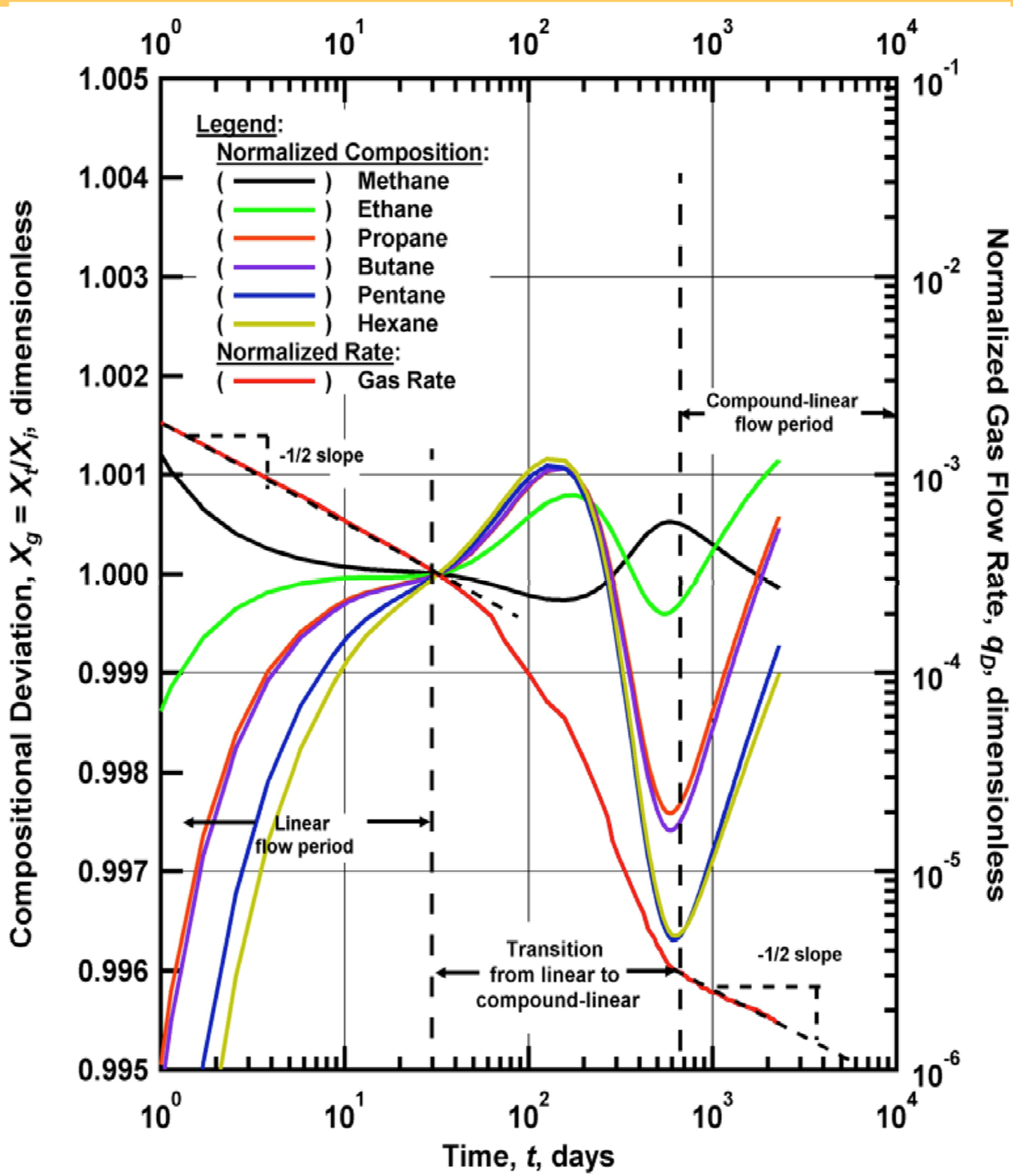
### System Specifics: Type I

- **Type I**
- **Gas Composition**
  - CH4 : 80%
  - $C_2H_6$ : 7%
  - $C_3H_8$ : 5%
  - $C_4H_{10}$: 5%
  - $C_5H_{12}$: 2%
  - $C_6H_{16}$: 1%



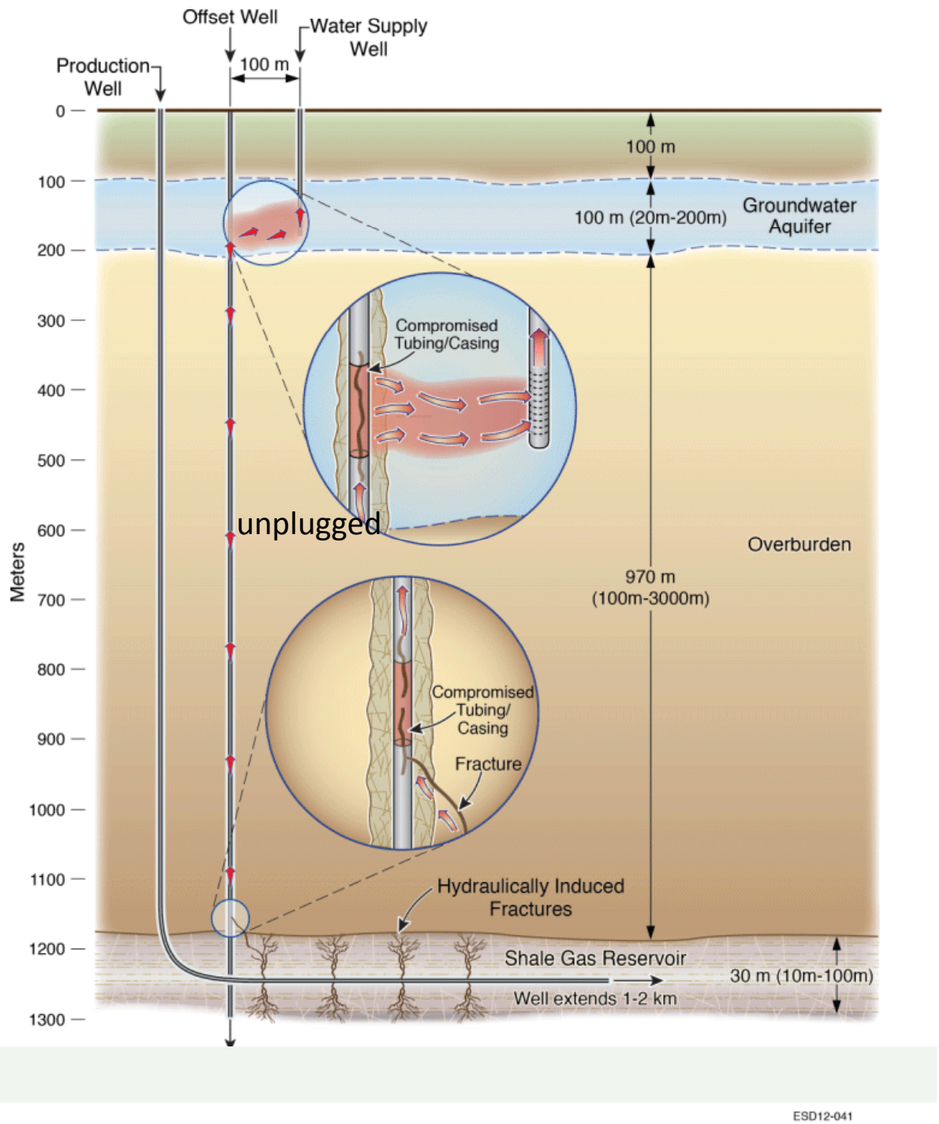
# APPLICATION EXAMPLES: Problem A3

**Numerical simulation results: 800,000 elements (Freeman et al., 2012)**

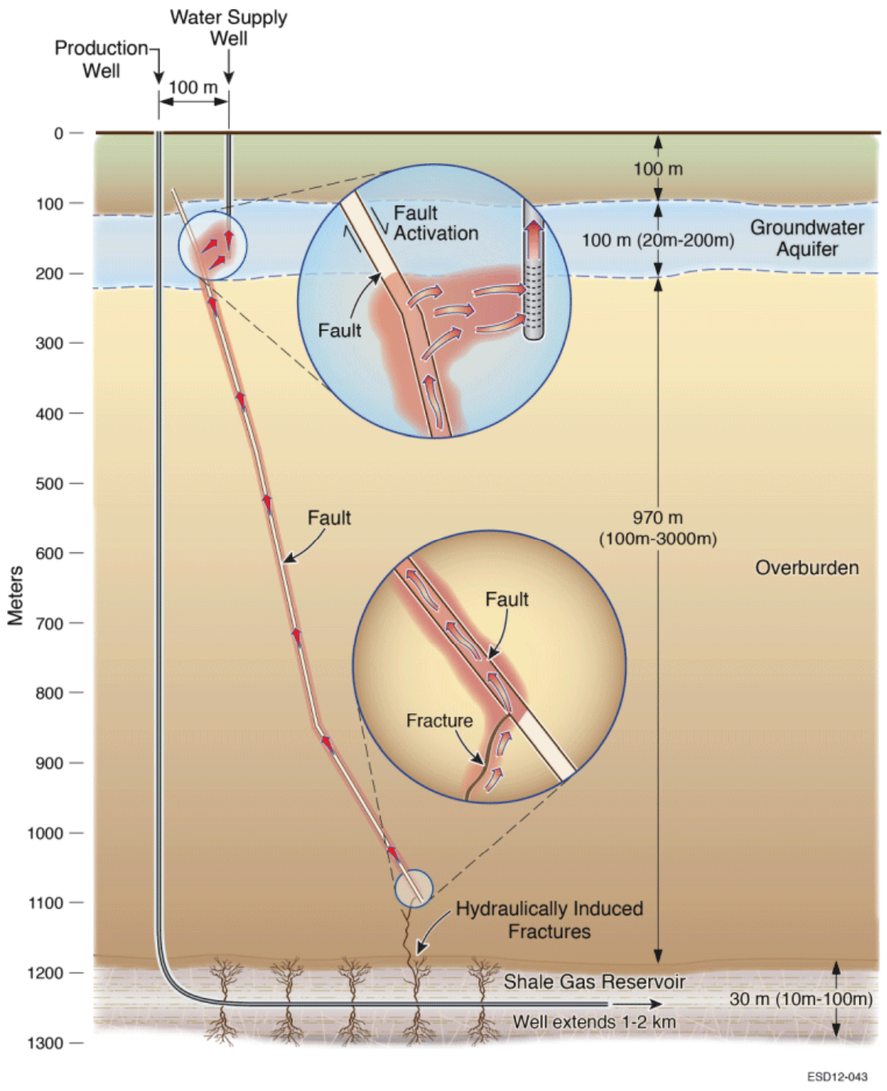


# Modeling Failure Scenarios:  Wells, Faults and Fractures

## Artificial Pathways: Well(s)




## Natural Pathways: Faults or Fractures






(1) Physically possible?  **(2) Potential for fluid migration?**

# Mesh Generation Process

MeshVoro code for unstructured mesh generation developed for complex 3D geometries.

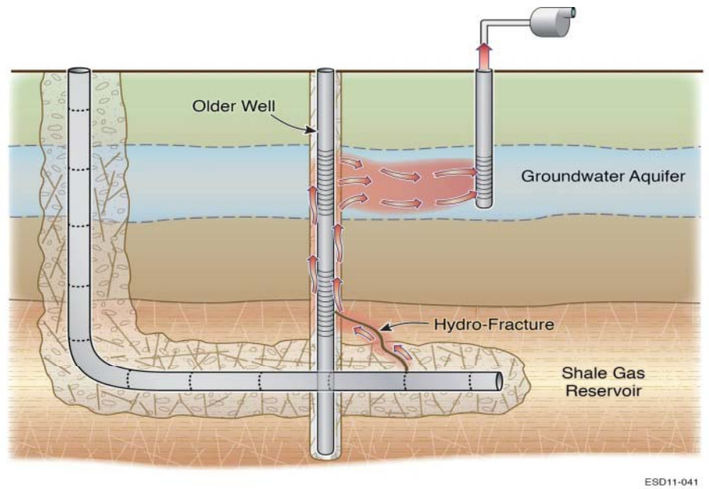



**Figure 1.a: Conceptual schematic.**

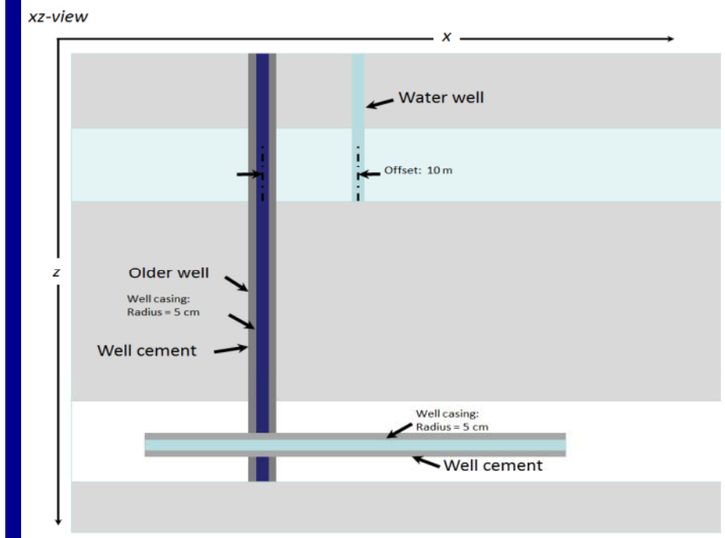



**Figure 1.b: Engineering detail.**

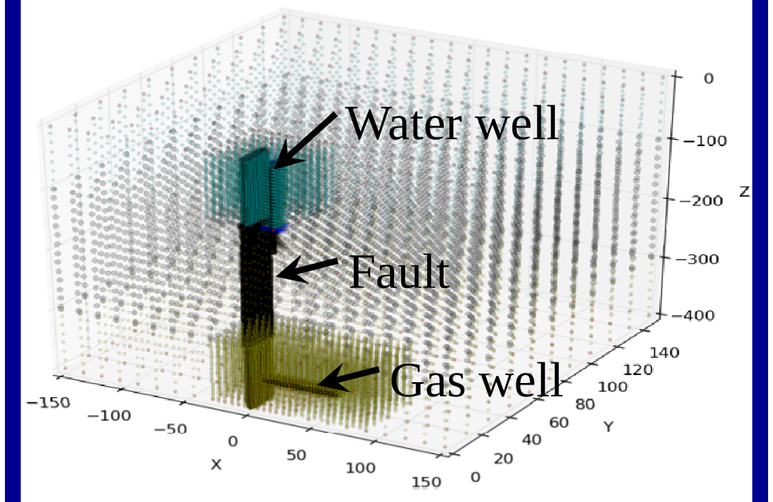



**Figure 1.c: Pointcloud rendering.**

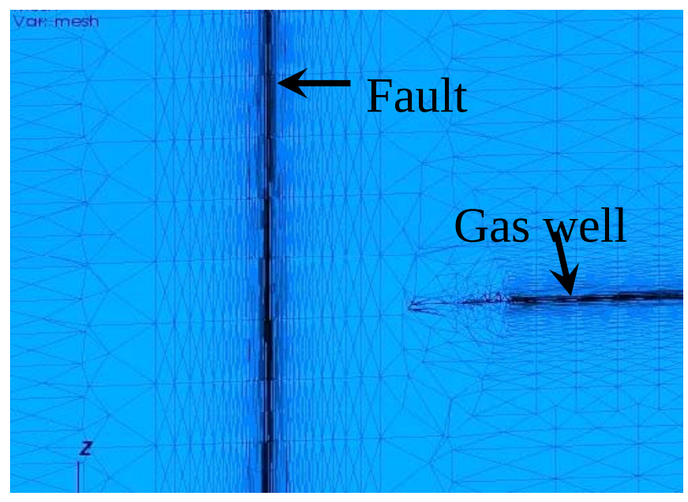
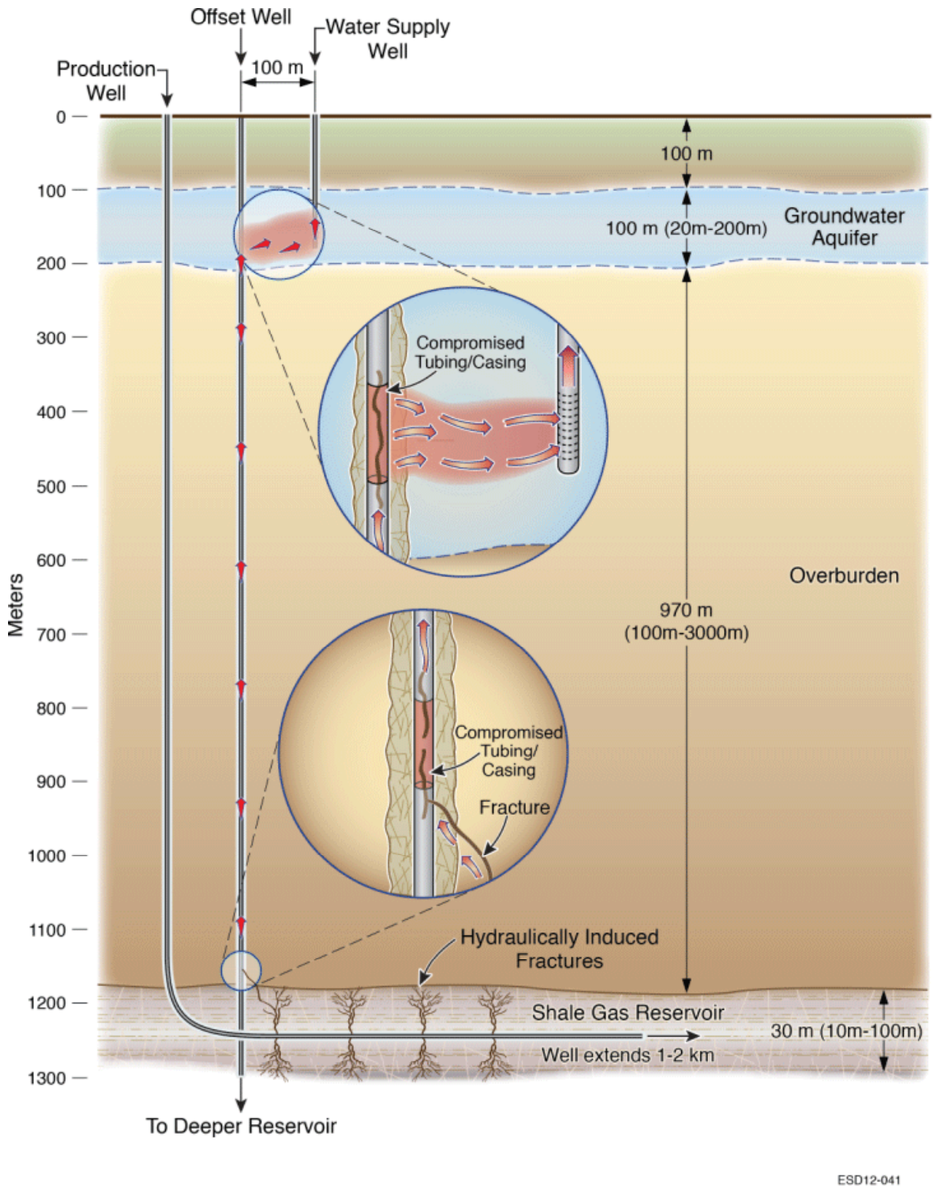


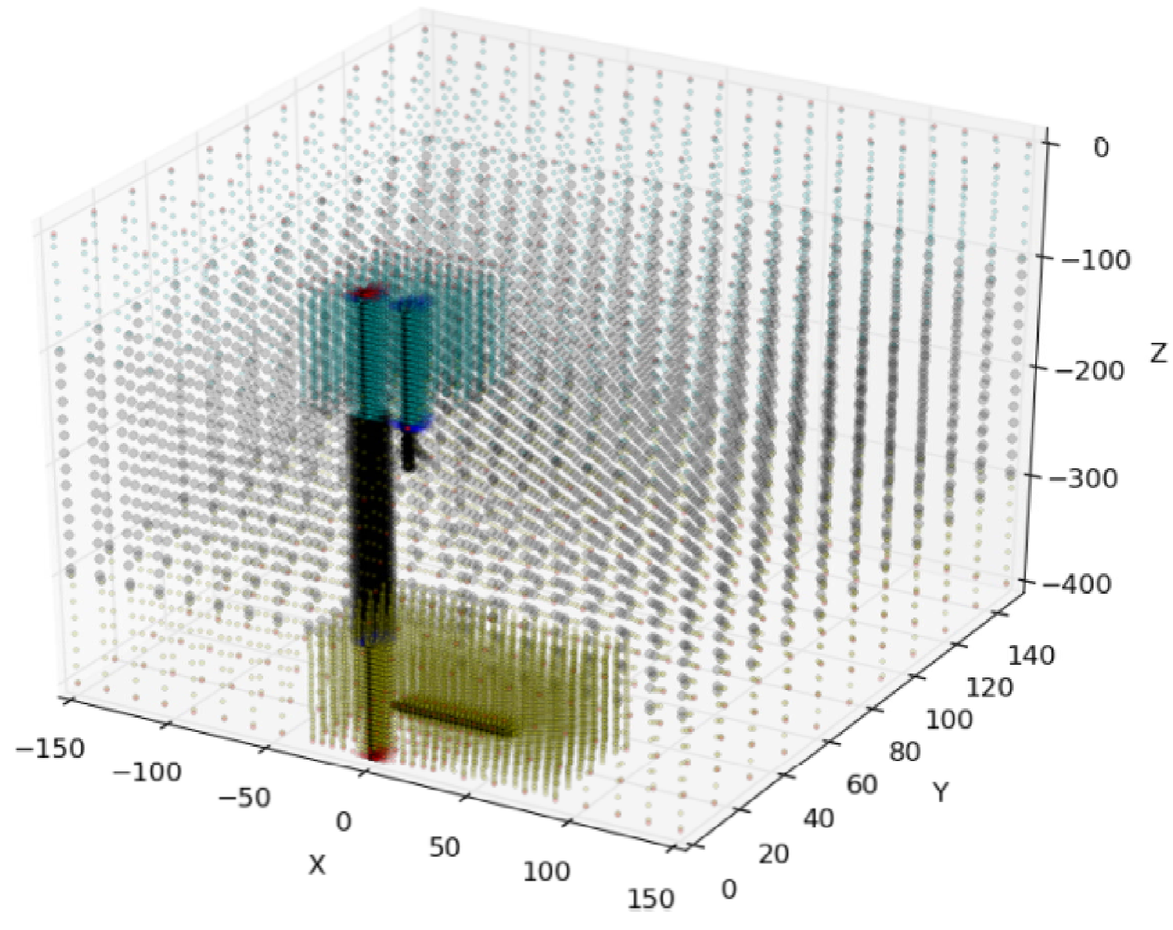

**Figure 1.d: Close-up of Voronoi mesh.**

**Workflow for generation of complex Voronoi meshes using the MeshVoro code base. The generated meshes typically possess between 100,000 and 500,000 elements.**

# Conceptual Model Building:

## Scenarios: Well(s) as a Pathway

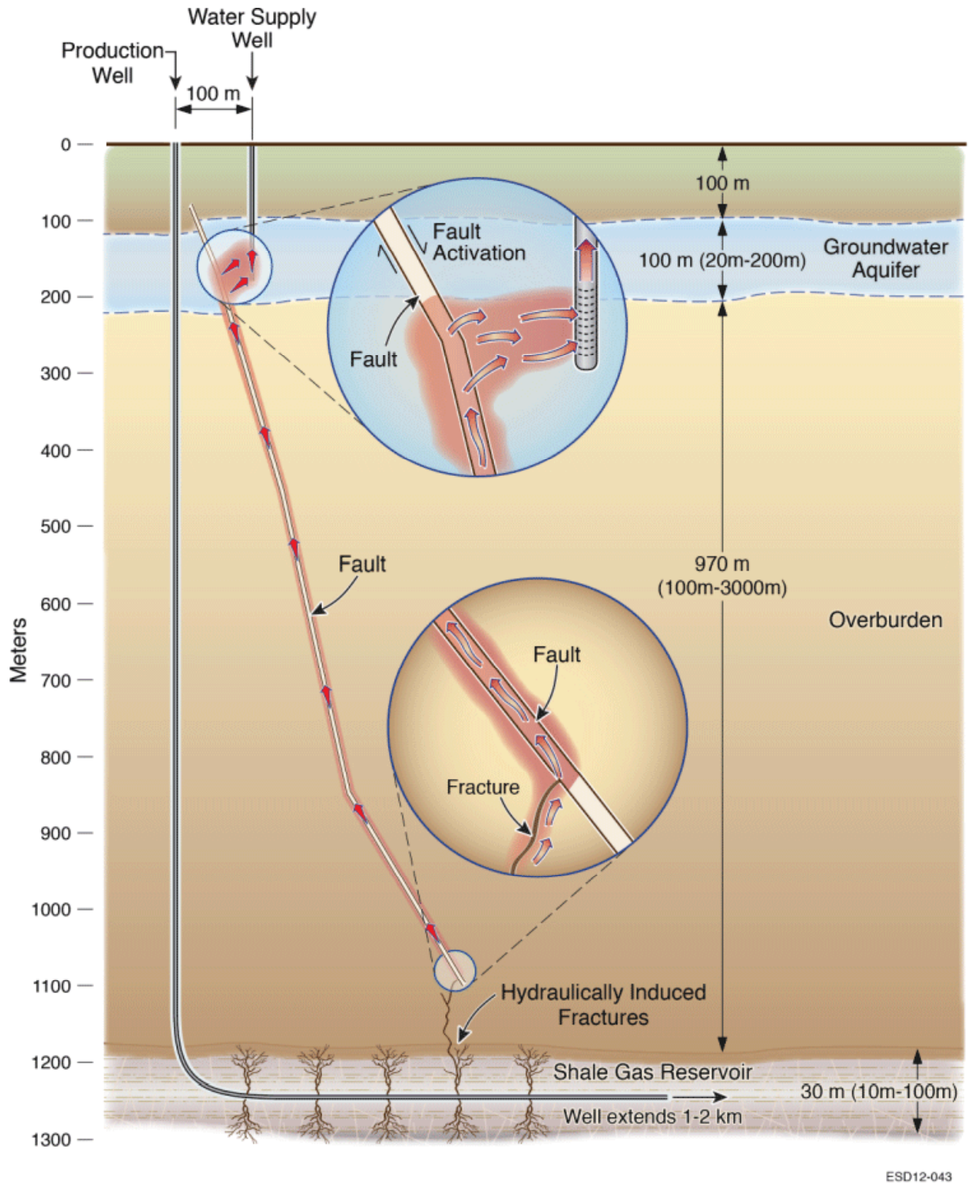


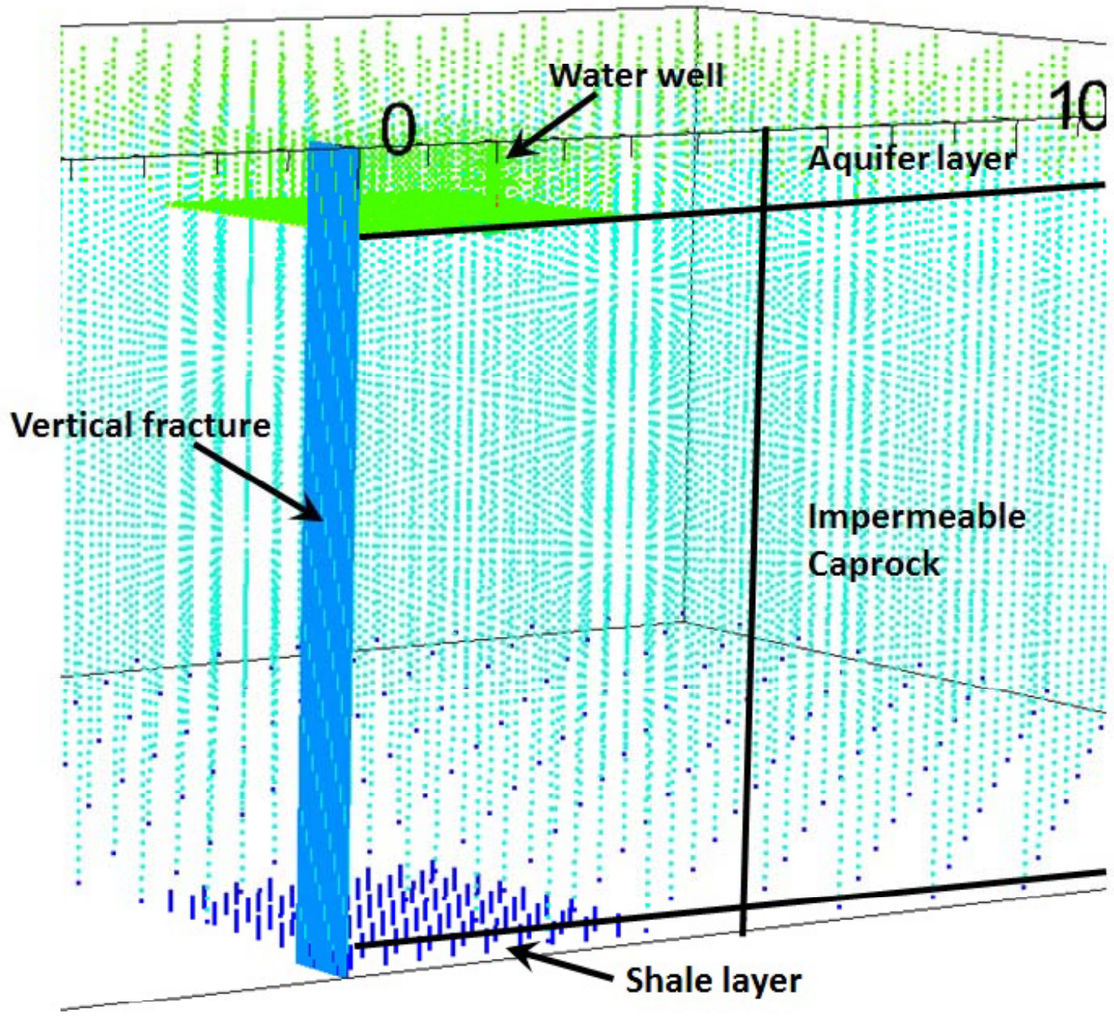




Various zones of the simulated system. Colors denote different material types.

# Conceptual Model Building:

## Scenarios: Fault/Fractures Pathway




Annotated view of the various zones of the simulated system. Colors denote different material types.

# Some properties & conditions of systems under investigation

**Abandoned leaking well**

| $k_{shale}$ ($m^2$) | $k_{well}$ ($m^2$) | Well Production Rates: Shale well (kg/s) | Well Production Rates: Water well (gpm) |
|---|---|---|---|
| 3.00E-19 | 3.00E-09 | **1.00E-03** | 0.00E+00 |
| 3.00E-19 | 3.00E-09 | **1.00E-04** | **1.00E-01** |
| 3.00E-19 | **3.00E-14** | 0.00E+00 | 0.00E+00 |
| **3.00E-18** | **3.00E-14** | 0.00E+00 | 0.00E+00 |

**Penetrating fracture**

| $k_{shale}$ ($m^2$) | $k_{frac}$ ($m^2$) | Shale well (kg/s) | Water well (gpm) |
|---|---|---|---|
| 3.00E-18 | 3.00E-13 | 0.00E+00 | 0.00E+00 |
| 3.00E-19 | 3.00E-13 | 0.00E+00 | 0.00E+00 |



Partial lists

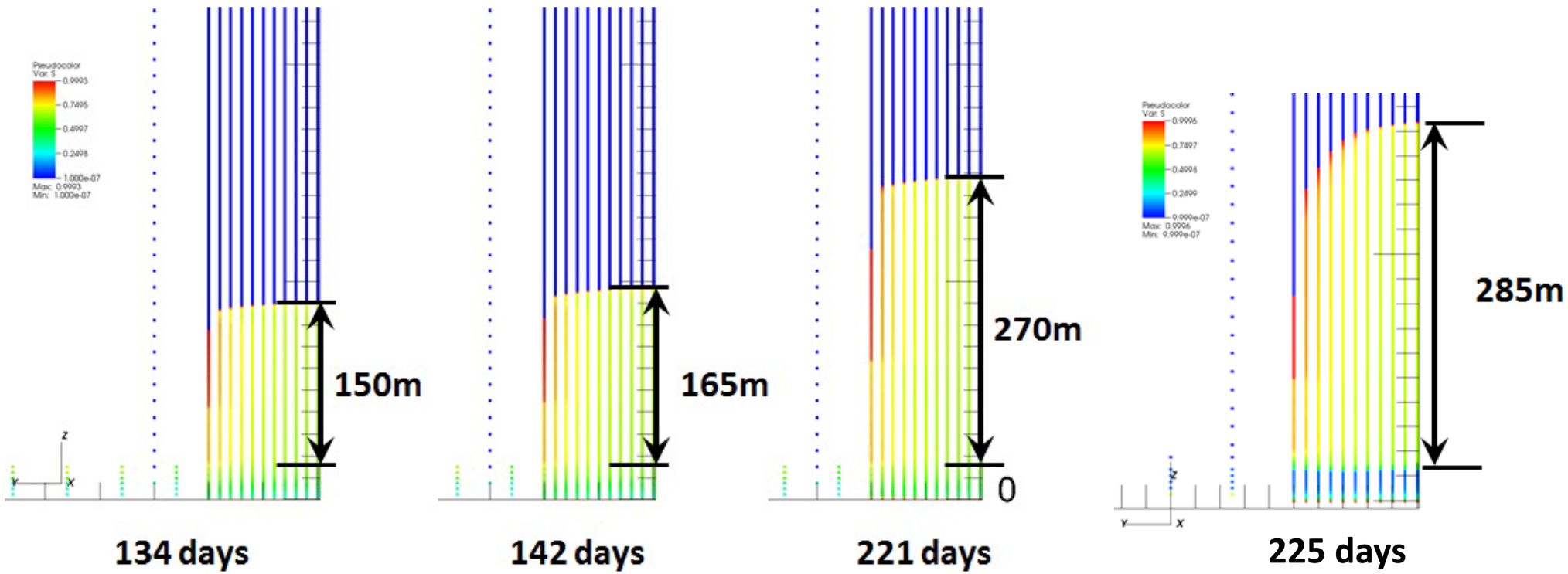
# Sensitivity Analysis:

## Characterize the problem space

1) Sensitivity parameters:
   - Conductivity of the leaking pathway (well/fault/fracture)
   - Production rate from **water** well
   - Production rate from **shale** well
   - Permeability of the shale
   - Vertical distance between gas-bearing shale and aquifer
   - Relative pressure regimes between the aquifer and the shale (as affected by respective production rates)

# Results:

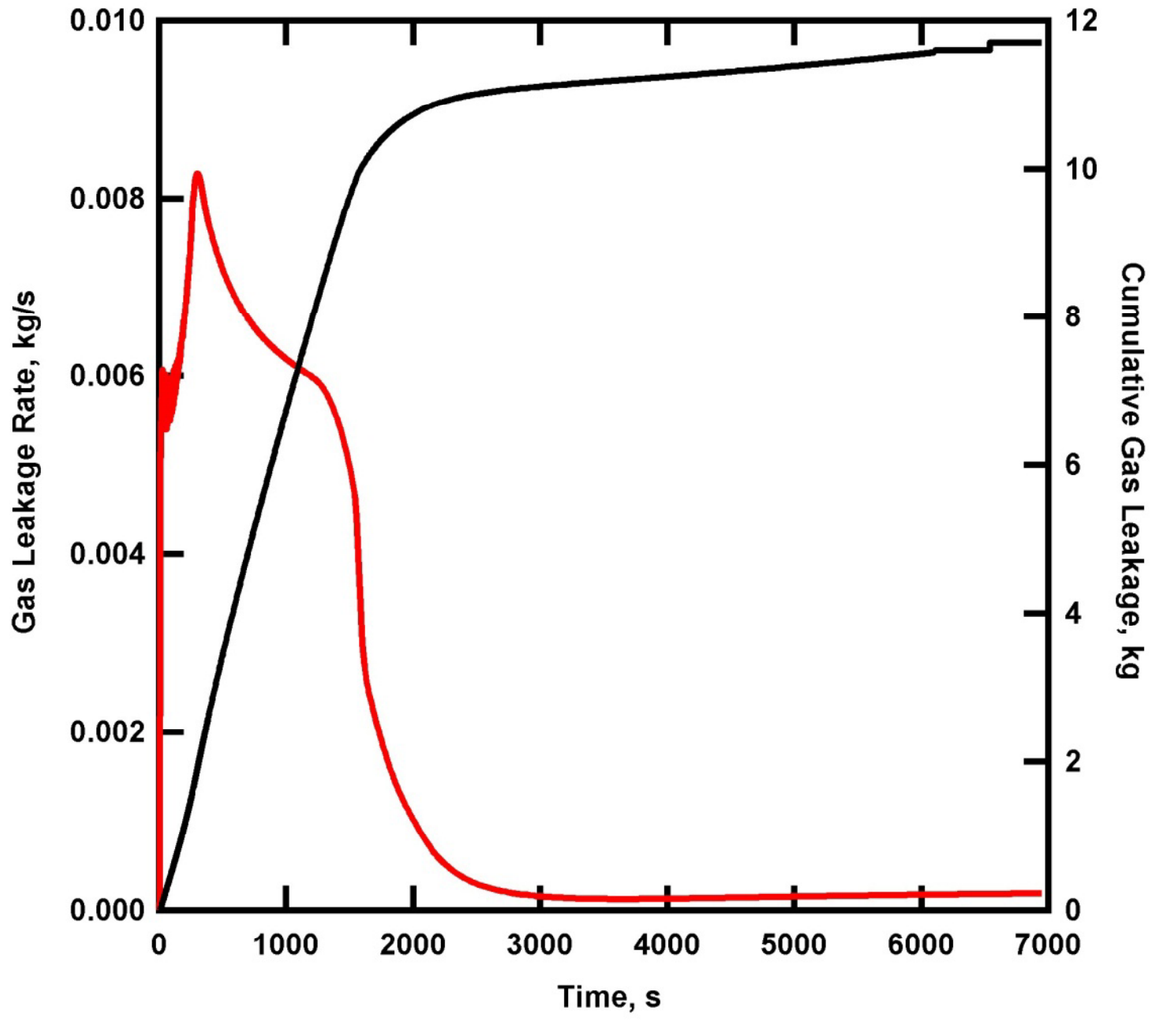
## Gas plume rises through fracture




**Saturation distribution at along the fracture at time snapshots of 134 days, 142 days, 221 days, and 225 days depicting the behavior of the gas plume over time with an overlying water well providing suction.**

# Results:

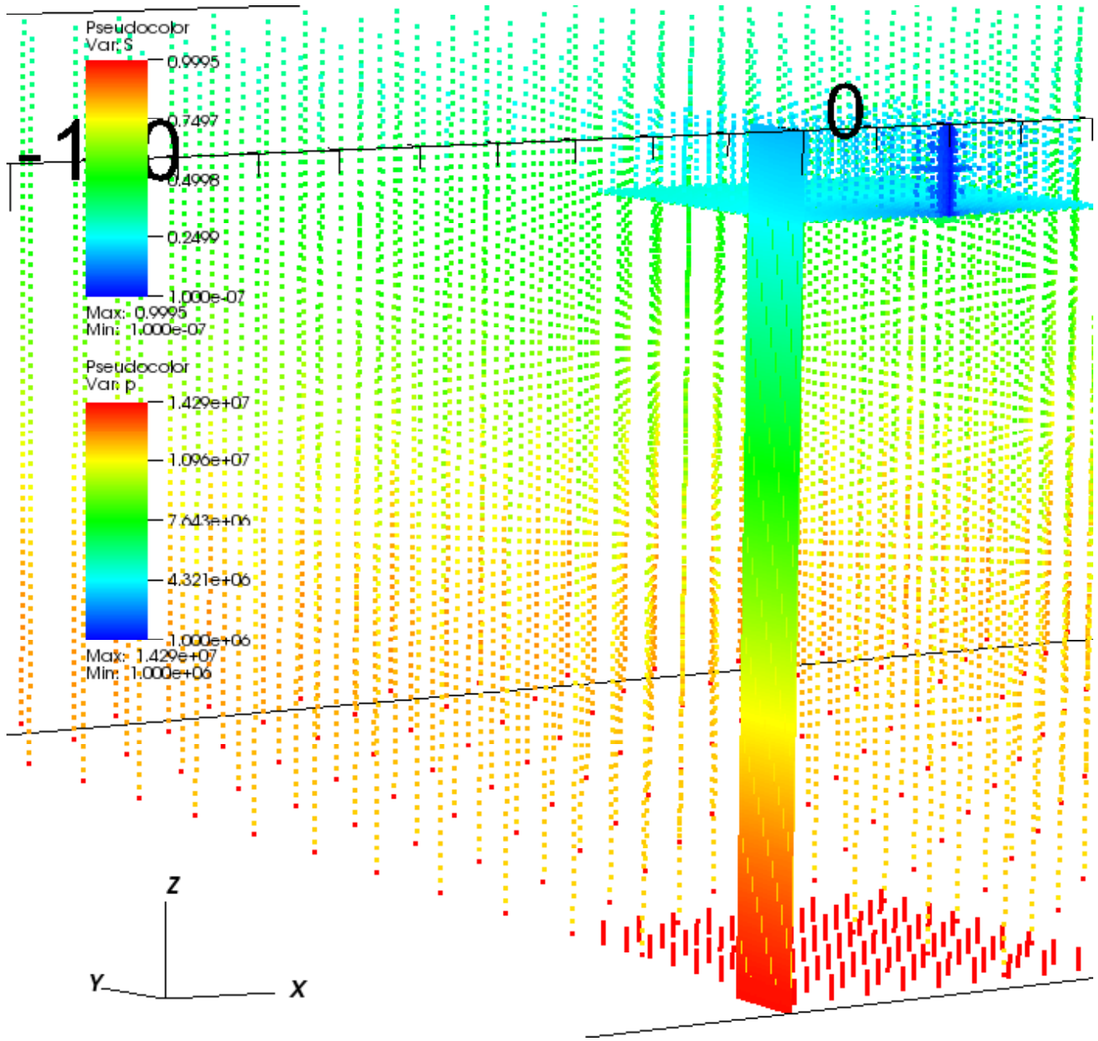
## Gas plume rises through wellbore



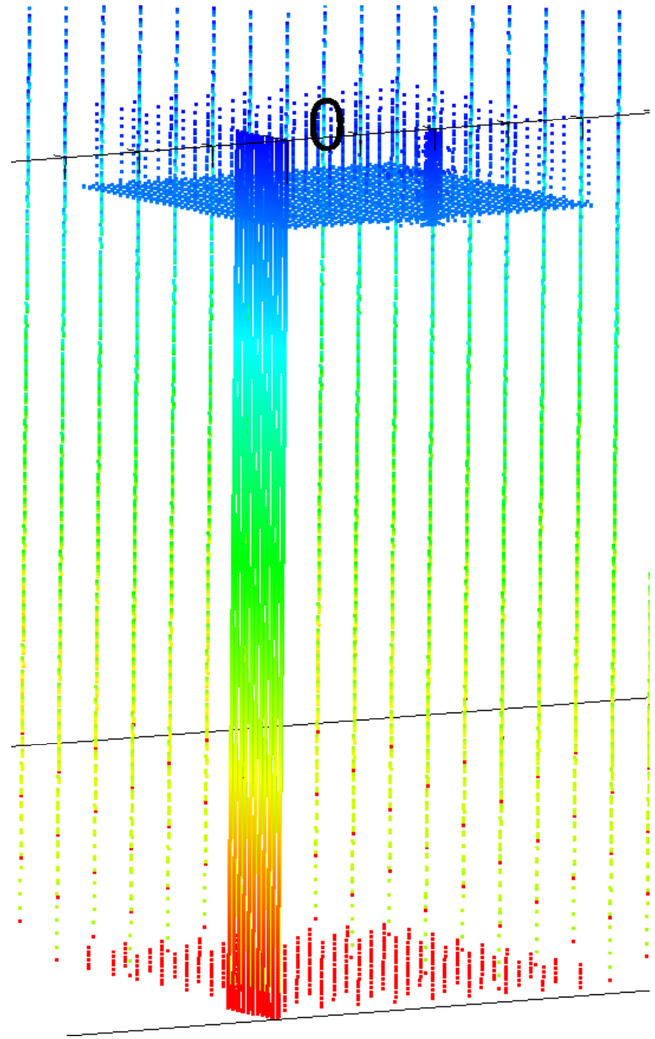

**Gas leakage rate and cumulative leaked gas through an old abandoned well, with a shale layer permeability of 3.0e-18 $m^2$ and a wellbore permeability of 3.0e-9 $m^2$. After an initial "bubble" of gas (~11 kg) percolates to the aquifer, the leakage rate drops to approximately 2.2e-4 kg, or 19.0 kg/day, and then rises very gradually.**

# Results:
# Drawdown of aquifer

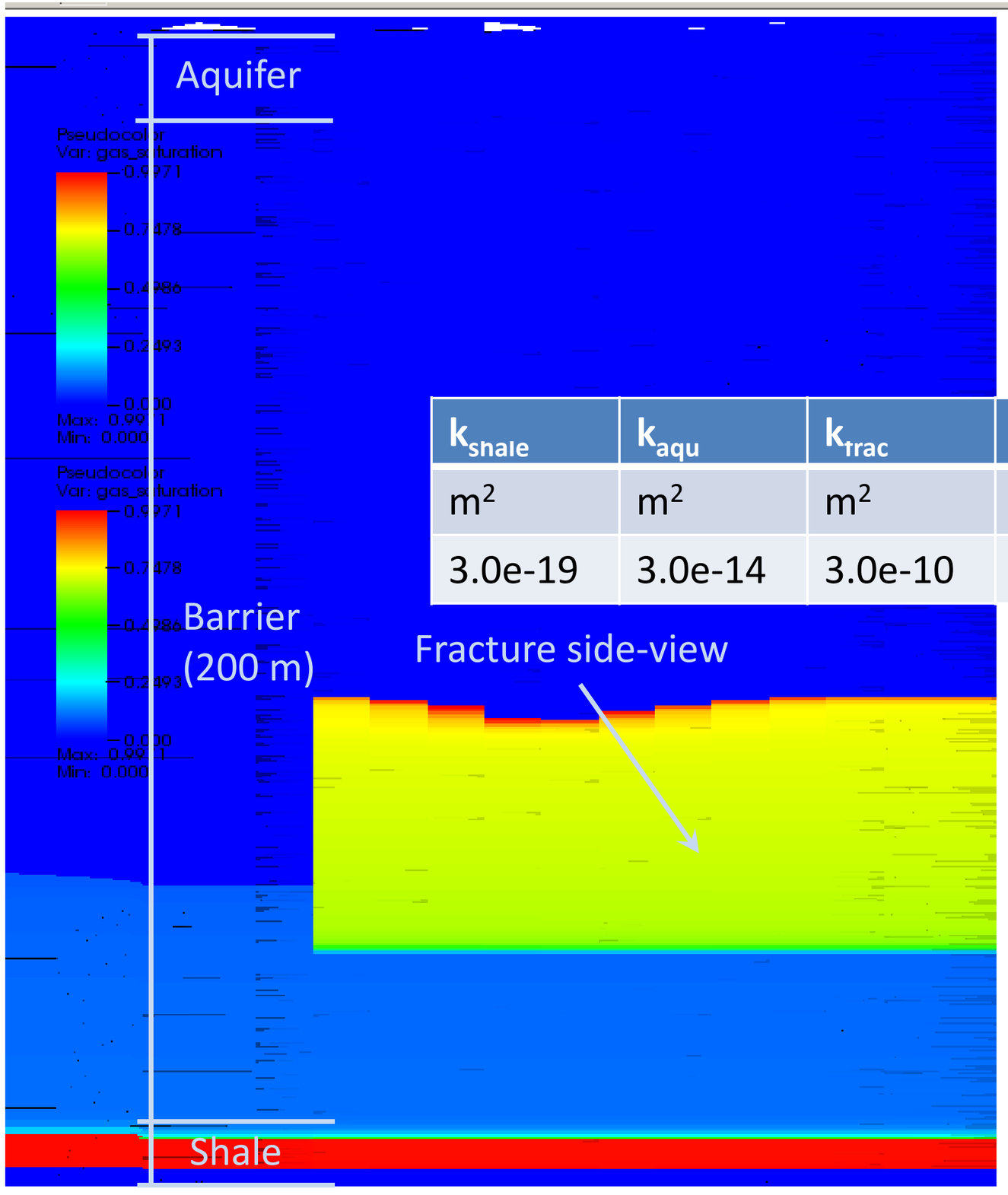
a.




b.

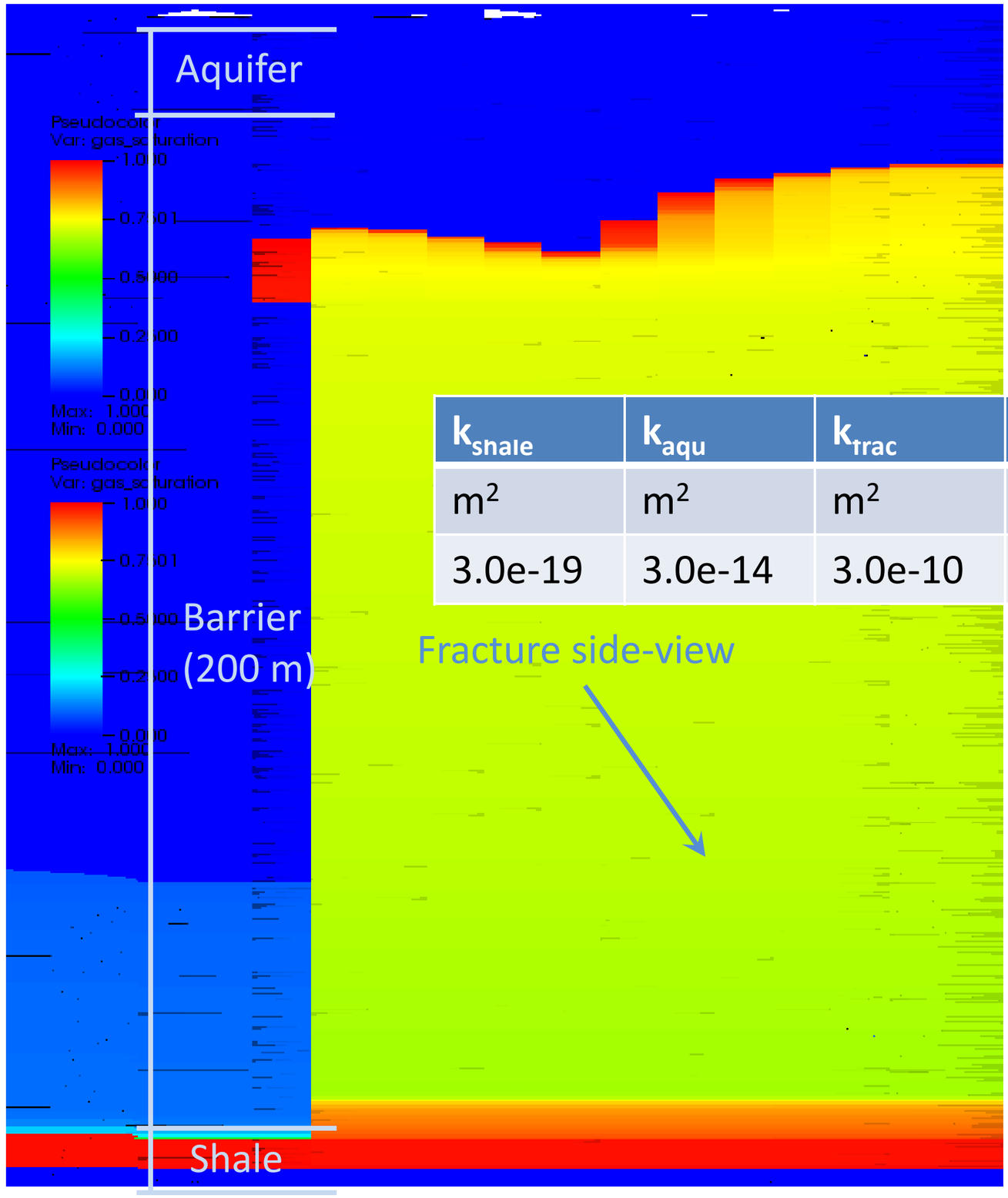



**a.** Pressure distribution at 134 days with water well producing at 1.0e6 Pa bottomhole pressure;
**b.** Pressure distribution at 221 days with water well producing at 1.0e6 Pa bottomhole pressure




| $k_{snale}$ | $k_{aqu}$ | $k_{trac}$ | $q_{water}$ |
|---|---|---|---|
| $m^2$ | $m^2$ | $m^2$ | kg/s |
| 3.0e-19 | 3.0e-14 | 3.0e-10 | 0.0 |

3000 seconds
Case 161



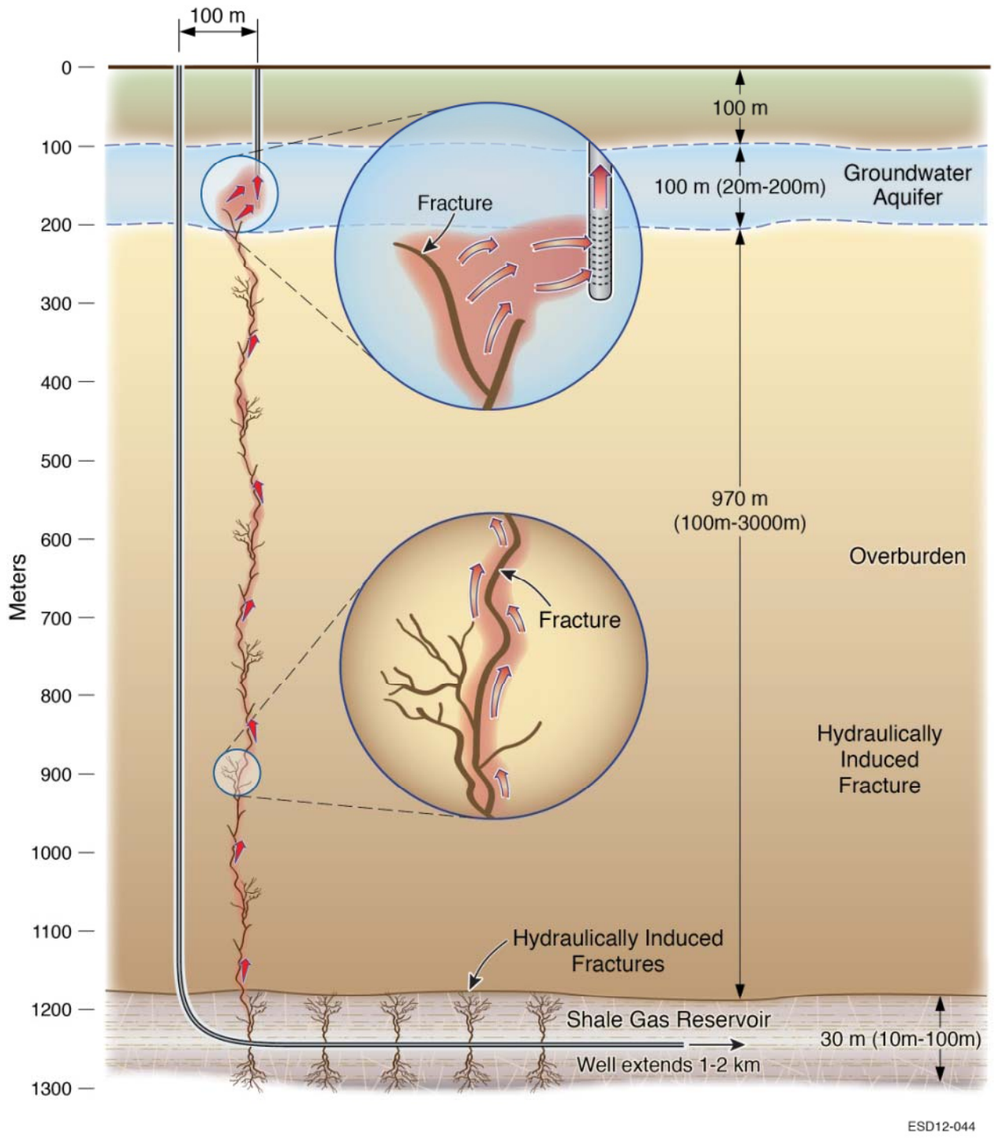

| $k_{shale}$ | $k_{aqu}$ | $k_{trac}$ | $q_{water}$ |
|---|---|---|---|
| $m^2$ | $m^2$ | $m^2$ | kg/s |
| 3.0e-19 | 3.0e-14 | 3.0e-10 | 0.0 |

12000 seconds
Case 161

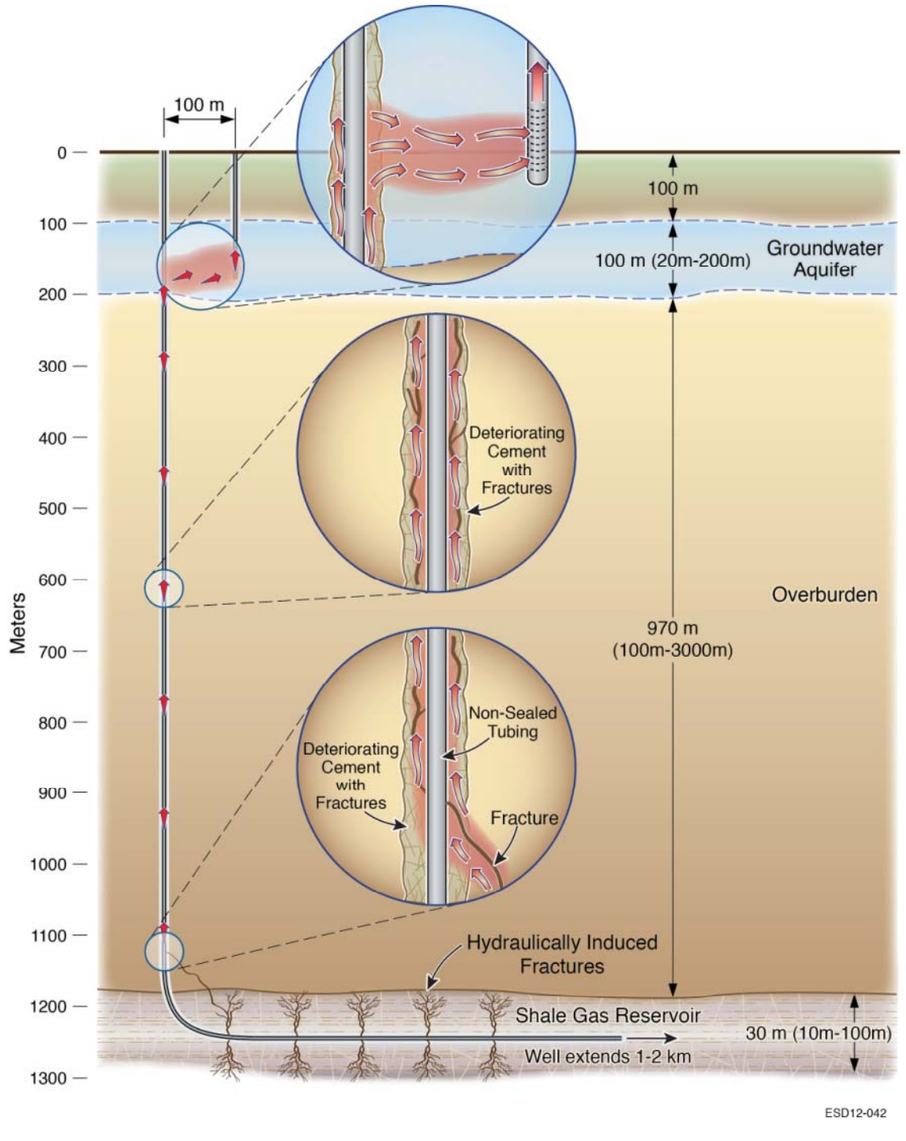
# Conclusions

1) Primary drivers for accelerated gas leakage:
   - Conductivity of the leaking pathway
   - Relative pressure regimes
   - Shale permeability
   - Shale-aquifer separation

# Modeling Failure Scenarios: Extensive Fracture Development and Fault Activation

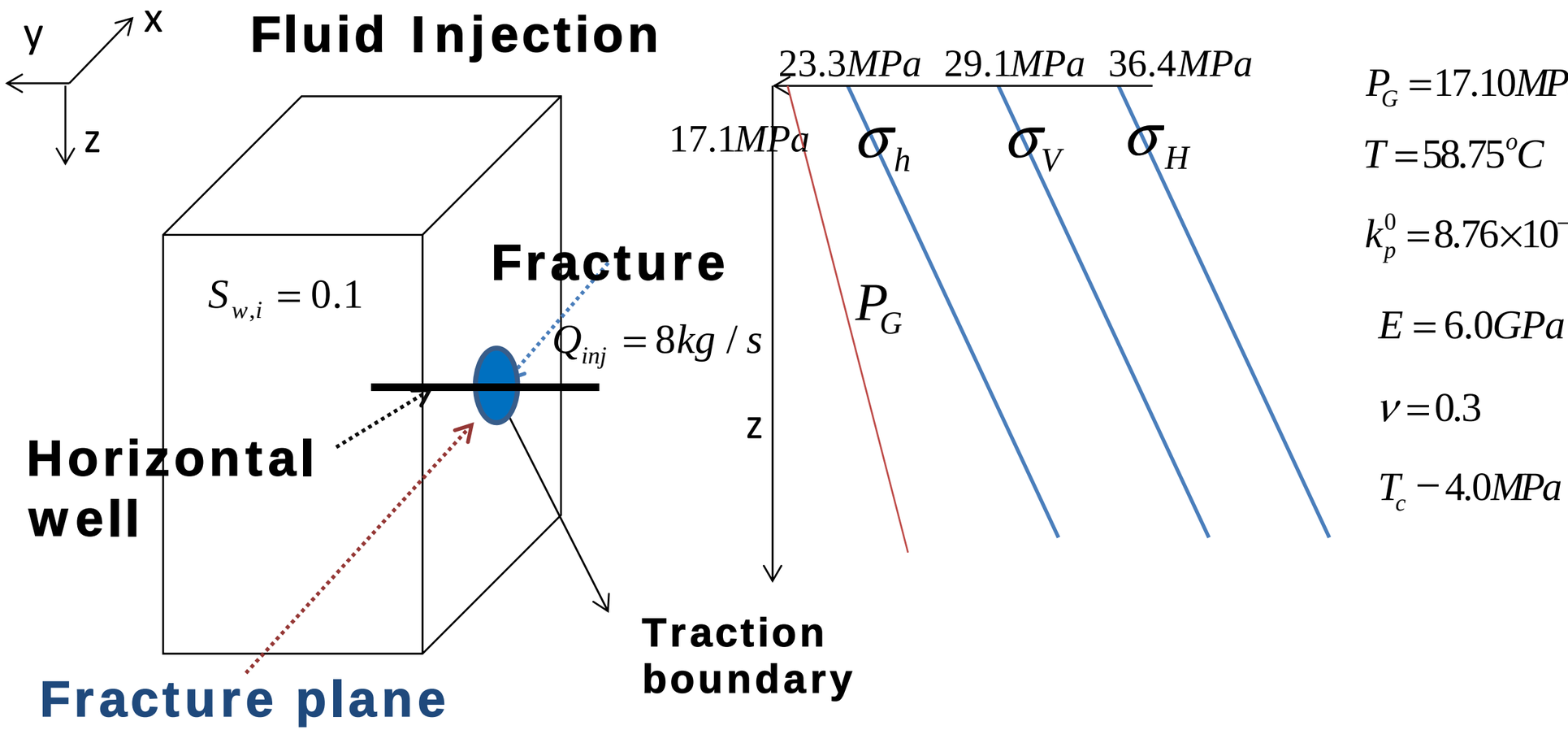



**HF extending from shale to shallow aquifer through the overburden**




**HF extending from shale to shallow aquifer through weak cement (not discussed)**

# 3D Domain




$P_G = 17.10MPa$

$T = 58.75^oC$

$k_p^0 = 8.76\times10^{-7}\,D$

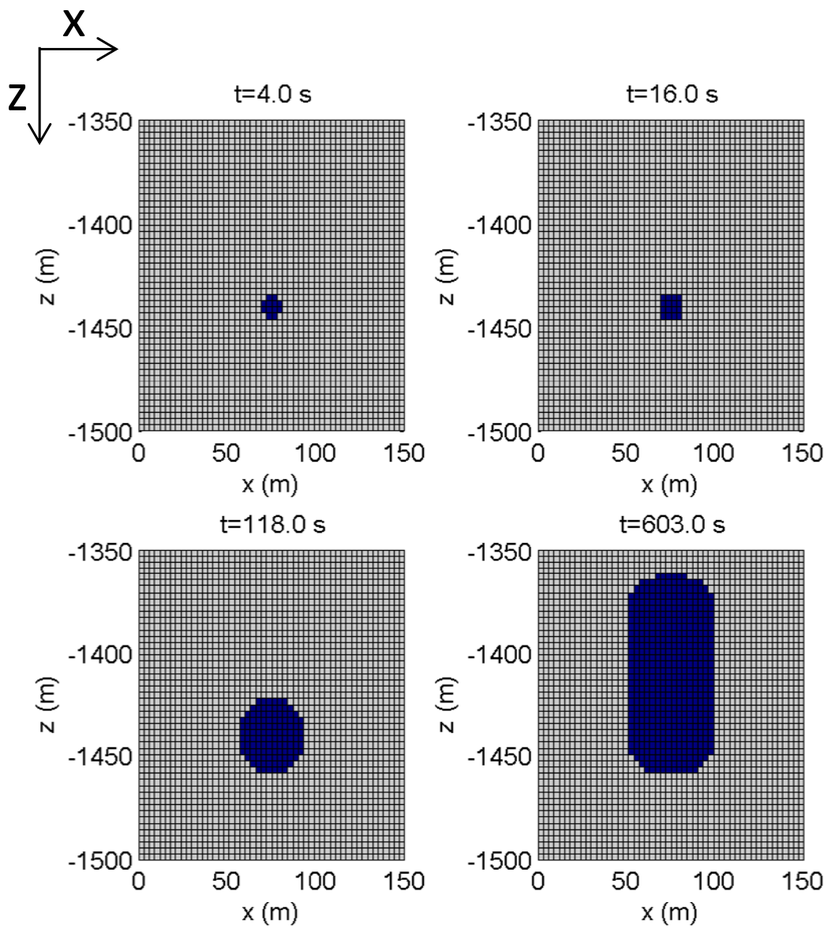
$E = 6.0GPa$

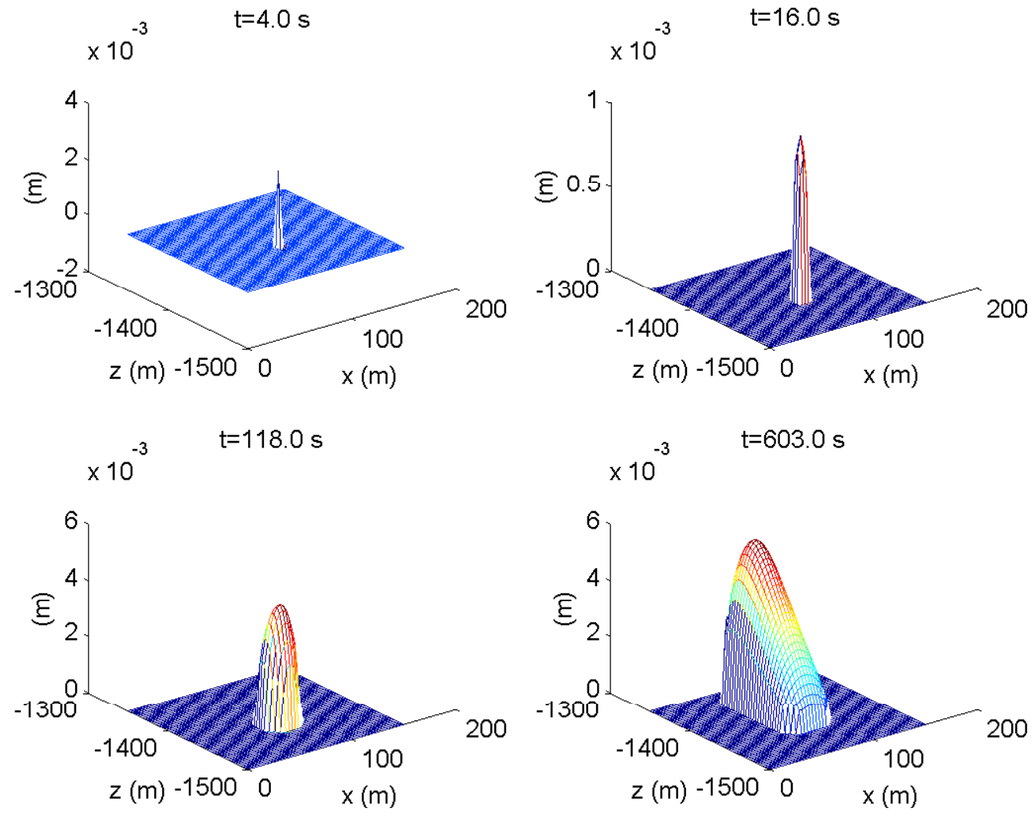
$\nu = 0.3$

$T_c - 4.0MPa$

Investigate fracture propagation in shale gas reservoirs - **properties of Marcellus shale**

# Fracture Propagation (I)



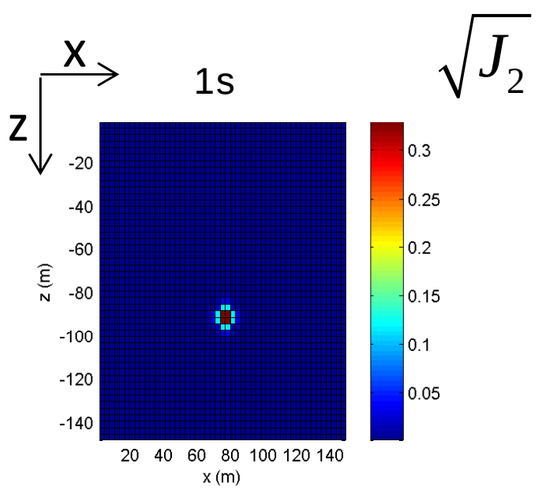



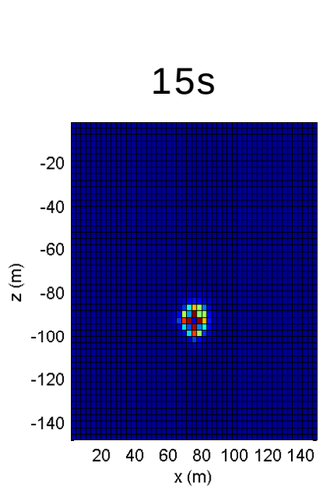

**Fractured areas** **Fracture aperture**

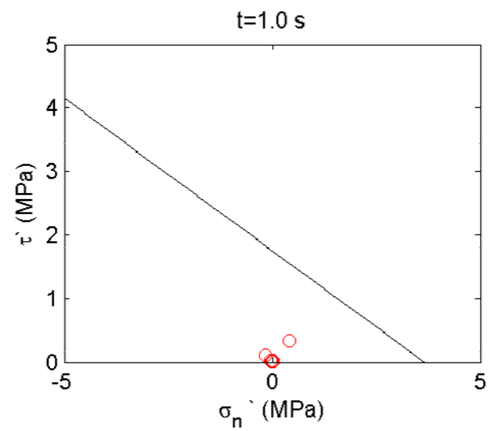
Example of fracture propagation

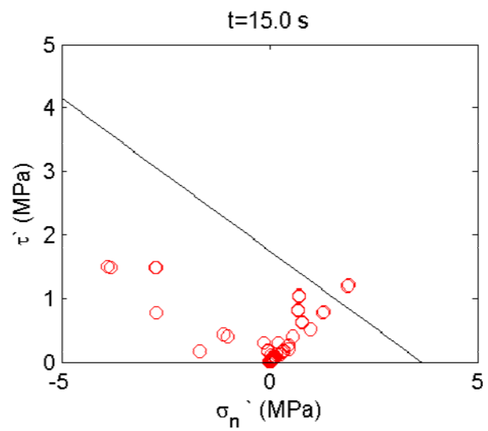
Larger fracture aperture near the fracture top

# Effective Stress



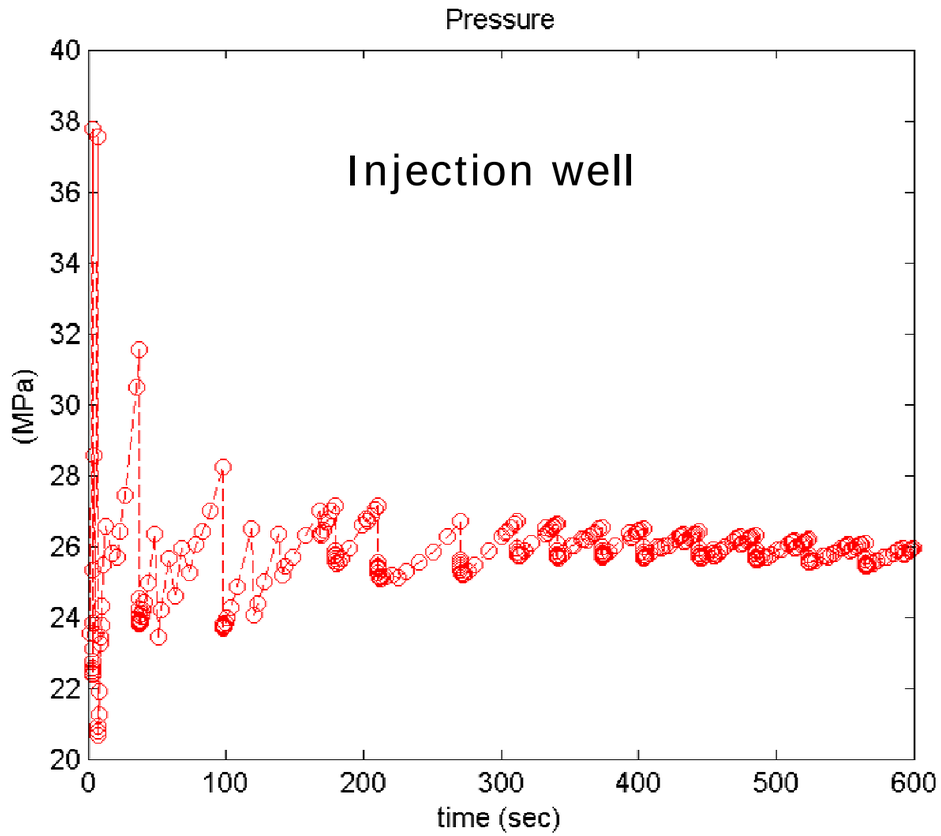



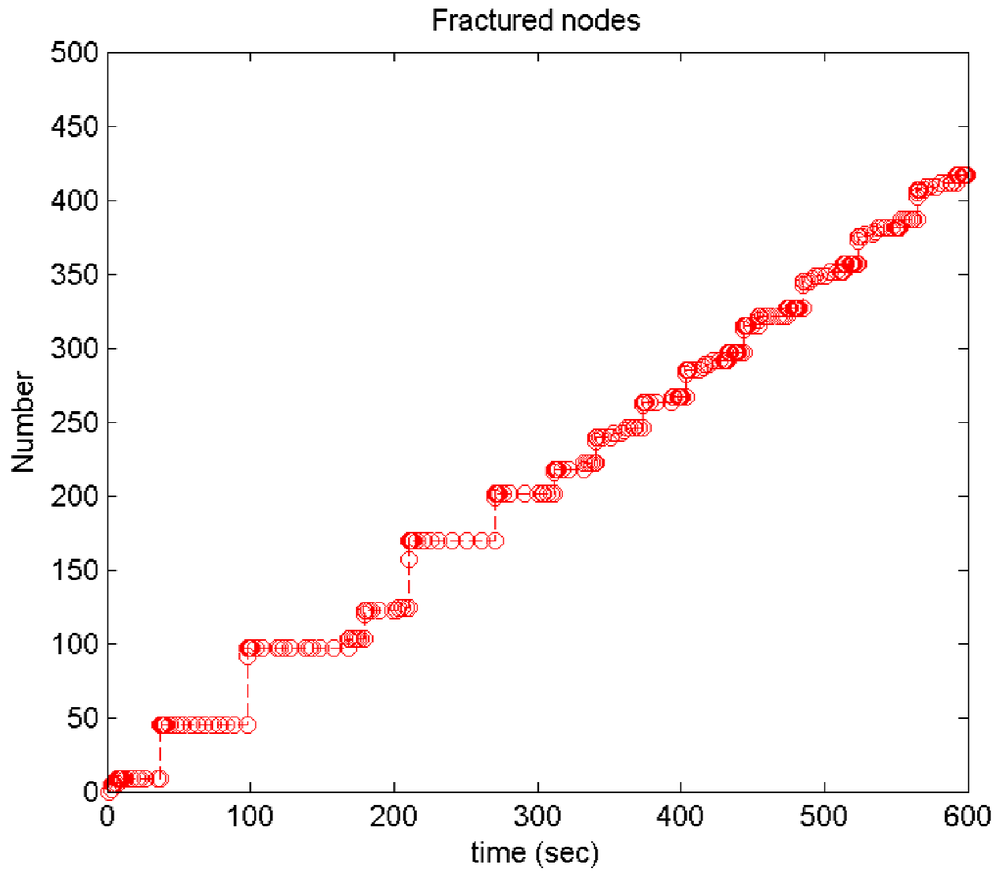




High shear stress near the fracture tips

Shear failure is possible when shear strength is low.

# Evolution of Pressure



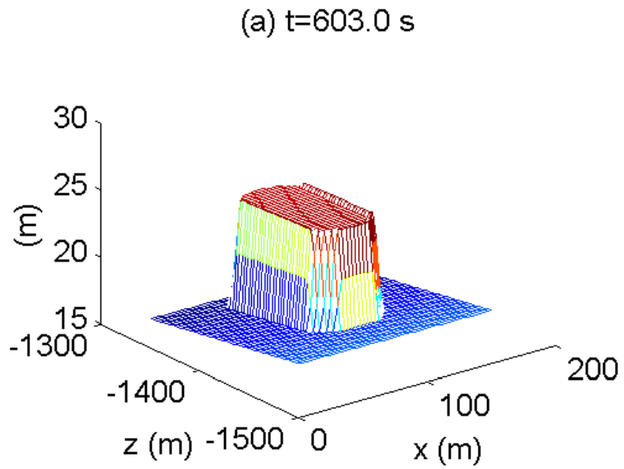



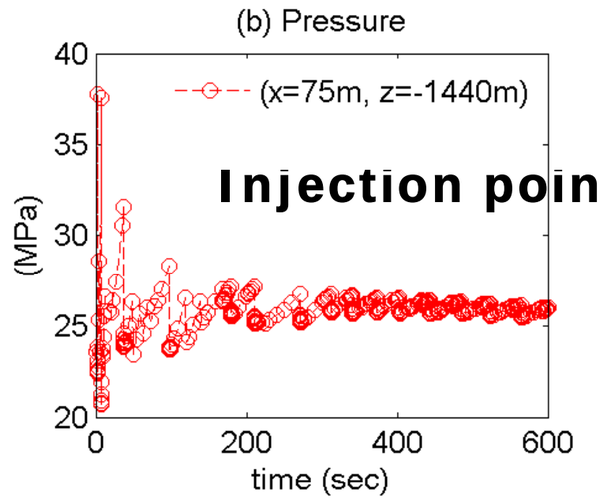

High pressure is required for fracturing, but the pressure decreases at late time

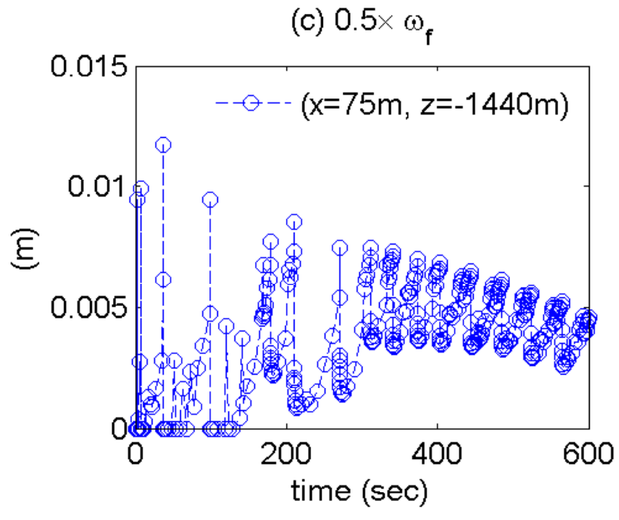
Stable fracture propagation

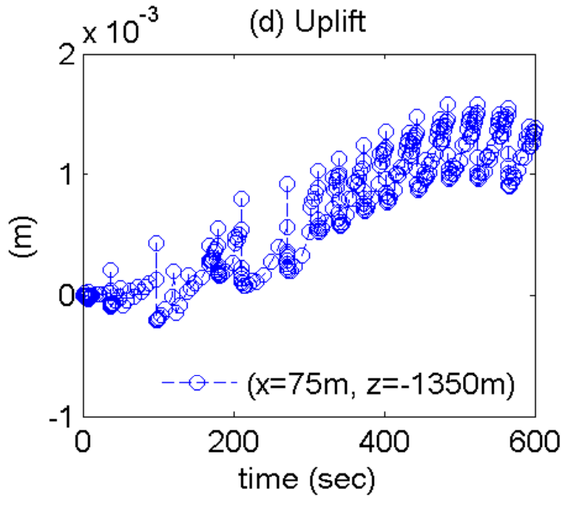
# Fracture Propagation (II)

**Fast pressure diffusion due to high permeability**



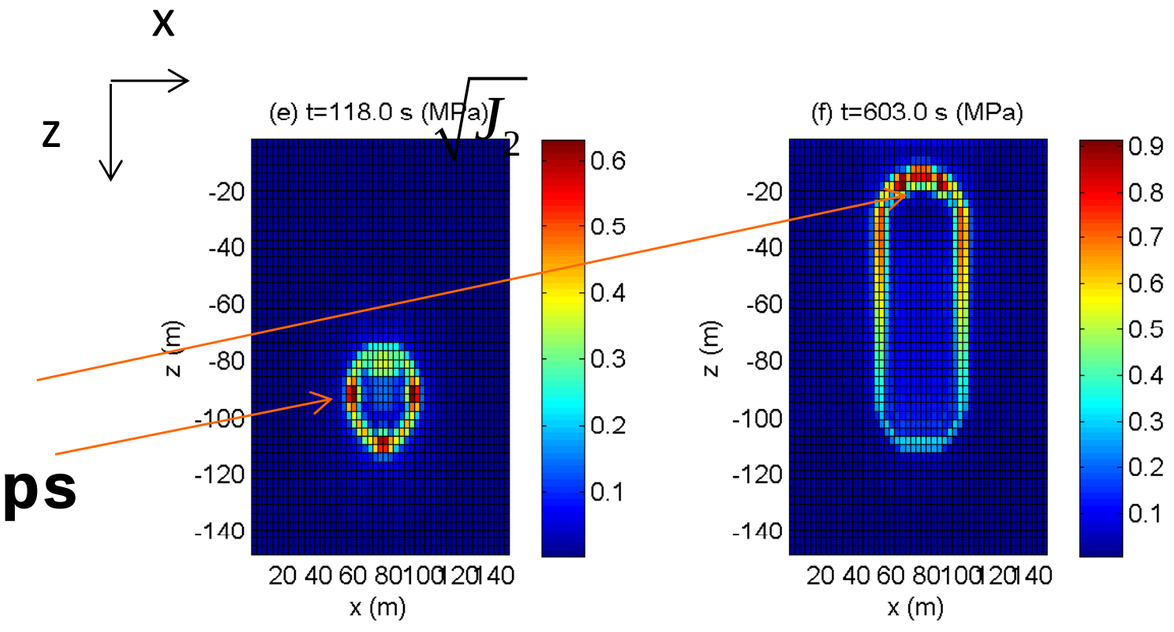




Saw-tooth (oscillatory) pressure, fracture aperture, displacement

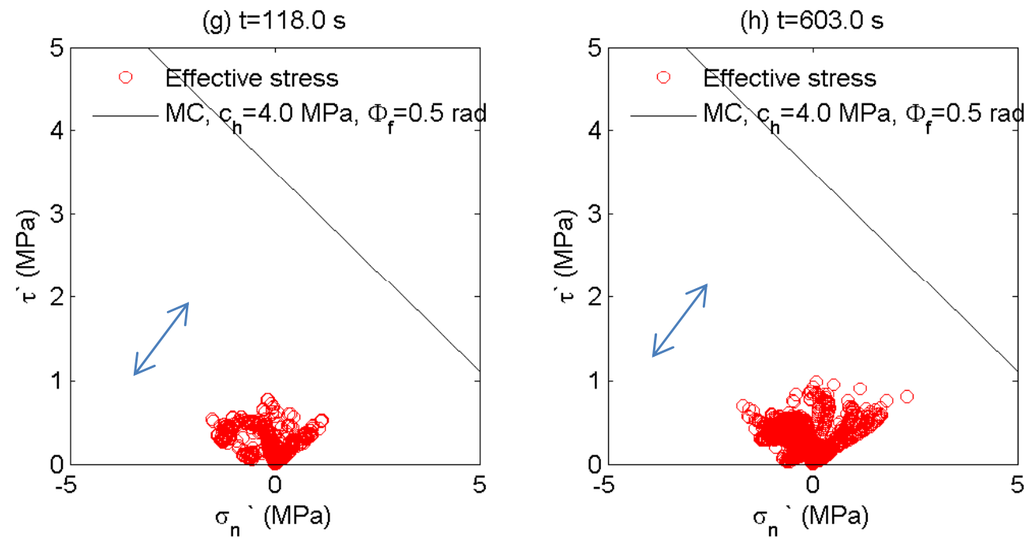
**Can be considered as microearthquakes induced by tensile failure**

# Shear stress study: an example

**High shear stress near the fracture tips**

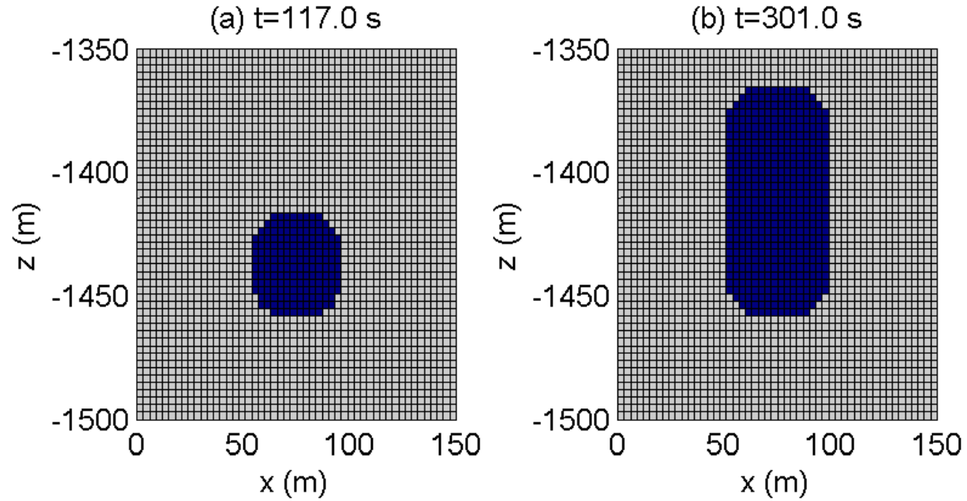



**Investigating the probability of shear failure**



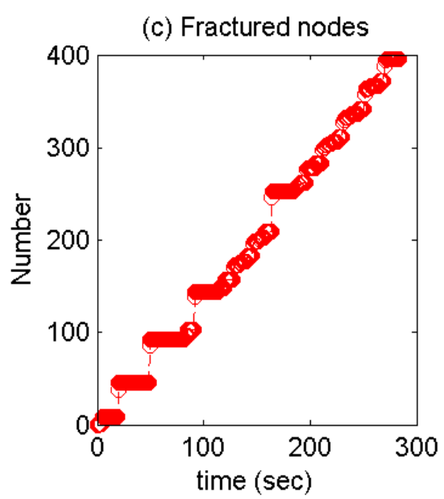
# Coexistence of water & gas

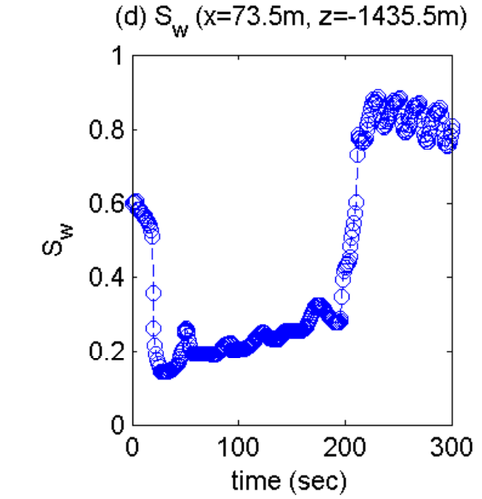
$$S_{w,i} = 0.6$$

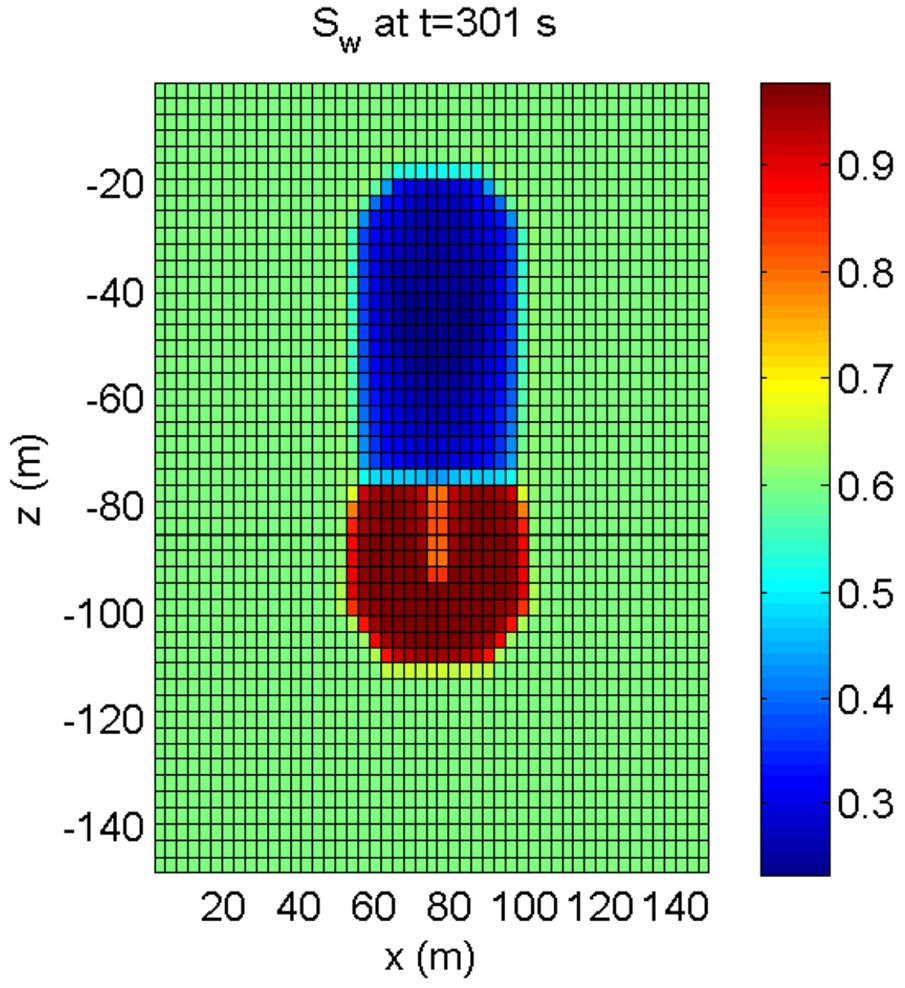








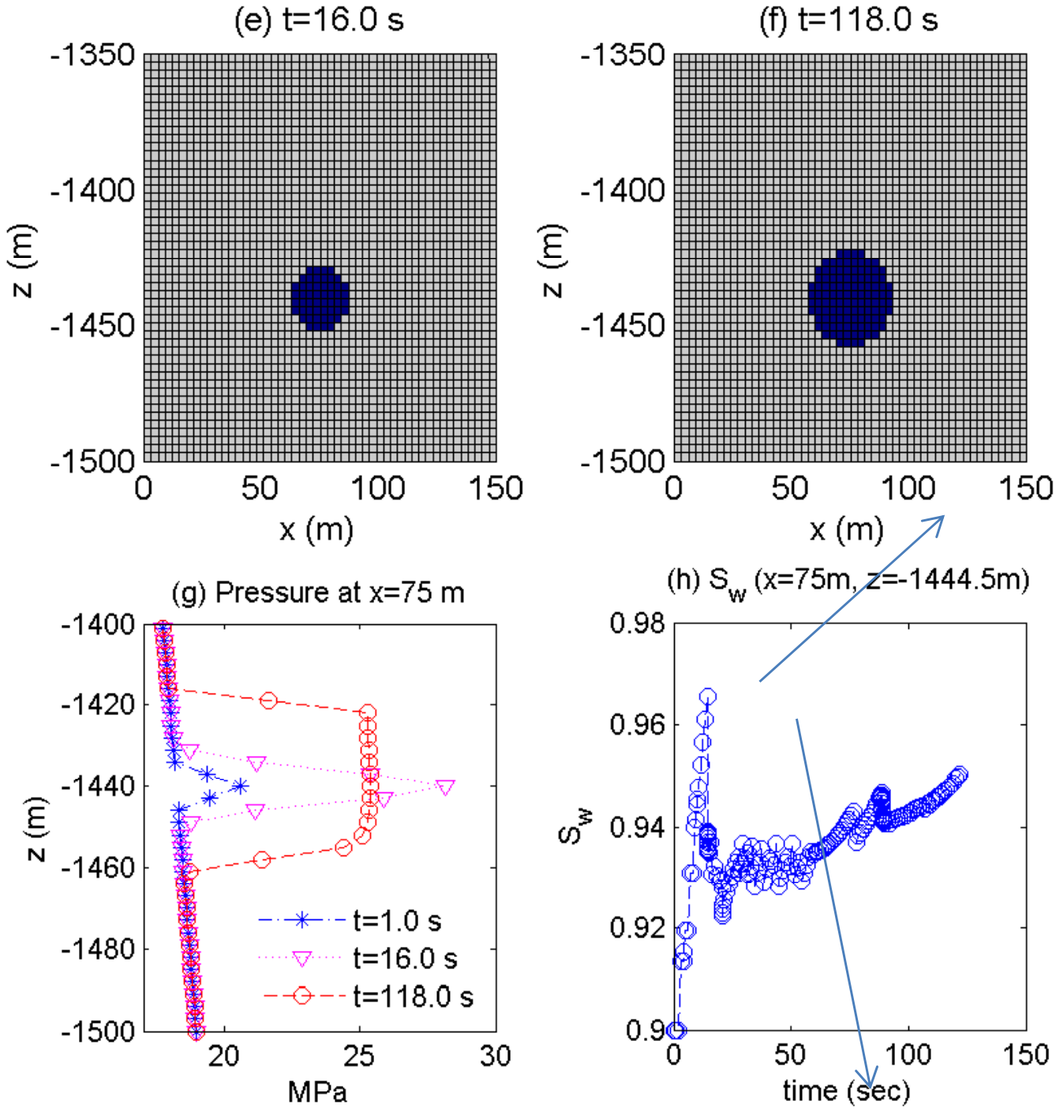




Simple calculation by only the injection volume might significantly underestimate the fracture volume and propagation.

Complex multiphase flow with gravity segregation within the fracture

# Water injection: fundamental issues

$S_{w,i} = 0.9$

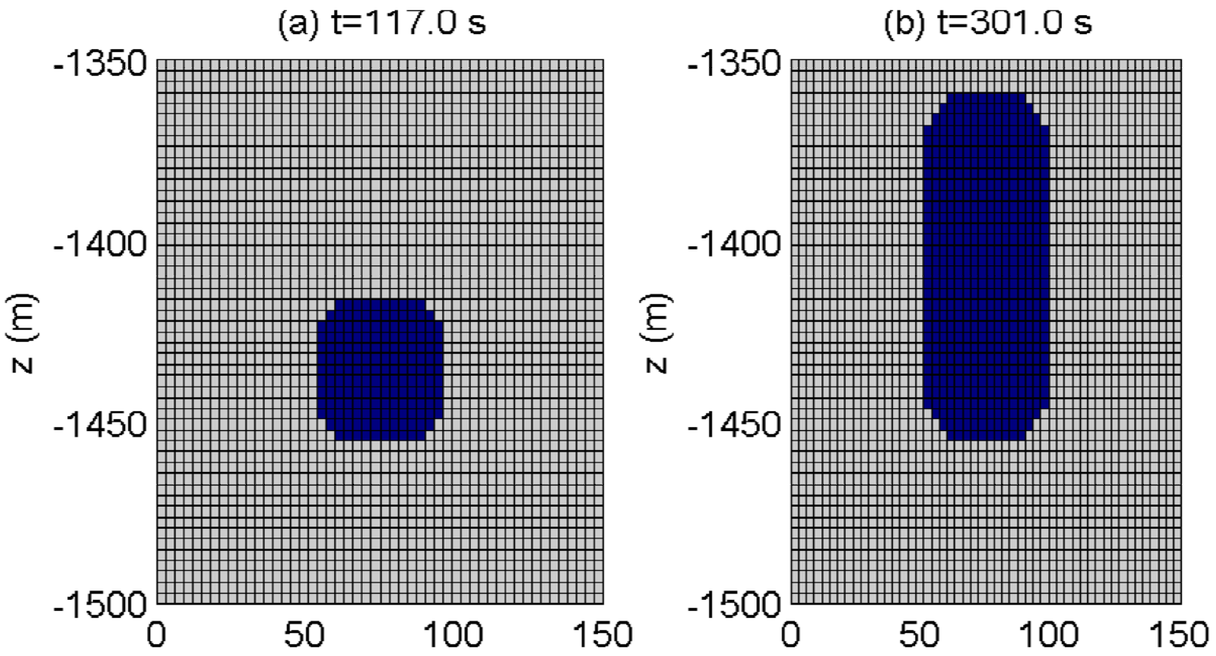



Does not approach
Sw = 1.0

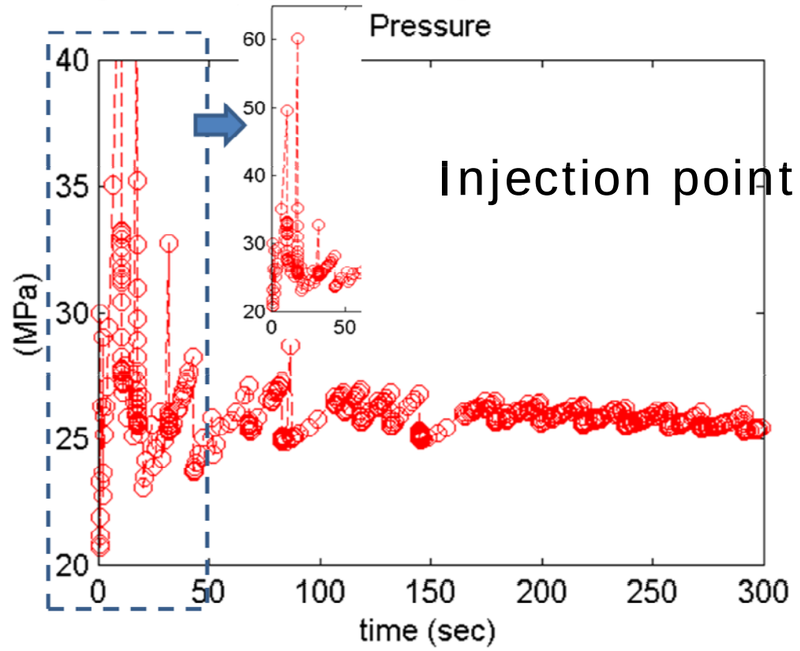
Water & gas still coexist within the fracture.
Water saturation drops at the time when fracturing occurs.

# Higher Injection Rate

$$Q_{inj} = 16 kg/s$$



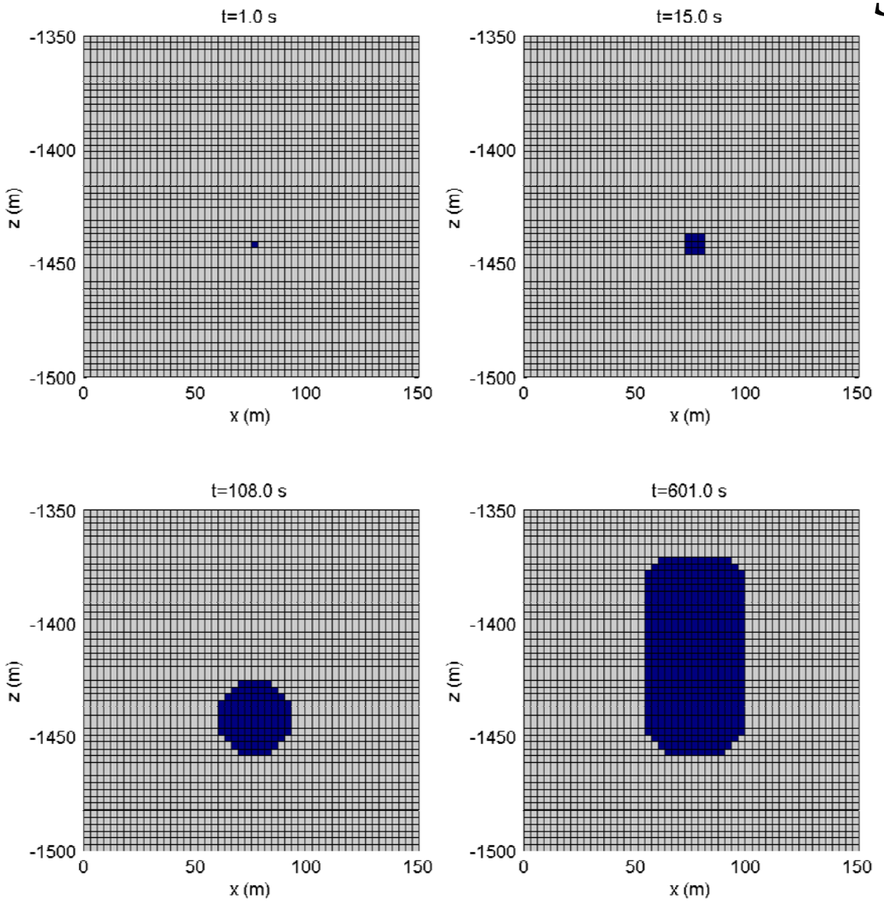

**Higher peak pressure**

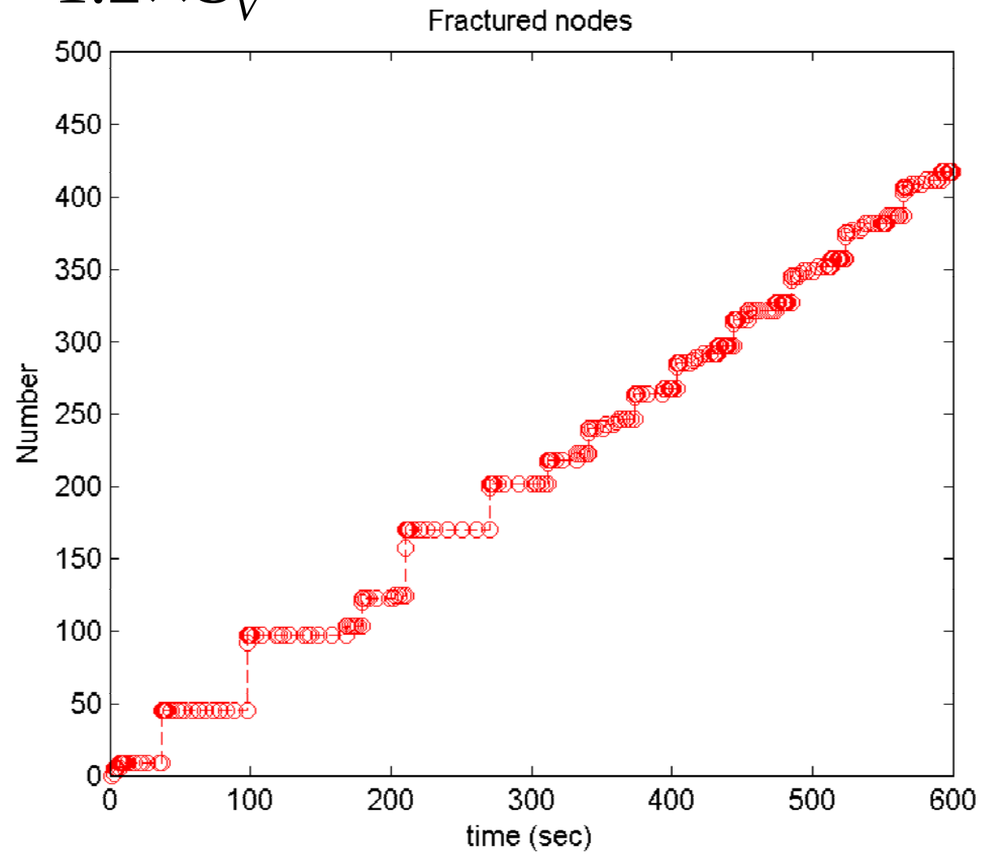



Higher injection rate = faster fracture propagation

# Maximum Horizontal Stress, $S_H$

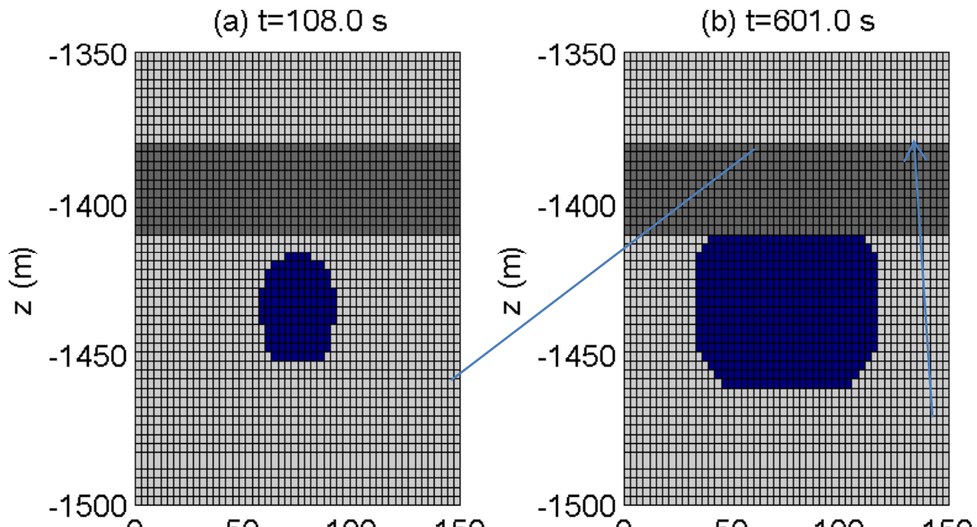
$$S_H = 1.2 \times S_V$$



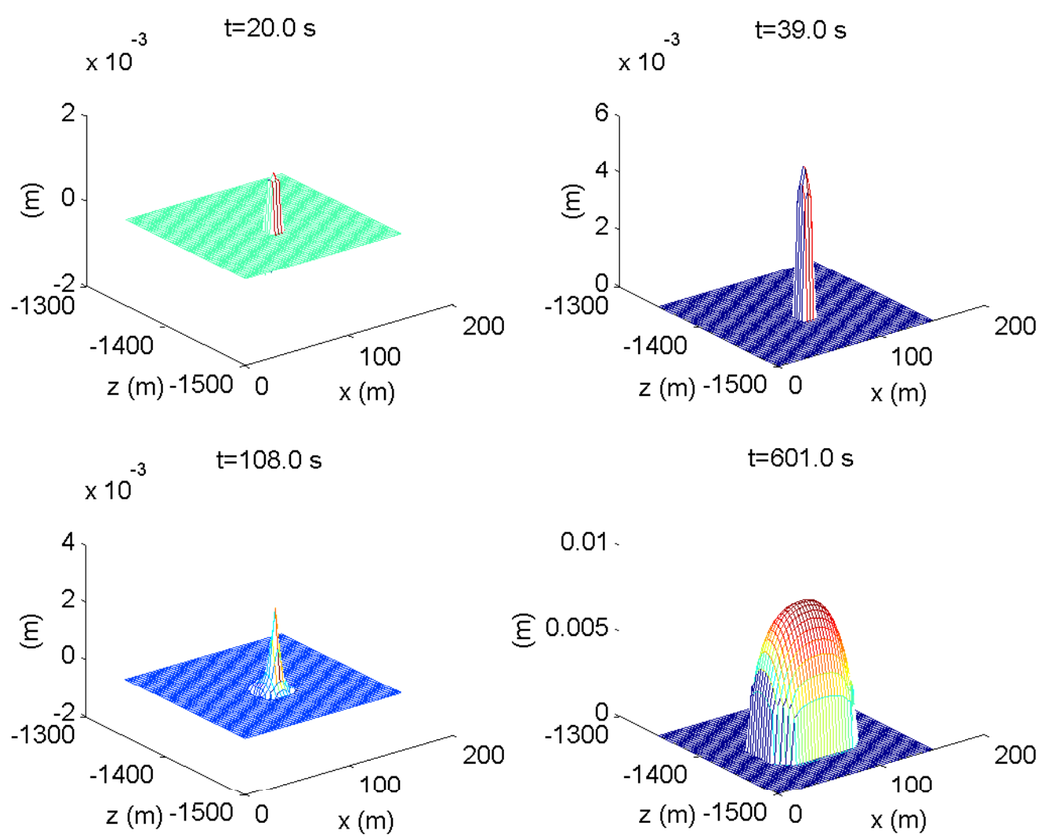

Change in $S_H$ induces slight change in the fracture shape.

# Heterogeneity effects




A strong geological formation with $\tau_c$ = 10 MPa

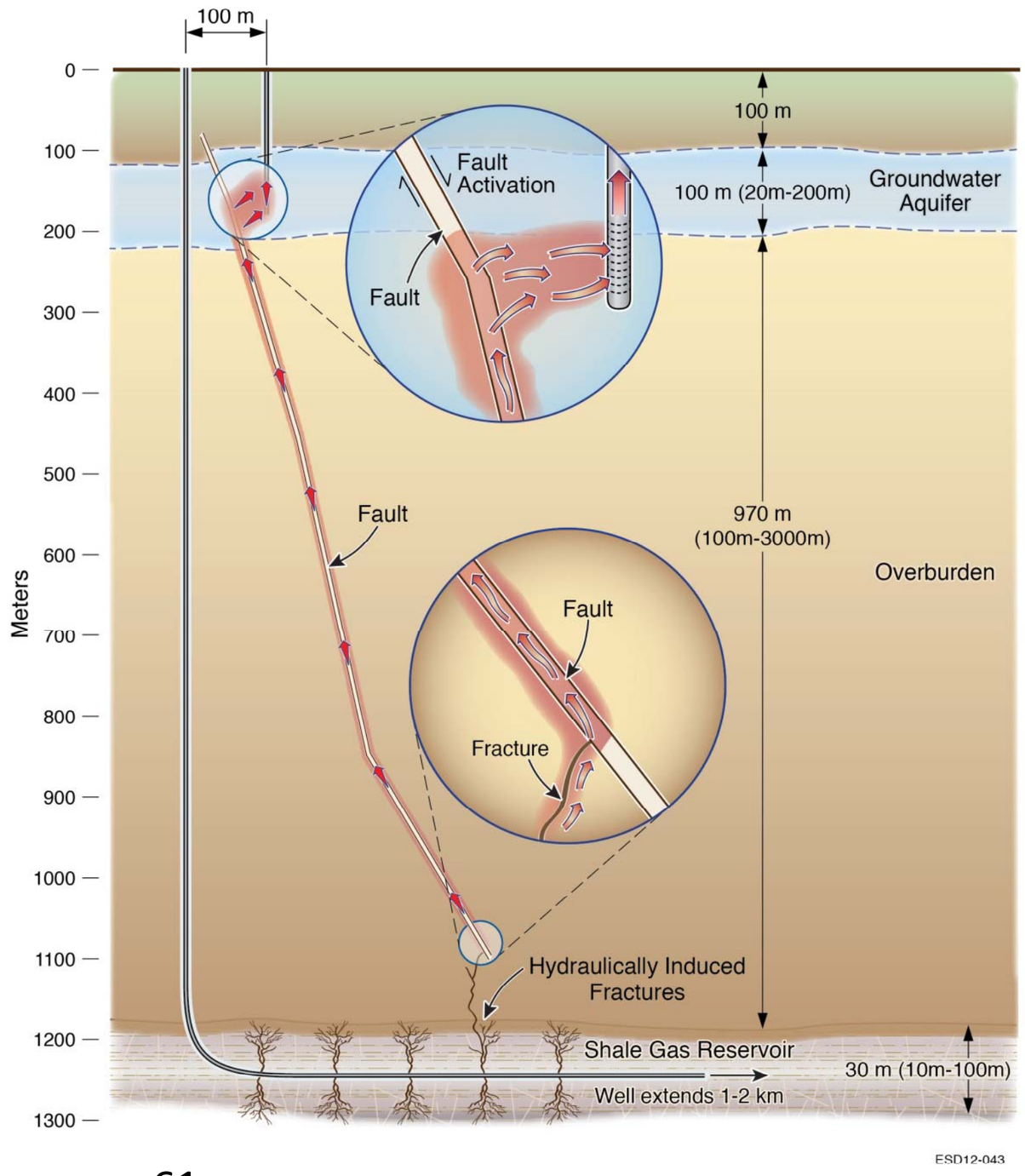
**A strong geological formation can block vertical fracture propagation**



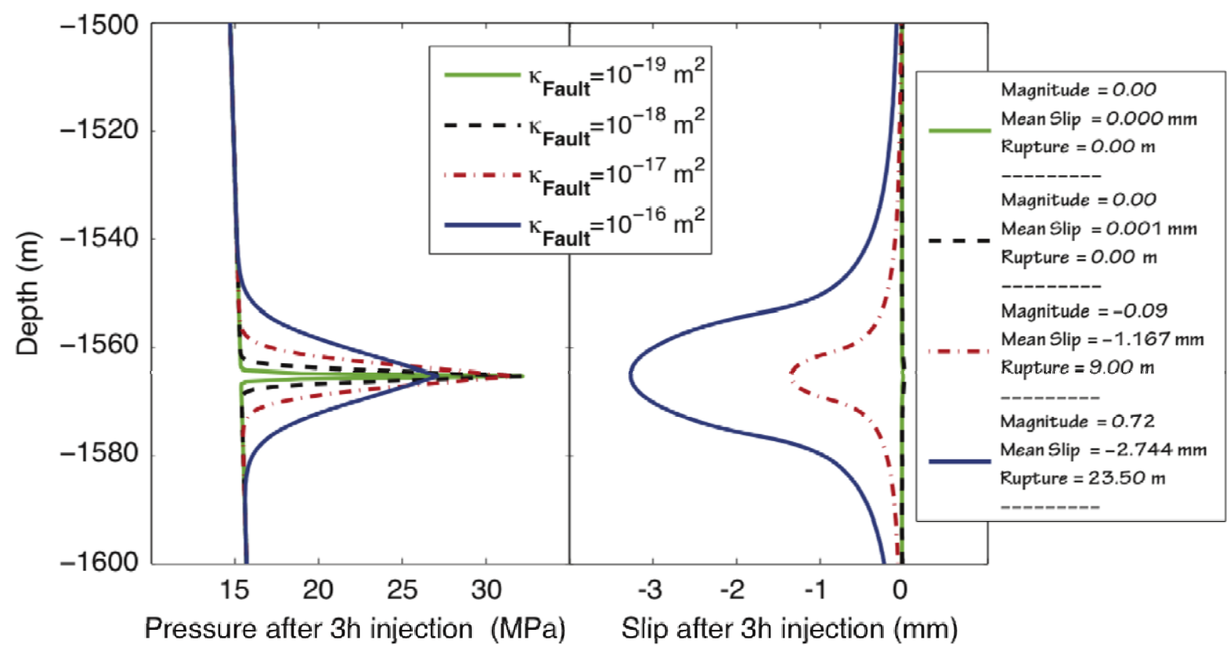
# Failure scenarios (?)

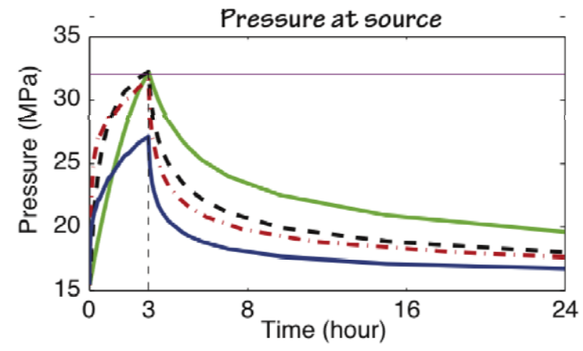
**Fault activation during the hydraulic fracturing process**

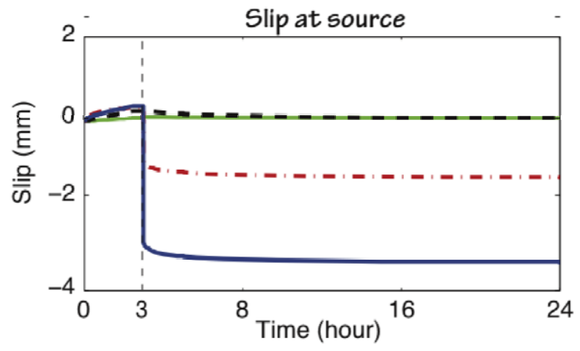
**Code:**
**TOUGH+**
**RealGasH2O+**
**FLAC3d**

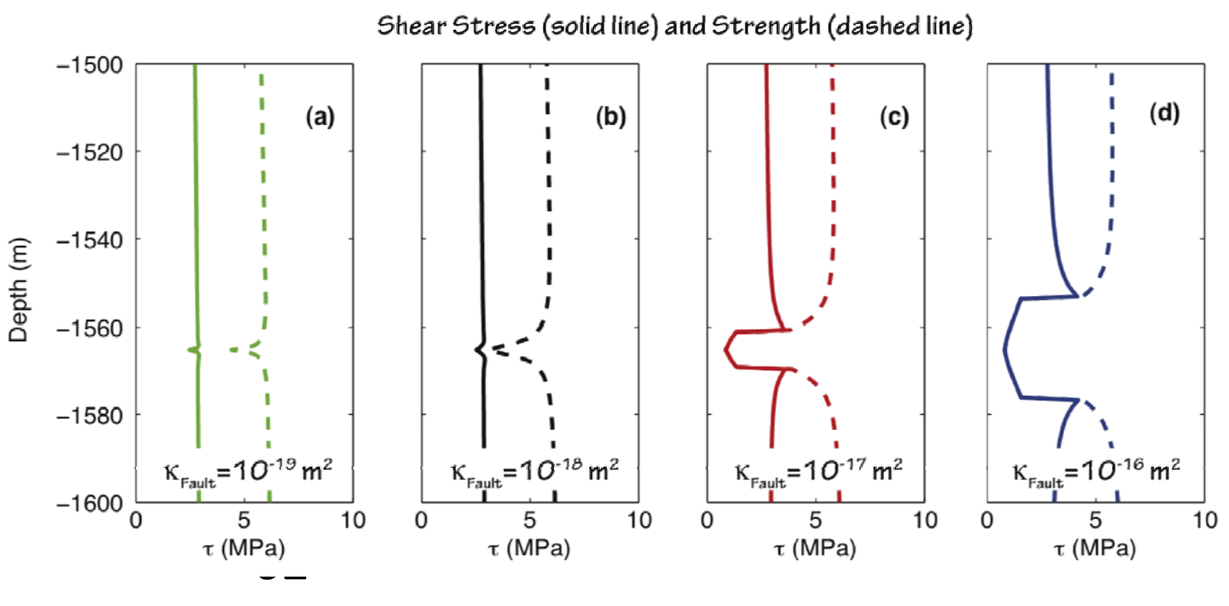


# Constant rate of P-increase

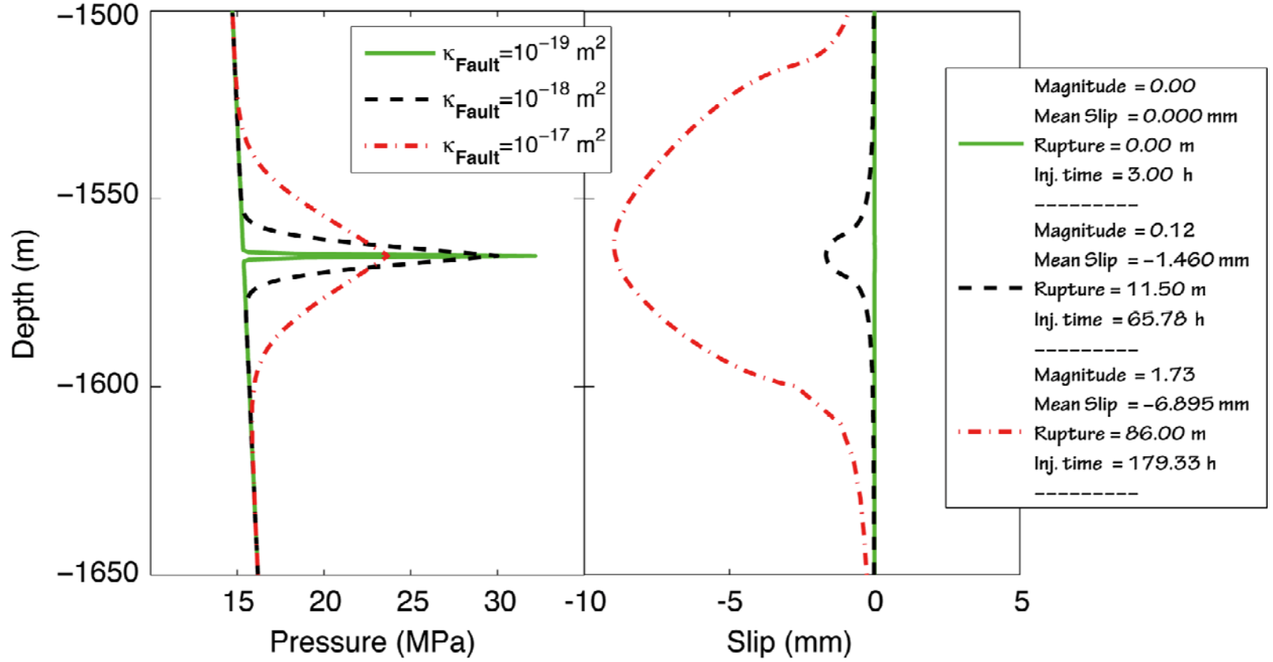


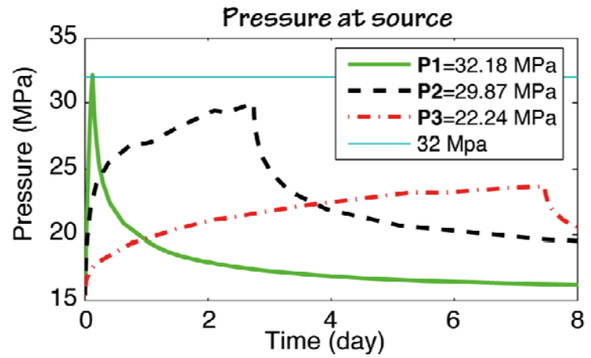



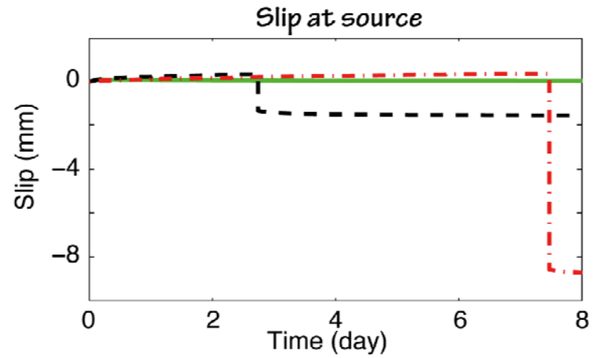



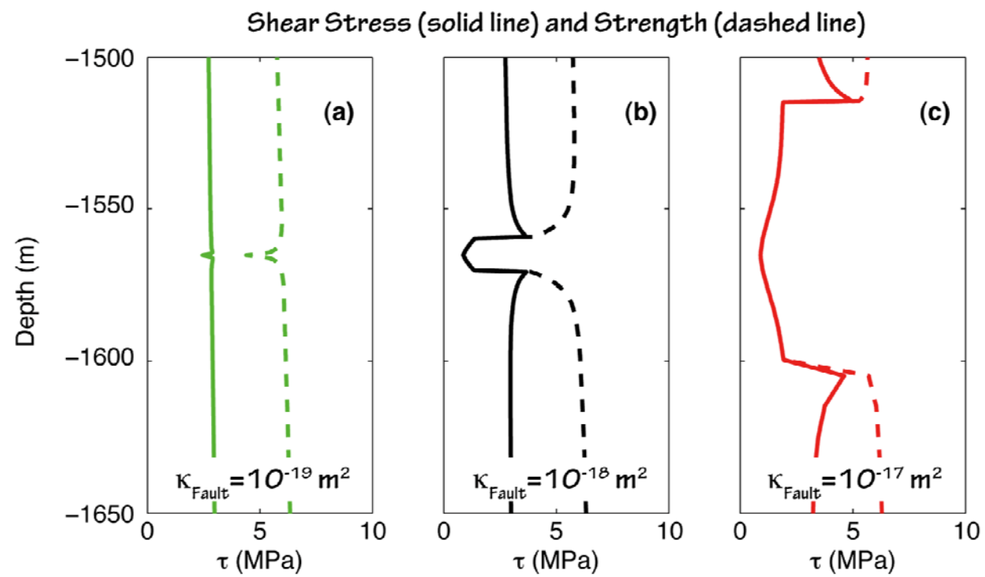



# Constant rate of injection



# Conclusions

- Developed a hydraulic fracturing simulator
- Investigated fracture propagation scenarios in Marcellus shales
- Identifying the factors controlling fracture propagation
- Estimation based on the  injection volume may significantly underestimate the fracture volume & its propagation

Rigorous modeling of fracture propagation & accurate geophysical monitoring are strongly recommended

# Acknowledgements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**Thank you**