Methane in subsurface: resource and hazard. Towards hybrid mathematical models and computational solutions.

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Methane \(CH_4\) ...

- ... is a naturally occurring gas; it is the major component (95 percent) of natural gas. [EPA]

- ... is a greenhouse gas that remains in the atmosphere for approximately 9-15 years. Methane is over 20 times more effective in trapping heat in the atmosphere than carbon dioxide over a 100-year period and is emitted from a variety of natural and human-influenced sources. [EPA]

- ... trapped in marine sediments as a hydrate represents such an immense carbon reservoir that it must be considered a dominant factor in estimating unconventional energy resources; the role of methane as a 'greenhouse' gas also must be carefully assessed. [William Dillon, USGS]
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CoalBedMethane ∩ MethaneHydrates

- Complex physical models
- Metastable states
  - hysteresis (CBM)
  - phase transitions (MH)
- Need hybrid models ... ?
Multiple phases and components

- \( p_1 \) (gas)
- \( p_2 \) liquid
- \( p_3 \) (gas)
- \( p_4 \) (water)
- \( p_5 \) (solid)

COMPONENTS:
- \( C_1 \)
- \( C_2 \)
- \( C_3 \)
- \( C_4 \)
- \( C_5 \)
- \( C_6 \)
- \( C_7 \)
- \( C_8 \)
Multiple phases and components
Multiphase multicomponent model

Gibbs rule:
\[ N_F = N_C - N_P + 2 - N_R \]

Variables
\[ \{ P_p, T, X_{pC}, S_p, N^C, u_p, V^C \}_p,c \]
phase pressures \( P_p \), saturations \( S_p \), velocities \( u_p \), viscosities \( \mu_p \), densities \( \rho_p \), component concentrations \( N^C \), fluxes \( V^C \), mass fractions \( X_{pC} \).
NEED: Equation of State (EOS) [Lake’89], [JWheeler,MFWheeler, P’99-, P’05]

Definitions and conservation laws

Mass conservation:
\[ \frac{\partial}{\partial t} \phi N^C + \nabla \cdot (V^C_{ADV} + V^C_{DIFF}) = q^C + R^C \]
\[ N^C = \sum_p S_p \rho_p X_{pC} \]
\[ V^C_{ADV} = \sum_p \rho_p X_{pC} u_p; \quad u_p = -K \frac{k_p}{\mu_p} (\nabla P_p - \rho_p g) \]
\[ V^C_{DIFF} = -\sum_p \rho_p D^C_p \nabla X_{pC} \]
Volume:
\[ \sum_p S_p = 1; \quad \sum_c X_{pC} = 1 \]
Capillary forces:
\[ P_p = P_{p,ref} + P_{cp} \]
Reaction:
\[ R^C = \phi \sum_p S_p r^C_p + (1 - \phi) r_s^C \]
Equilibrium and Kinetic models

Generic model for mass conservation of a component $C$

\[ \text{storage} \quad \text{advection} \quad \text{diffusion} \quad \text{source} \]

\[ \text{Sto}_C + \text{Adv}_C + \text{Diff}_C = q_C, \text{ in } \Omega \]

can be written in

- per each $C$ (phase summed form)
- per each $C$/each phase (must define mass transfer)

Evolution of a mobile component $X$ with immobile $Y$

\[
\frac{\partial}{\partial t} (X + Y) + \text{Adv}_X + \text{Diff}_X = 0.
\]

... must be supplemented with a definition of $\frac{\partial Y}{\partial t}$ ...

EQUILIBRIUM

\[ Y = f(X) \]

KINETIC

\[ \frac{dY}{dt} = r(f(X) - Y) \]

As $r = \frac{1}{\tau} \rightarrow \infty$, KINETIC $\rightarrow$ EQUILIBRIUM.
Equilibrium or kinetic?

- many processes are equilibrium type (large $r$)
- no issues with time stepping
- requires algebraic phase equilibrium solver

- many processes are kinetic with (fixed $r$)
- for large $r$ requires small time steps (stiff system)
- "regularization" or "pseudo-transient solvers" of equilibrium processes

In applications of interest: $EQU \cup KIN$ phenomena

- multicomponent adsorption (CBM)
- adsorption hysteresis (CBM)
- coal matrix swelling (CBM)
- coal macro-meso-micro porosity (CBM)
- solubility constraints (MH)
- mass transfer models (MH)
- phase transitions (MH)
Coalbed Methane Recovery

- Pilot projects evaluated ECBM as a potential carbon sequestration technology
  \[\text{Wolf08, Goodman07, Yu07, ShiMazumder08, vanBergen09, Gensterblum10, Fujioka10}\]
- Modeling using reservoir simulation \[\text{ShiMazumder'TiPM'07, JessKovcsek'TiPM'07}, \text{more in Intl. J. Coal Geology, Fuel.}\]
  \[\text{Also Elsworth et al}\]
- **Modeling** (fit adsorption rates to experimental data) \[\text{Clarkson99, Clarkson99b, Busch2004, PanConnell10, Massarotto2010, Siriwardane2009b, ConnellDet2009}\]
- Multiphase multicomponent + double porosity (Warren-Root)
  \[\text{KingErtekan'86 in SPEFE}\]
- Coal **swelling** and pore deformation
  \[\text{Ceglarska95'-08, Zarębska'02, Czerw’10}\]
Coal structure and ECBM mechanism

Image from Atlas petrograficzny, AGH, Poland
Adsorption in ECBM Recovery

**MULTICOMPONENT**

- **equilibrium**
- **non-equilibrium**

**kinetic**
- triple - porosity
- hysteretic

**TRANSPORT**
- advection/diffusion

- **Multicomponent** adsorption: (competitive/selective/preferential).
- Beyond Extended Langmuir (EL):
  - Ideal Adsorbate Solution (IAS)
- Many processes are **kinetic** (e.g. coal swelling)
- Macropore + mesopore + micropore = triple porosity
- Adsorption-desorption **hysteresis**
Multiple phases and components: CBM

- **M** methane
- **D** carbon dioxide
- **N** nitrogen
- **g** (gas)
- **a** (adsorbed)
- **w** (water)

**COMPONENTS**
CBM flow+transport model

Cleats: \( p = g(\text{as}) + w(\text{ater}) \), \( C = M, D, N \) (mostly advection during recovery, then diffusion)

\[
\frac{\partial (\phi S_p \rho_p x_{pC})}{\partial t} - \nabla \cdot \left( K \rho_\alpha x_{pC} \frac{k_{r,\alpha}}{\mu_\alpha} \nabla P_\alpha \right) + Q_C = q_C, \ \forall C
\]

Matrix: \( p = g(\text{as}), a(\text{dsorbent}) \) (simplified) (diffusion + competitive/hysteretic adsorption)

\[
\frac{\partial (\phi_m x_{gC})}{\partial t} + \frac{\partial (x_{aC})}{\partial t} - \nabla \cdot (D_{mC} \nabla x_{pC}) - Q_C = q_C, \ \forall C
\]

Exchange term \( Q_C := \) flux of \( C = M, D, N \) from matrix to cleats \( Q_{AC} := \) rate of adsorption

In many models \( Q_C \approx Q_{AC} \).
Exchange terms $Q_C$ and adsorption $Q_{AC}$

Single component $X$ in gas phase, adsorbed $Y$

Have $\frac{\partial}{\partial t}(X + Y) + \text{Adv}_X + \text{Diff}_X = 0$. Need $\frac{\partial Y}{\partial t}$!

- equilibrium $Y = f(X)$ with isotherm $f(\cdot)$
- kinetic $\frac{\partial Y}{\partial t} = \frac{1}{\tau}(f(X) - Y)$
- double-porosity+adsorption models “$Y = \kappa \ast f(X)$”
  - bidisperse pore [Ruckenstein’71, ShiDur’03]
  - double-porosity: [Arbogast et al, Showalter et al, P’92-, PShow’07]
Exchange terms $Q_C$ and adsorption $Q_{AC}$

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Multiple components $C = M, D, N$ with $x_{pC}, p = a, g$

- single porosity equilibrium models [Kovcsek etal]
  $Q_C \approx Q_{AC} = \frac{\partial(x_{AC})}{\partial t}$ plus isotherm $x_{AC} = f_C(\{x_{gi}\}_i)$
- quasistatic (Warren-Root) double-porosity model $\equiv$ kinetic adsorption model [Shi etal]
  $Q_C \approx Q_{AC} = \frac{\partial(x_{AC})}{\partial t}, \frac{\partial(x_{AC})}{\partial t} = \frac{1}{\tau} (x_{AC} - f_C(\{x_{ai}\}_i))$
- NEED “triple-porosity + multicomponent adsorption” models ??
Adsorption beyond Langmuir ... IAS

Let $X = \{x_{gC}\}_C$, $Y = \{x_{aC}\}_C$ in $\frac{\partial}{\partial t} (X + Y) + \text{Adv}_X + \text{Diff}_X = 0$. But ... multicomponent $Y = f(X)$ difficult to find experimentally.

- **Extended Langmuir: (EL)**
  - simple but ill-fitting with questionable thermodynamics

- **Ideal Adsorbate Solution (IAS) [Do’98-08], ECBM-IAS [Yu’10]**
  - needs pure component isotherms
  - assumes equality of potentials à la vapor-liquid equilibria (Raoult’s law)
  - analytical form unavailable: requires a nonlinear solver

**EXAMPLE: binary CH₄/CO₂ or CH₄/N₂ recovery with EL/IAS**

**NEED: multi-porosity IAS multicomponent model?**
Adsorption beyond Langmuir ... IAS

Let \( X = \{ x_{gC}\} C, \ Y = \{ x_{aC}\} C \) in \( \frac{\partial}{\partial t}(X + Y) + \text{Adv}_X + \text{Diff}_X = 0. \)

But ... multicomponent \( Y = f(X) \) difficult to find experimentally.

- **Extended Langmuir:** (EL)
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  - assumes equality of potentials à la vapor-liquid equilibria (Raoult’s law)
  - analytical form unavailable: requires a nonlinear solver

**EXAMPLE:** binary \( CH_4/CO_2 \) or \( CH_4/N_2 \) recovery with EL/IAS

**NEED:** multi-porosity IAS multicomponent model?
Adsorption-desorption hysteresis

Consider \( \frac{\partial}{\partial t} (X + Y) + \text{Adv}_X + \text{Diff}_X = 0 \), with \( Y \in f(X) \).

**Significant hysteresis in ECBM**

image from [Kovcsek et al'08]

**Differential (Preisach) model**

[\textit{PShow'97}]

image from [\textit{P'11 current work}]

Given input \( X \), define output \( Y \):

\[
\begin{align*}
\frac{dY_s}{dt} + c_s (Y_s - X) & \geq 0 \\
Y(t) &= \int_0^S Y_s(t) \psi''(s) \, ds
\end{align*}
\]

where \( c_s \) is a max. monotone graph, and \( \psi \) the (convex) isotherm.
Adsorption hysteresis computing example

Consider model problem

\[
\frac{\partial}{\partial t} (X + Y) + \frac{\partial X}{\partial x} = 0, \\
\frac{\partial Y}{\partial t} + \text{sgn}^{-1}(Y - X) \ni 0
\]

Use \( \tau \)-regularization of \( \text{sgn}^{-1} \)

Analytical solution from \([P\text{Show}'97]\), numerics: \([P'11, \text{current work}]\)
Summary on coalbed methane

Continuum models and simulators: current work

- **hysteresis** in adsorption/desorption
  - Preisach model insufficient for description
  - Numerics difficult (very stiff when $\tau \downarrow 0$)
    - Use complementarity condition...
  - Extensions to multicomponent ??? IAS ???
- **merging kinetics** to describe swelling and stress evolution with triple (macro-meso-micro) porosity
  ... multiscale multicomponent adsorption models ???
- **models for porosity evolution and deformation**
  $\phi = \phi(X, Y), K = K(X, Y)$ beyond Carman-Kozeny correlations

Need hybrid models? Or experiments/porescale imaging?

[Wolf08], [Mazum’06], [Czerw’10]
Methane Hydrates: Ice That Burns

Methane Hydrate \textit{(methane ice, methane clathrate)}: greenhouse gas, source of energy, \textcolor{red}{drilling hazard}

- Programs: DOE NETL, CSM, Ocean Drilling, USGS. (MH Reservoir Simulator Code Comparison Study: TOUGH+HYDRATE, STOMP-HYD and other ...), \textit{[Fire in the Ice Newsletter, MH_Primer2011]}

\textit{[Sloan, Koh’2008], [TréhuTorres’04-], [DavieBuffet’01-03-05], [Zatsepina,Buffet] [LiuFleming’08,Garg et al’08], [PTrorrTre’10]}

\textit{image from MH at surface. Hands: R.}
Methane Hydrate: phase properties

image from Trehu, Ruppel, Dickens, et al, Oceanography’2006
Methane Hydrate: thermodynamics

**phases**
- g (methane)
- l (brine)
- s (hydrate)
- p (precipitate)

**COMPONENTS**

Variables: \((P, T), \{x_{pC}, S_p, N_C, u_p\}_{p,c}\)

Constraints: \(x_{IM} \leq x_{IM}^{EQ}(P, T, x_{IS})\)

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**Graphs**
- Pressure vs. Temperature for I+h and I+g with different salinity levels.
- Methane solubility and maximum solubility vs. Reservoir pressure for I+h and I+g with different salinity levels.
Model for Methane Hydrates

Variables: \((P, T), \{x_{pC}, S_p, N_C, u_p\}\),
Constraints: \(x_{IM} \leq x_{IM}^\text{EQ}(P, T, x_{IS})\)

\((\text{EQ})\) Mass cons. for each \(C\) use \(\sum_{\text{phases}}\)
- Use variable switching \([\text{Class,Helmig'02}].\)
- Partition between phases: equilibrium data \([\text{LF'08,Garg'08}].\)

\((\text{KIN})\) Mass cons. for each \(C\), for each phase
- Mass transfer via kinetics (first order) \([\text{DB'01,DB'03,TT'04}].\)
- Rates ?
- Time scale of interest !
Model for Methane Hydrates

Variables: \((P, T), \{x_{pC}, S_p, N_C, u_p\}\)
Constraints: \(x_{IM} \leq x_{IM}^{EQ}(P, T, x_{IS})\)

(EQ) Mass cons.: \(storage + advection + diffusion = source\),
use \(\sum_{\text{phases}}\)

\[
\begin{align*}
\frac{\partial}{\partial t} (\phi S_g \rho g + \phi S_l \rho l x_{IM} + \phi S_h \rho h x_{hM}) + \nabla \cdot (\phi S_g \rho g u_g + \phi S_l \rho l x_{IM} u_l + \phi S_h \rho h x_{hM} u_r) &- \nabla \cdot (D_m \phi S_l \rho l \nabla x_{IM}) = f \\
\frac{\partial}{\partial t} (\phi S_l \rho l x_{lW} + \phi S_h \rho h x_{hL}) + \nabla \cdot (\phi S_l \rho l x_{lW} u_l + \phi S_h \rho h x_{hW} u_r) &- \nabla \cdot (D_S \phi S_l \rho l \nabla x_{lS}) = 0
\end{align*}
\]
energy equation
phase equilibria and volume, capillary and thermodynamic constraints
Model for Methane Hydrates

**Variables:** \((P, T), \{x_{pC}, S_p, N_C, u_p\}_{p,c}\)

**Constraints:** \(x_{IM} \leq x_{IM}^{EQ}(P, T, x_{IS})\)

(KIN) **Mass cons. for** \(C = M, p = l, h\)

\[
\begin{align*}
\frac{\partial}{\partial t} (\phi S_I \rho_I x_{IM}) + \text{advection} - \nabla \cdot (D_m \phi S_I \rho_I \nabla x_{IM}) &= f - f_{hM} \\
\frac{\partial}{\partial t} (\phi S_h \rho_h x_{hM}) &= f_{hM} \\
\frac{\partial S_h}{\partial t} &= \mathcal{R}(x_{IM} - x_{IM}^{EQ}) \mathcal{H}(S_h)
\end{align*}
\]
MH evolution example: **EQ**

[PTorresTrehu’10]
Discretize \((h, \Delta t)\)... the coupled nonlinear system
\((P, T\ 	ext{fixed}: \text{isothermal, no advection})\)
solve fully implicitly or with a **sequential model**

Solve for \(N_M, N_S\)  
\[
F_M(N_M) = 0 \\
F_S(N_S) = 0
\]

Solve for \(N_{M,h}^{n+1}, N_{S,h}^{n+1}\)  
\[
F_M^n(N_{M,h}^{n+1}) = 0 \\
F_S^n(N_{S,h}^{n+1}) = 0
\]
MH evolution simulation
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Overview
Motivation
Preliminaries
Continuum models
Coalbed methane
Interlude: recap
Methane hydrates
Hybrid models
Porescale models
Porescale discrete models
MH evolution simulation
MH evolution simulation
MH evolution simulation
Introduce **KINETICS** to relax equilibria
Introduce KINETICS to relax equilibria
Compare EQ and KIN

\[\text{KleinP'10}\]
Compare EQ and KIN

[KleinP’10]
Compare EQ and KIN

\[\text{[KleinP'10]}\]
Analysis of MH model: EQ

Simplified model of solubility constraints in hydrate zone:

\[
\frac{\partial}{\partial t} \left( x_{IM}(1 - S_h) + S_h R \right)_{NM} - \nabla \cdot (D(S_h, x) \nabla x_{IM}) = 0
\]

\((x_{IM}, S_h) \in F := [0, x_{IM}^{\text{max}}) \times \{0\} \cup \{x_{IM}^{\text{max}}\) × (0, 1).

Analysis of EQ/KIN:

\[
\frac{\partial N_M}{\partial t} - \nabla \cdot (D(N_M, x) \nabla m(N_M, x)) = 0
\]

- Nonlinear evolution problem [Showalter'96] [current work]
- Phase transitions: non-isothermal [Visintin'96]
- Kinetic and equilibrium adsorption with non-Lipschitz nonlinearity [BarretKnabner'9*]
- Solubility constraints: [Jaffre et al'09, BenGharbia’10] [Bourgeat et al’09], [Eck/Knabner] as complementarity condition (IP, primal-dual active set)
  [IMA Workshop on Uncertainty & Optimization’ Oct’10]
Energy balance for methane hydrates

\[ \frac{\partial}{\partial t}(C(T)) - \nabla \cdot (\lambda \nabla T) = 0 \]

- **static:** \(-\nabla \cdot (\lambda \nabla T) = 0\)
- **dynamic, no latent heat:**
  \[ C(T) = \begin{cases} 
  C_1 T, & T < T_{eq}, \\
  C_2 T, & T \geq T_{eq} 
  \end{cases} \]
  \[ \lambda(T) = \begin{cases} 
  \lambda_1, & T < T_{eq}, \\
  \lambda_2, & T \geq T_{eq} 
  \end{cases} \]
- **dynamic with latent heat (Stefan-type model):** [KelkarSloan'98]
  \[ C(T) = \begin{cases} 
  C_1 T, & T < T_{eq}, \\
  C_2 T + L \mathcal{H}(T), & T \geq T_{eq} 
  \end{cases} \]
  \[ \lambda(T) = \begin{cases} 
  \lambda_1, & T < T_{eq}, \\
  \lambda_2, & T \geq T_{eq} 
  \end{cases} \]
- **dynamic with latent heat (sink-type model):** [Ahmadi'07,Lichtner'07]
  \[ C(T) = \sum_{phases} \cdots , \]
  \[ \lambda(T) = \sum_{phases} \cdots \]
  In addition, we have a source term
  \[ \frac{\partial}{\partial t}(C(T)) - \nabla \cdot (\lambda \nabla T) = -\alpha(T) \frac{\partial S_h}{\partial t} \]
Discretization: coupled nonlinear system

Original system solved for $N_M, N_S, T$
($P$ is frozen: no advection)

\begin{align*}
F_M(N_M) &= 0 \\
F_S(N_S) &= 0 \\
F_T(T) &= 0
\end{align*}

Discretize $\Delta t$... solve fully implicitly or with a sequential model

\begin{align*}
F_M^n(N_{M,h}^{n+1}) &= 0 \\
F_S^n(N_{S,h}^{n+1}) &= 0 \\
F_T^{n+1/2}(T_{h}^{n+1}) &= 0
\end{align*}

Static 
Dynamic, no latent heat 
Dynamic, with sink model 
Dynamic, with Stefan-like model
Dependence of $Q(u)$ on the choice of the energy model

Quantity of interest $Q(u)$: methane flux to the ocean

![Methane flux to the ocean with respect to time [nondimensional], medium grid](image)
Open problems and current work (MH)

Have/Need:

- Have computational models for methane hydrates with different variants of energy balance, and phase equilibria in EQ/KIN [PTT10,KPcmwr10] / Need better phase equilibrium model
- Have some analysis / Need more analysis

Challenges:

- porosity and permeability evolution in the presence of hydrate [Jaines/Juanes’10]
- pore-filling vs pore-coating models $\phi = \phi(S_h), K = K(S_h) =$?
- three-phase coexistence ($S_w > 0, S_h > 0, S_g > 0$) zone?
- kinetics of hydrate formation and dissociation

Need hybrid models? Or experiments/porescale imaging?

Image from BatzleElder et al

Image from Rydzy/Batzle et al’10
Hybrid models: why

Recall **challenges** in CBM ∩ MH:
- Complex coupled physical models
- Metastable states with multiple components
  - hysteresis (CBM)
  - phase transitions (MH)
- Multiple scales (spatial/temporal) are important
- Models of **porescale evolution** lack precision

Oh, so we need “bigger” continuum simulators?

- Need better solvers for metastable states
- Need more physics
  - physics porescale ≠ physics Darcy scale
  - [Tartakovsky et al’10]:
    - “adsorption @ porescale” ≠ “ adsorption @ Darcy scale
- Need more models at porescale
  - static
  - dynamic
  - dynamically coupled?

*Hybrid := an offspring resulting from cross-breeding*
Hybrid models: why

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Hybrid := an offspring resulting from cross-breeding
Porescale models for flow and transport

- Different approaches: LB, pore network ....

Our approach (with A. Trykozko (ICM, University of Warsaw)

- Traditional Navier-Stokes solvers for flow ...
- Pre-/post-processing [Chippada, Dawson, Martinez, Wheeler'1998]
- Transport (e.g., Godunov)
- Upscaling which recovers anisotropy (non-periodic geometries)

[PTrykozkoAugustson'09, PTry’09, PTrySob’09, PTryKen’10]
Several projects underway (OSU, PNNL, LANL) to image reactive processes at porescale for the needs of \(\text{CO}_2\)-sequestration

**But**

- How representative are the porescale simulations?
- Current porescale models too expensive for a dynamic model

**Image from Dorthe Wildenschild**

**Porescale Benchmark**: [PeszProdanovicWildenschild]
Try discrete models

Other applications where hybrid=discrete + continuum are used:


Ex.: Ising-like models of adsorption and phase transitions 
...[IMA Workshop on Molecular Dynamics May’09]

Mean field theory/MD/GMC [Sarkisov, Monson’00, Woo, Sarkisov, Monson’01], [Ornstein/Zernike]

Given chem. potential $\mu$, temp. $T$; $1/\beta = k_B T$, fluid-fluid interaction $J$, wettability $yJ$

- generate porescale geometry realizations of solid $t$; quench a $t$
- generate realizations of fluid occupancy $n$, form averages weighted with $e^{-\beta H}$ where $H$ is the Hamiltonian

$$H[n_i, t_i] = -J \sum \langle ij \rangle n_i n_j t_i t_j - \mu \sum_i n_i t_i -$$

$$yJ \sum \langle ij \rangle [n_i t_j (1 - t_i) + n_j t_i (1 - t_j)]$$

- loop only over equilibrium configurations found by iteration

Result:

- adsorbed amount for a given pressure i.e. isotherm
- reveals hysteretic nature of adsorption
Try discrete models

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- generate porescale geometry realizations of solid $t$; quench a $t$
- generate realizations of fluid occupancy $n$, form averages weighted with $e^{-\beta \mathcal{H}}$ where $\mathcal{H}$ is the Hamiltonian
  $\mathcal{H}[n_i, t_i] = -J \sum \langle ij \rangle n_i n_j t_i t_j - \mu \sum_i n_i t_i - yJ \sum \langle ij \rangle [n_i t_j (1 - t_j) + n_j t_i (1 - t_i)]$
- loop only over equilibrium configurations found by iteration

Result:
- adsorbed amount for a given pressure i.e. isotherm
- reveals hysteretic nature of adsorption
Last word

Beauty

Utility

Truth
Last word
Methane in subsurface: resource and hazard
M. Peszyńska et al

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Continuum models
Coalbed methane
Interludium: recap
Methane hydrates

Hybrid models
Porescale models
Porescale discrete models

Interludium: recap