GH-3PAD – a new numerical solver for multiphase transport in porous media - new insights on gas hydrate and free gas co-existence

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START

Pre-processing

Setting up depositional history of the basin

- Time of the first deposition
- Fluctuating sedimentation rates
- Varying lithology (initial porosity and compaction length scale)
- Varying productivity (degradable organic matter input)
- Potential fluxes of fluids and/or gas phases

Setting up modeling parameters

- Water depth
- Salinity
- Initial temperature profile
- Initial pressure (incl. compressible fluids and gas phases)
- Initial concentration of chemical species (CH_4, SO_4, DIC, POC)

Adjusting parameters

- Initial box definition
- Time-step limited to the flux of fluid or gas phase (Courant number)
- Vertical resolution of the basin

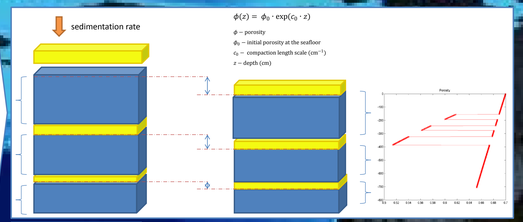
Variables obtained:
P_{ini}, $Temp_{ini}$, ρ_f, ρ_g, ρ_h, ρ_s, μ_f, μ_g, λ_f, λ_g, λ_h, λ_s, Cp_f, Cp_g, Cp_h, Cp_s

Simulation

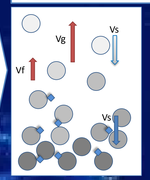
Deposition of a new sedimentary layer

Compaction of the sediment package

- Solid velocity calculation due to the mesh movement



- Intrinsic and relative permeability calculation for 3-phase system



Variables obtained:
new modeling box size,
new ϕ, k, k_f, k_g, V_s

Pressure update

- 3-phase compressible solver
- Darcy' velocity update (2-phase)

Phases:
- **solid** (incompressible grains)
- **fluid** (compressible pore fluids)
- **gas hydrate** (incompressible)
- gas (pure methane)

Sf + Sg + Sh = 1

Temperature update

- Bulk thermal conductivity
- Bulk heat capacity
- Temperature advection
- Temperature diffusion

$$(\rho C_p)_{bulk}\frac{\partial T}{\partial t} = -(\rho C_p)_{bulk}\overrightarrow{V_s}\cdot\nabla T - \rho_f C_{p_f}\overrightarrow{U_f}\cdot\nabla T - \rho_g C_{p_g}\overrightarrow{U_g}\cdot\nabla T + \nabla\cdot(\lambda_{bulk}\nabla T) + Q$$

Bulk heat capacity
$(\rho C_p)_{bulk} = (1-\phi)\rho_s C_{p_s} + \phi S_f \rho_f C_{p_f} + \phi S_g \rho_g C_{p_g} + \phi S_h \rho_h C_{p_h}$

Bulk thermal conductivity
$\lambda_{bulk} = \lambda_s^{(1-\phi)}\lambda_f^{S_f\phi}\lambda_g^{S_g\phi}\lambda_h^{S_h\phi}$

Advection

- Advection of chemical species in the pore fluids
- Advection of gas phase

Diffusion

- Diffusion of chemical species in the pore fluids
- Tortuosity calculation
- Diffusion coefficients of CH_4, SO_4, and DIC in marine sediments

Variables obtained:
P, Temp, V_s, U_f, U_g,

$$\frac{\partial((1-\phi)\rho_s)}{\partial t} = -\nabla\cdot\left((1-\phi)\rho_s\cdot\overrightarrow{V_s}\right)$$ Mass balance for solids

$$\phi S_f\left(\overrightarrow{V_f}-\overrightarrow{V_s}\right) = -\frac{kk_f^f}{\mu_f}\left(\nabla P+\rho_f\vec{g}\right)$$ Mass balance for solutes

$$\phi S_g\left(\overrightarrow{V_g}-\overrightarrow{V_s}\right) = -\frac{kk_r^g}{\mu_g}\left(\nabla P+\rho_g\vec{g}\right)$$ Mass balance for gas phase

$$\frac{\partial((1-\phi)\rho_s)}{\partial t} = -\nabla\cdot\left((1-\phi)\rho_s\cdot\overrightarrow{V_s}\right)$$ Mass balance for hydrates

$$\frac{\partial(\phi S_f C)}{\partial t} = \nabla\cdot\left(\phi S_f D\nabla C\right) - \nabla\cdot\left(\phi S_f C\cdot\overrightarrow{V_f}\right) + Q$$ Mass balance for chemical species dissolved in fluids

Rate	Kinetic rate law
Anaerobic Oxidation of Methane ($mmol\cdot yr^{-1}$)	$R_{AOM} = k_{AOM}\cdot C(SO_4)\cdot C(CH_4)$
Methanogenesis ($mmol\cdot yr^{-1}$)	$R_M = 0.5\cdot\frac{K_{SO_4}}{C(SO_4)+K_{SO_4}}\cdot R_{POC}\cdot r_C$
Sulfate reduction ($mmol\cdot yr^{-1}$)	$R_{SR} = 0.5\cdot\frac{C(SO_4)}{C(SO_4)+K_{SO_4}}\cdot R_{POC}\cdot r_C$
Constant	**Value**
k_{AOM} ($dm^3\cdot mmol^{-1}\cdot yr^{-1}$)	10^{-8}
K_{SO_4} (mM)	1
Conversion factor	**Formulation**
r_C from (wt. %) into (mM)	$r_C = \frac{\phi\cdot MW_C}{(1-\phi)\cdot d_s\cdot 10^6}$ *where* ϕ – porosity, MW_C – molecular weight of carbon ($g\cdot mol^{-1}$), d_s – density of dry sediments ($g\cdot cm^{-3}$)

Burwicz et al., 2011, GCA

A kinetic rate law of organic matter decomposition
(based on Middelburg J., 1989; modified by Wallmann K., 2006)

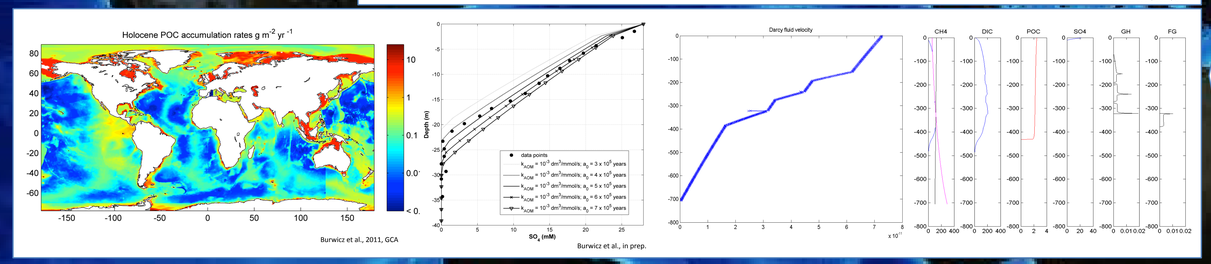
$$R_{POC} = \frac{K_c}{C(DIC)+C(CH_4)+K_c}\cdot k_x\cdot G(POC)$$

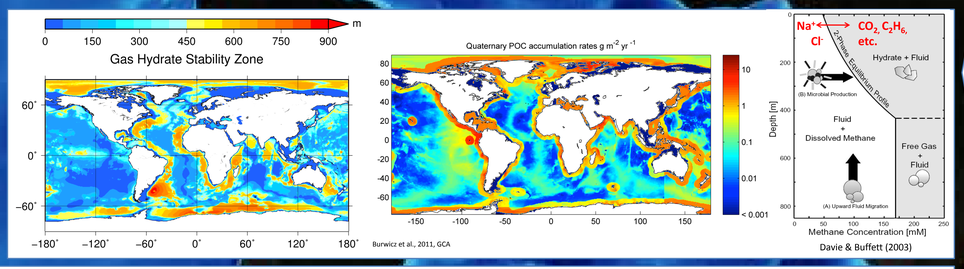
$$k_x = 0.16\cdot\left(a_0+\frac{z}{\omega}\right)^{-0.95}$$ → assumes a depth- decreasing reactivity of metabolites

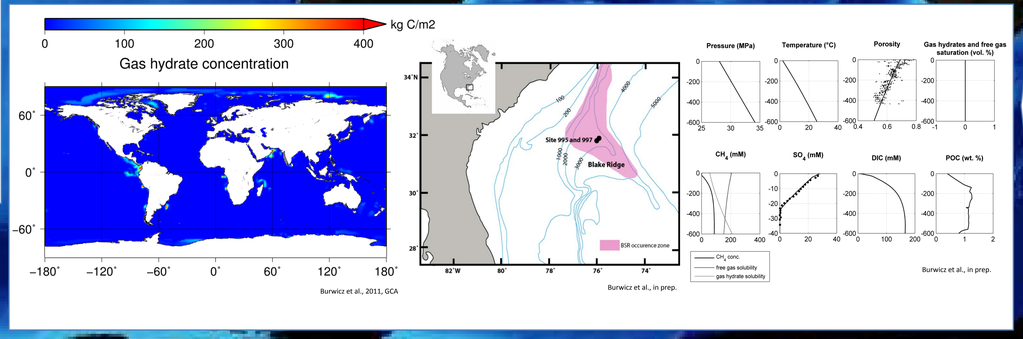
R_{POC} – rate of POC degradation (wt. % $\cdot yr^{-1}$)
K_c – Monod inhibition constant (mM)
k_x – age – dependent kinetic constant (yr^{-1})
C, G – concentration of dissolved (mM) and solid (wt. %) species, respectively
a_0 – initial age of organic matter decomposition (yr)
z – depth (cm)
ω – burial velocity of solid species ($cm\cdot yr^{-1}$)

→ controls the gradient of organic matter decomposition within a bioturbation zone- upper 10cm of sediments where AOM process occurs

Burwicz et al., 2011, GCA







Simulation

Chemical reactions solver

- In-situ POC degradation kinetics
- Kinetically-controlled bio-chemical reactions of methanogenesis, sulfate reduction and anaerobic oxidation of methane (AOM)
- Calculation of gas hydrate and free gas solubility in brine
- Gas hydrate and free gas formation (kinetics vs. thermodynamics)

Variables obtained:
new concentrations of dissolved chemical species

Post-processing

Equation-of-state for 3-phase system H_20-NaCl-CH_4 + GH

Variables obtained:
volumes and masses of phases, new ρ_f, ρ_g, S_f, S_g, S_h

Results

- P,T profiles
- Depth-resolved profiles of chemical species concentrations, gas hydrate and free gas saturations
- Full compaction history
- Local/global gas hydrate estimates

END

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