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Modelling Coupled Phase Transitions in Gas Hydrate Geosystems

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[1]GEOMAR Helmholtz Center for Ocean Research Kiel
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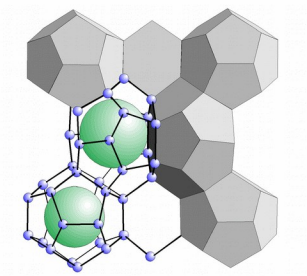
Gas Hydrates



gas
H_2O

Image source: J.Greinert, Geomar

- Gas hydrate → ice-like solid, immobile(?)

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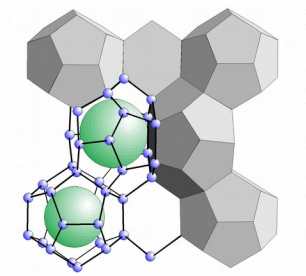

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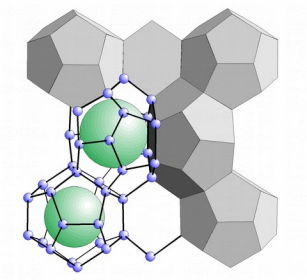

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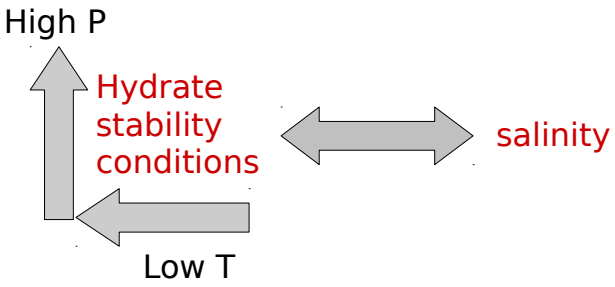
- Stable at high P, lo T
- Extremely sensitive to local thermodynamic state (P,T,salinity...)



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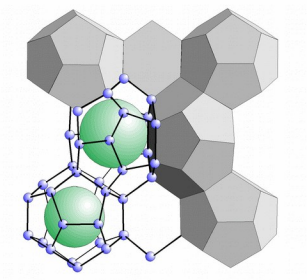

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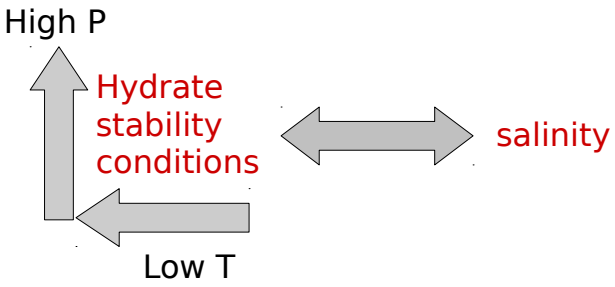


- Gas hydrate → ice-like solid, immobile(?)
- Stable at high P, lo T
- Extremely sensitive to local thermodynamic state (P,T,salinity...)

Challenges in modelling marine gas hydrates

- Predominantly **water saturated** domains
- environmental changes can locally destabilize hydrates
- **Free gas signatures as low as 0.5%!**
- Strong influence of salinity, **dilution effects**

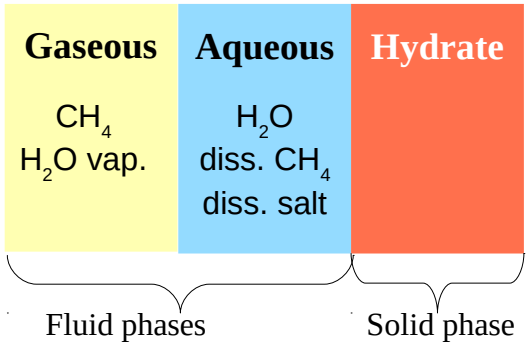
Mathematical Model

Four main components

CH_4 , H_2O , Hydrate , Dissolved salt

Three phases

Gaseous, Aqueous, Solid



Mathematical Model

GEOMAR

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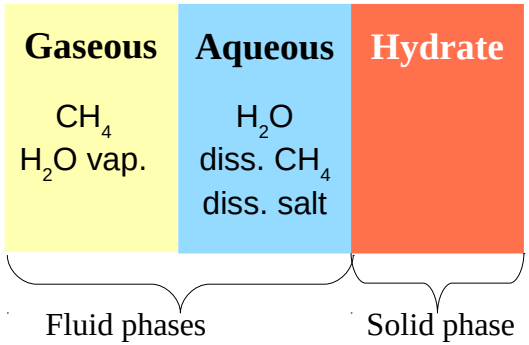
Model considers:

- Multi-phase, multi-component flow
- $CH_4 \leftrightarrow H_2O$ VLE
- Hydrate phase change
- Thermal effects due hydrate phase change



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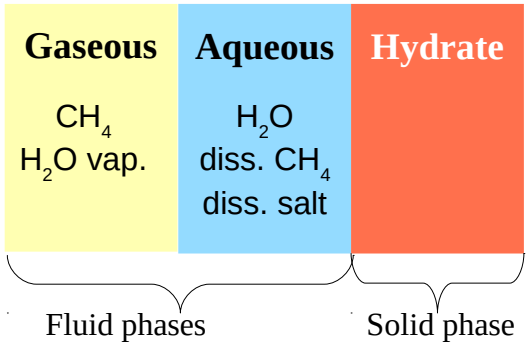
- Hydrate phase change → kinetic phase transition
- Thermal effects due hydrate phase change



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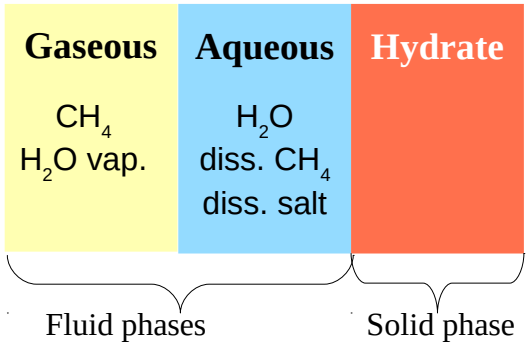

Governing equations

Mass balance for mobile components $\kappa = CH_4, H_2O$:

$$\Sigma_\alpha\left(\partial_t \phi \rho_\alpha S_\alpha \chi_\alpha^\kappa\right) + \Sigma_\alpha\left(\nabla \cdot \rho_\alpha \chi_\alpha^\kappa \boldsymbol{v}_\alpha\right) = \Sigma_\alpha\left(\nabla \cdot \phi S_\alpha \boldsymbol{J}_\alpha^\kappa\right) + \dot{g}^\kappa$$

where, $\boldsymbol{v}_\alpha = -\boldsymbol{K}\frac{k_{r,\alpha}}{\mu_\alpha}\left(\nabla P_\alpha - \rho_\alpha \boldsymbol{g}\right)$ and $\boldsymbol{J}_\alpha^\kappa = -\tau D_\alpha^\kappa \left(\rho_\alpha \nabla \chi_\alpha^\kappa\right)$

Mass balance for hydrate phase:

$$\partial_t \phi \rho_h S_h = \dot{g}_h$$

Mass balance for dissolved salt:

$$\partial_t \phi \rho_w S_w \chi_w^c + \nabla \cdot \rho_w \chi_w^c \boldsymbol{v}_w = \nabla \cdot \phi S_w \boldsymbol{J}_w^c$$

Energy balance:

$$\partial_t\left[(1-\phi)\rho_s u_s + \Sigma_\beta \phi \rho_\beta S_\beta u_\beta\right] + \Sigma_\beta \nabla \cdot \left(\phi \rho_\beta S_\beta \boldsymbol{v}_{\beta,t} h_\beta\right) = \nabla \cdot \left(-k_{eff}^{th} \nabla T\right) + \dot{Q}_h$$

Closure relations

summation condition for $\beta = g, w, h$: $\Sigma_\beta S_\beta = 1$

and, relation between fluid pressures: $P_g - P_w = P_c\left(S_w, S_h, \phi \ldots\right)$

$g^{\dot{CH}_4} + g^{\dot{H}_2O} + \dot{g}_h = 0$ and $\forall\, \alpha = g, w,\ \Sigma_\kappa \boldsymbol{J}_\alpha^\kappa = 0$

Hydraulic properties

$K = K_0 \cdot f_{S_h}^K\left(S_h\right)$, $P_c = P_c^{BC}\left(S_{we}\right) \cdot f_{S_h}^{P_c}\left(S_h\right)$

Mathematical Model

GEOMAR

Two main phase transitions

1. **non-equilinrium hydrate phase change**

P,T,salinity changes

$$CH_4 \cdot (H_2O)_{N_h} \Leftrightarrow CH_4 + N_h \cdot H_2O$$

$$\dot{g}_g = k_{reac} A_{rs} (P_g - P_{eqb})$$

where, $P_{eqb} = f(T, \chi^c_w)$,

$$k_{reac} = k^0_{reac} \exp\left(-\frac{\Delta E_a}{T}\right) \text{ , and } A_{rs} = A_{rs}(S_h, \phi, K)$$

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$$\dot{g}^{CH_4} + \dot{g}^{H_2O} + \dot{g}_h = 0 \quad \text{and} \quad \forall \alpha = g, w, \quad \Sigma_\kappa \boldsymbol{J}^\kappa_\alpha = 0$$

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2. Equilibrium fluid phase changes (VLE)

$\Sigma_\kappa \chi_\alpha^\kappa \leq 1 \quad \forall \alpha \quad$ and $\quad \Sigma_\kappa \chi_\alpha^\kappa = 1 \quad iff \quad S_\alpha > 0$

We can cast these inequality constraints as KKT complementarity conditions:

$1 - \Sigma_\kappa \chi_\alpha^\kappa \geq 0 \;,\; S_\alpha \geq 0 \;,\; S_\alpha (1 - \Sigma_\kappa \chi_\alpha^\kappa) = 0 \;.$

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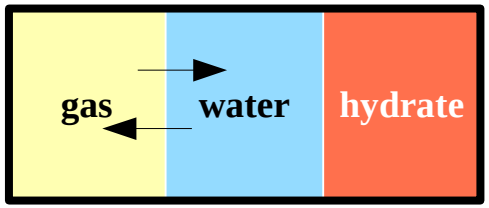

NUMERICAL SOLUTION

- Fully implicit cell centered finite volume method based discretization
  two-point finite difference flux approximation
  fully upwinded convective fluxes
- Nonlinear Complementary Constraints for vanishing gas phase, [Lauser,2011]
- **Semismooth Newton**'s method for Linearization,
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- SuperLU Linear Solver

Implementation in DUNE-PDElab framework [Bastian2010]
(http://www.dune-project.org)

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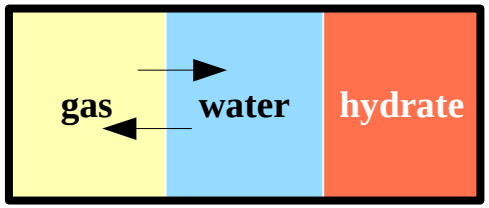

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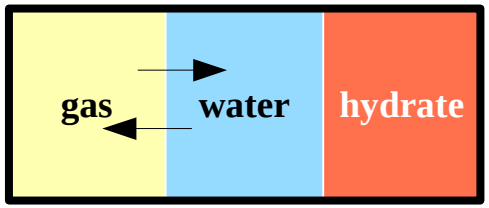
$$S_\alpha - \max\left\{0, S_\alpha - \left(1 - \sum_\kappa \chi_\alpha^\kappa\right)\right\} = 0\ , \quad \forall \alpha\ .$$

Equivalent form of the NCP non-differentiable, but semi-smooth

Mathematical Model



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$$S_\alpha - \max\left\{0, S_\alpha - \left(1 - \sum_\kappa \chi_\alpha^\kappa\right)\right\} = 0\ , \quad \forall \alpha\ .$$

$$\mathcal{A}_\alpha := \left\{ j \in \mathcal{N} : (S_\alpha)_j - \left(1 - \sum_\kappa (\chi_\alpha^\kappa)_j\right) > 0 \right\}$$

$$\mathcal{I}_\alpha := \mathcal{N} \backslash \mathcal{A}_\alpha$$

Field-scale Example
BCL System in Danube Paleo Delta

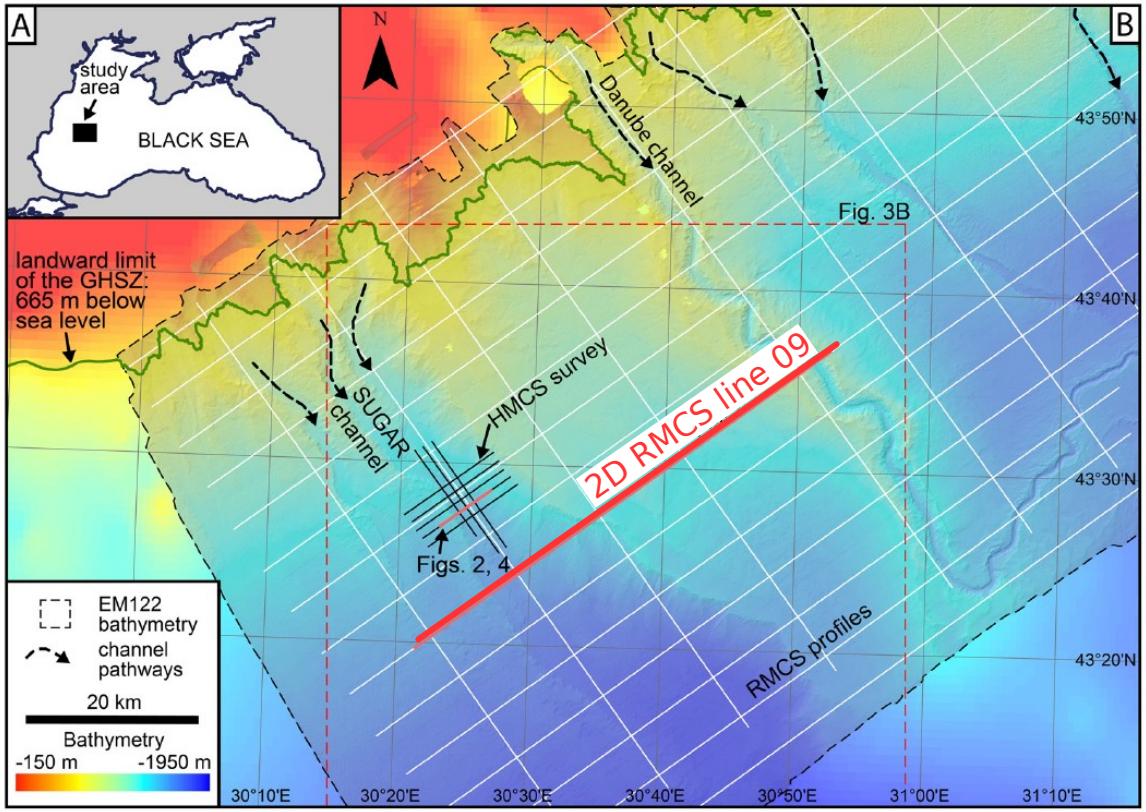

Fig.: Overview map of 2D high-resolution multichannel seismic (HMCS) survey, and 2D regional multichannel seismic (RMCS) survey.
Bathymetry and seismic data were acquired during **R/V Maria S. Merian cruise MSM34 in 2013–2014**.

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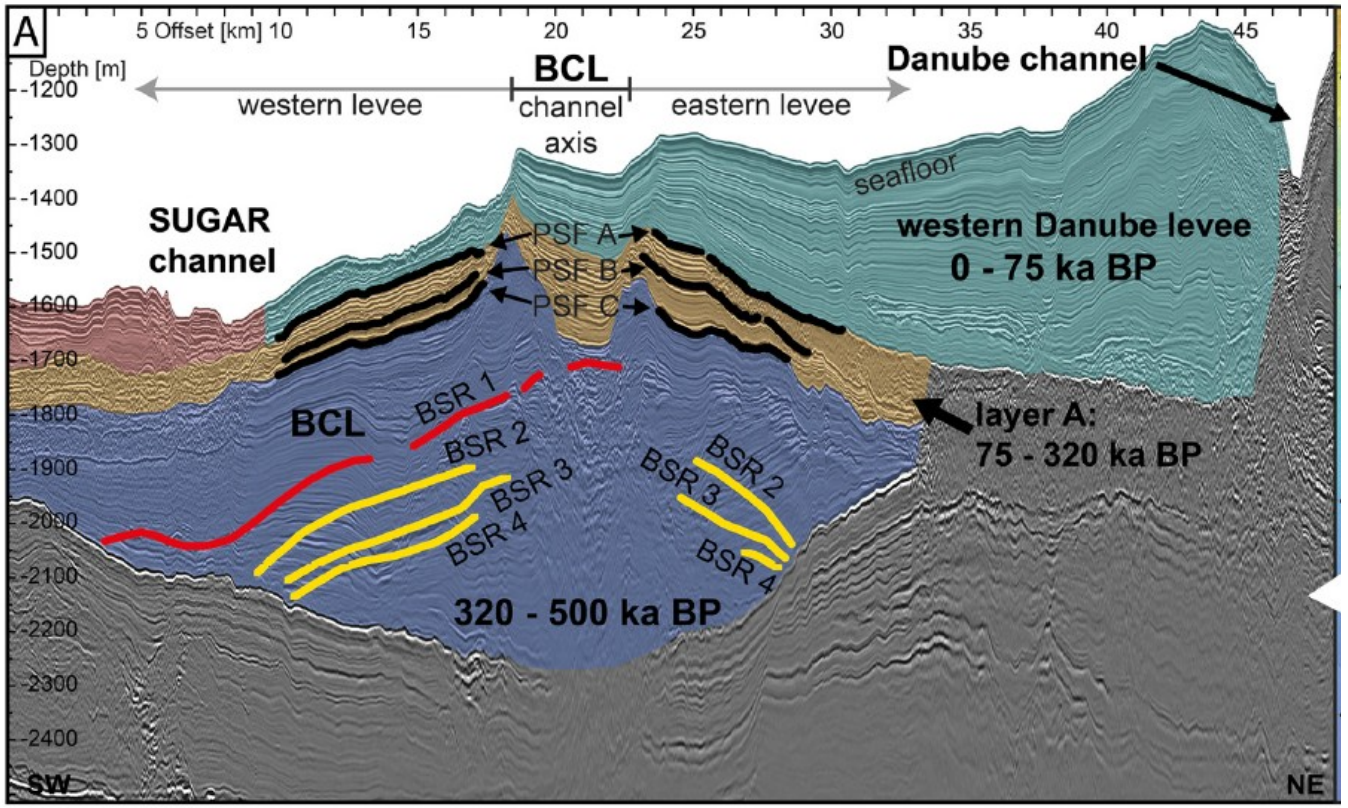

Fig.: 2D RMCS line 09
Interpretation of the seismic data [Zander2017]

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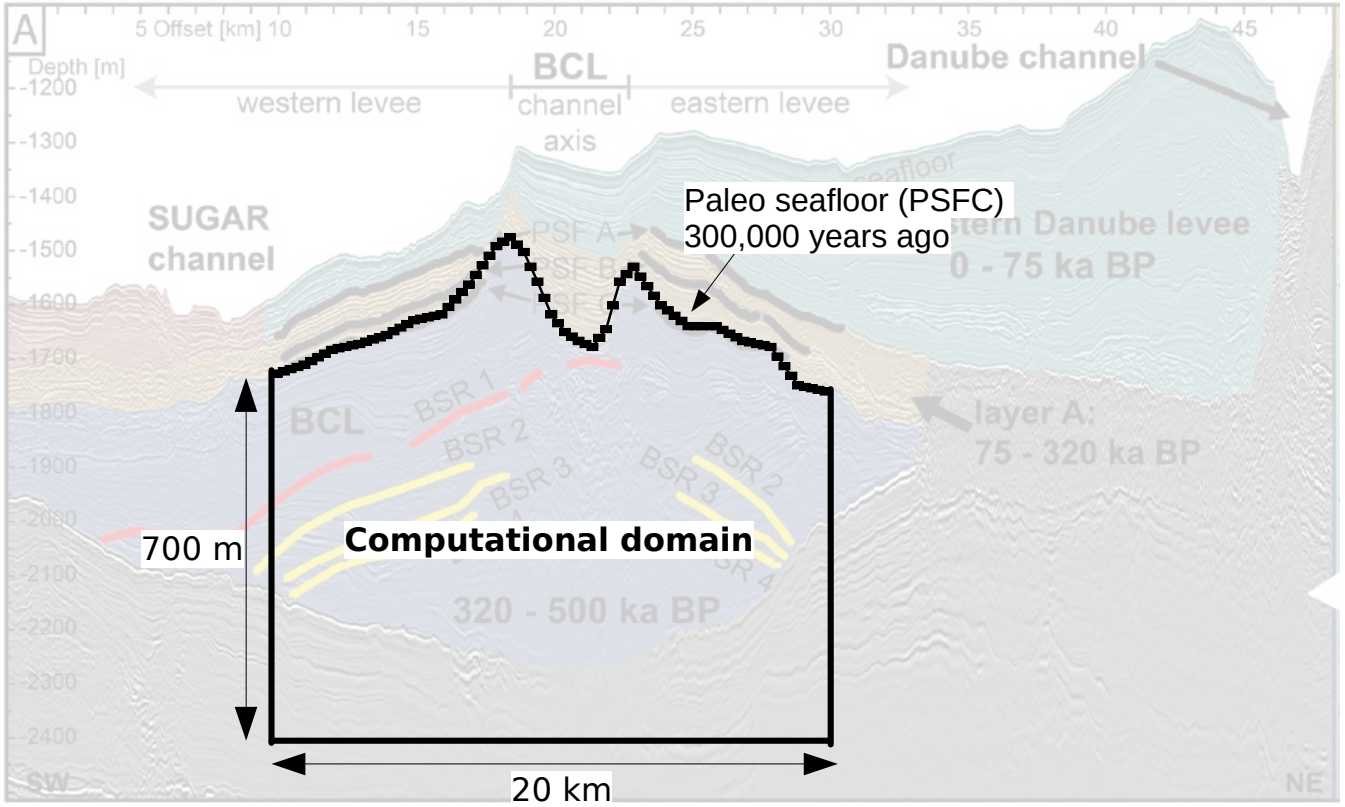

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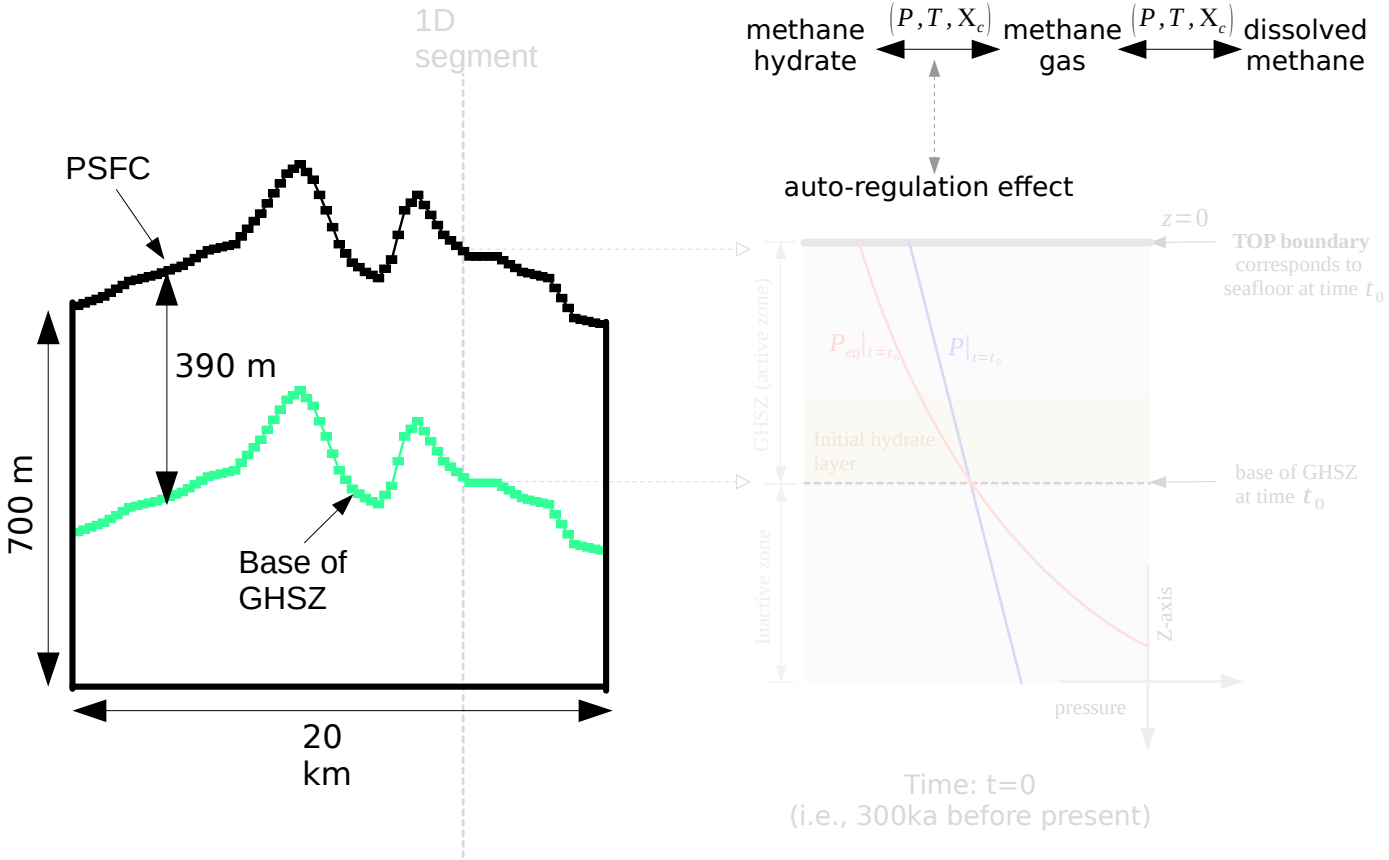

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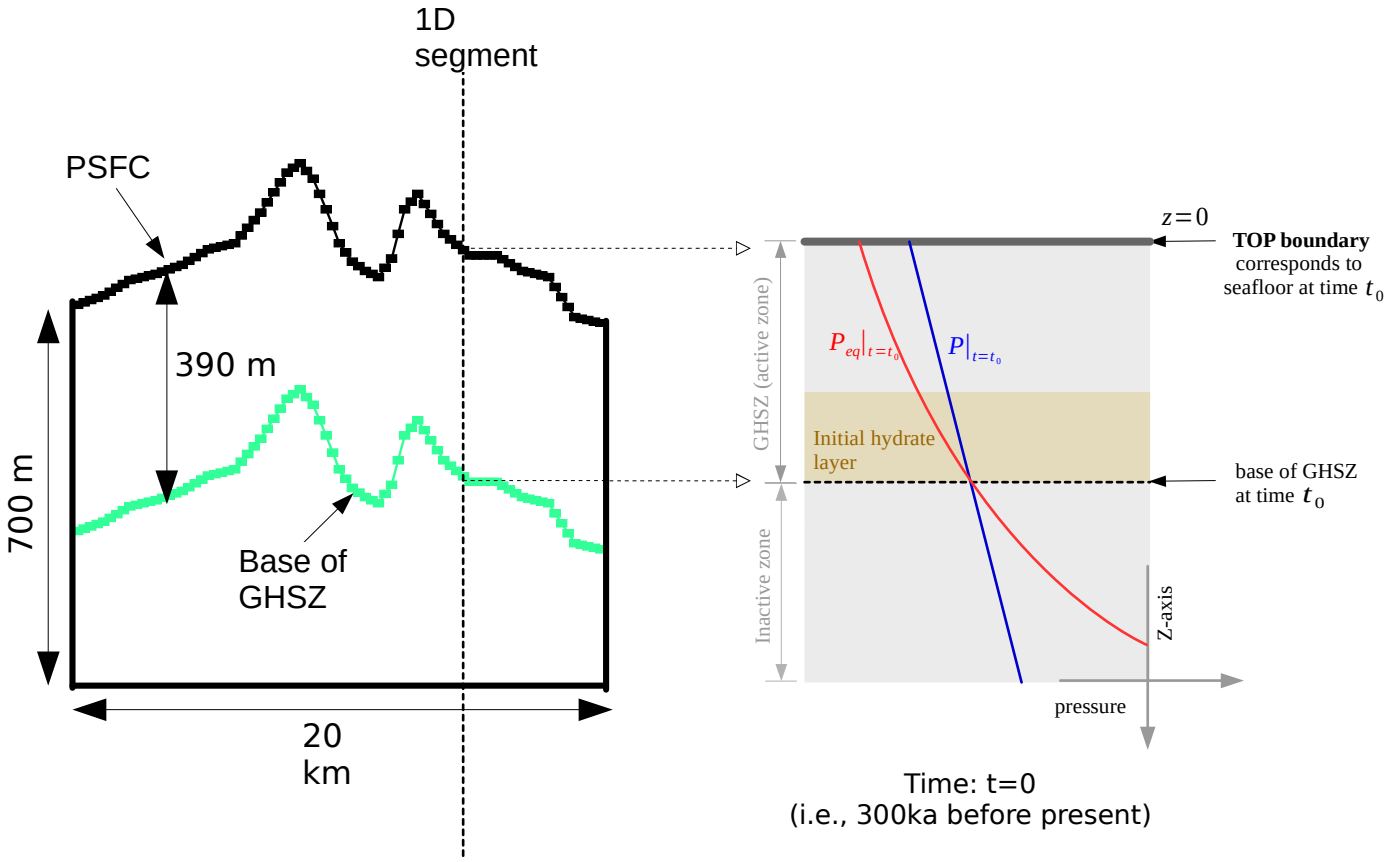

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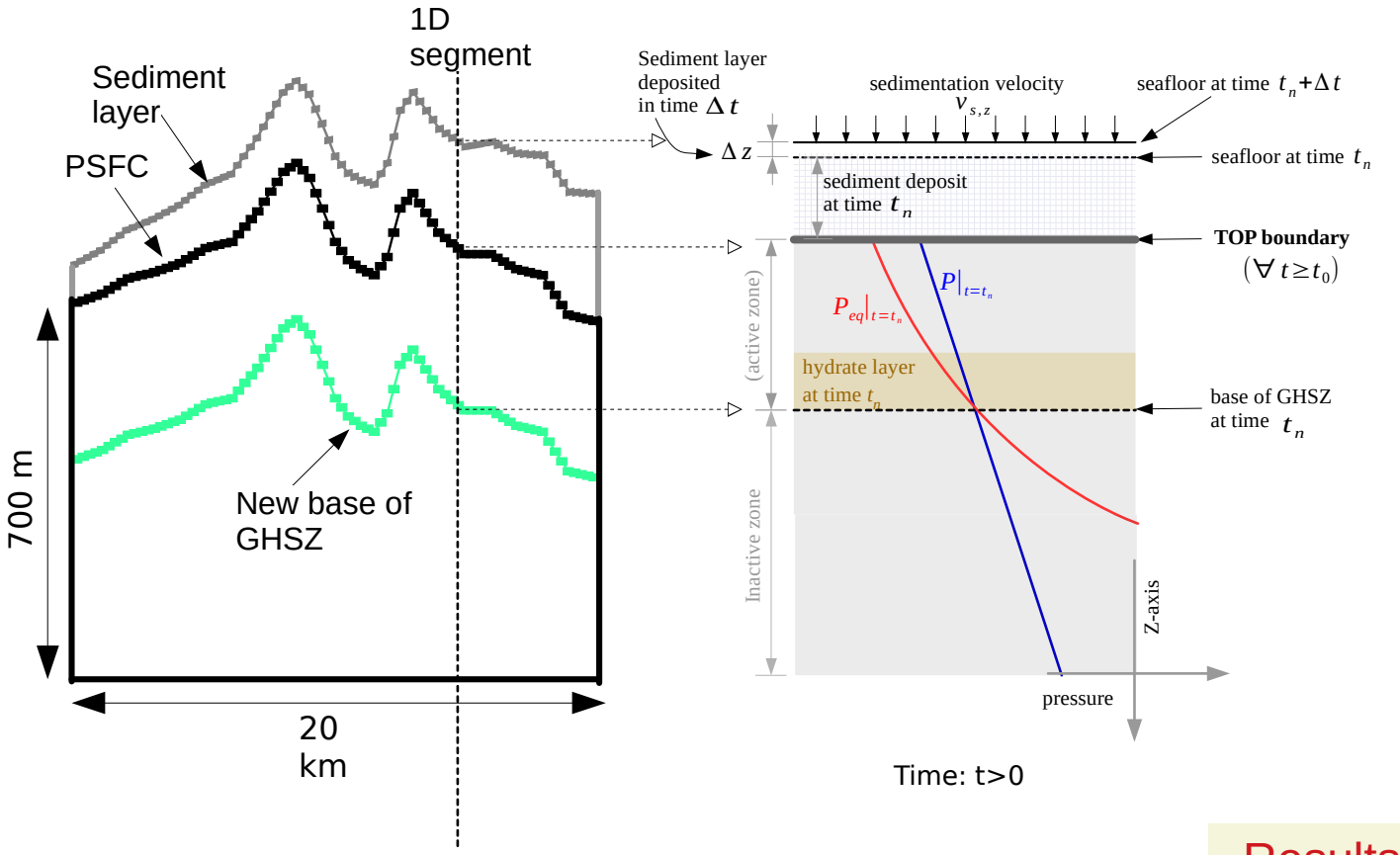
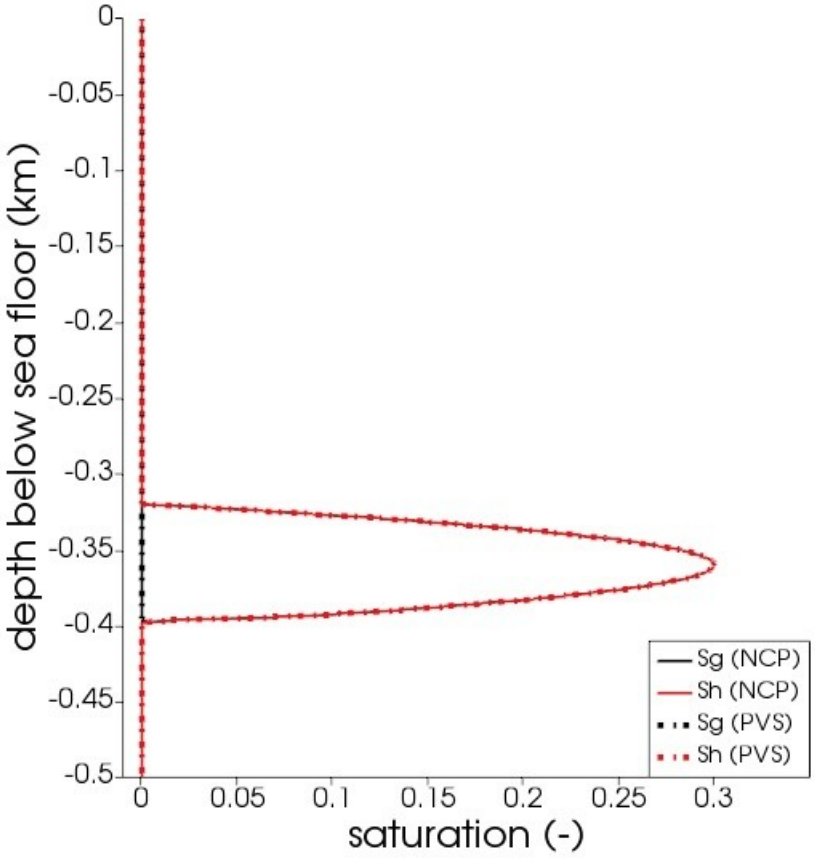


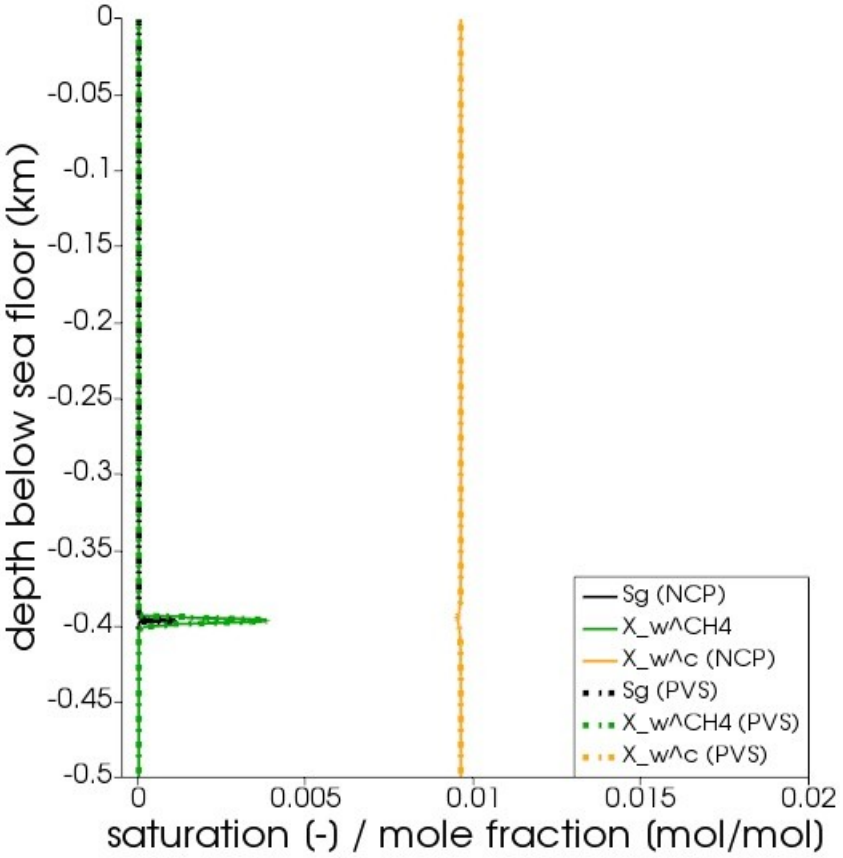
Results

Field-scale Example
BCL System in Danube Paleo Delta

GEOMAR

Time = 19,500 years





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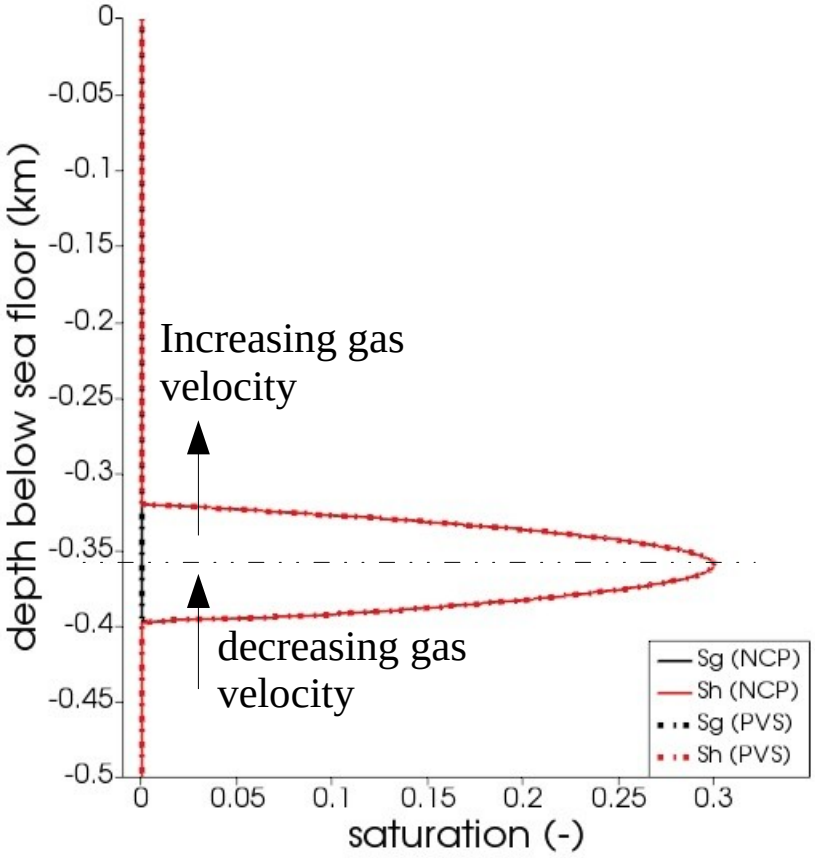

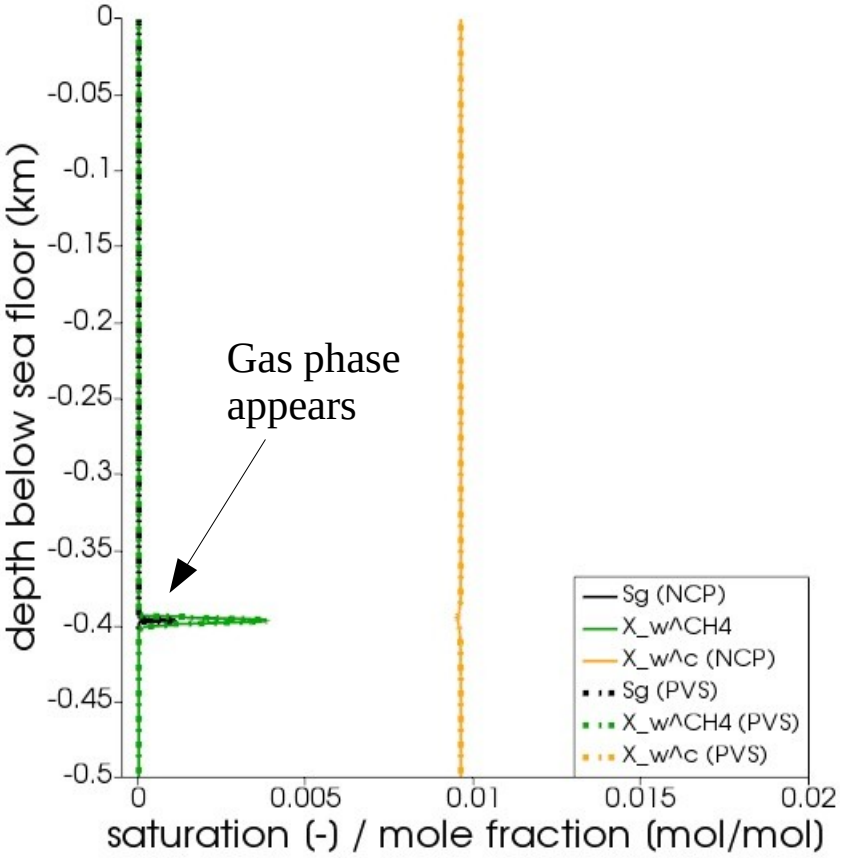

Field-scale Example
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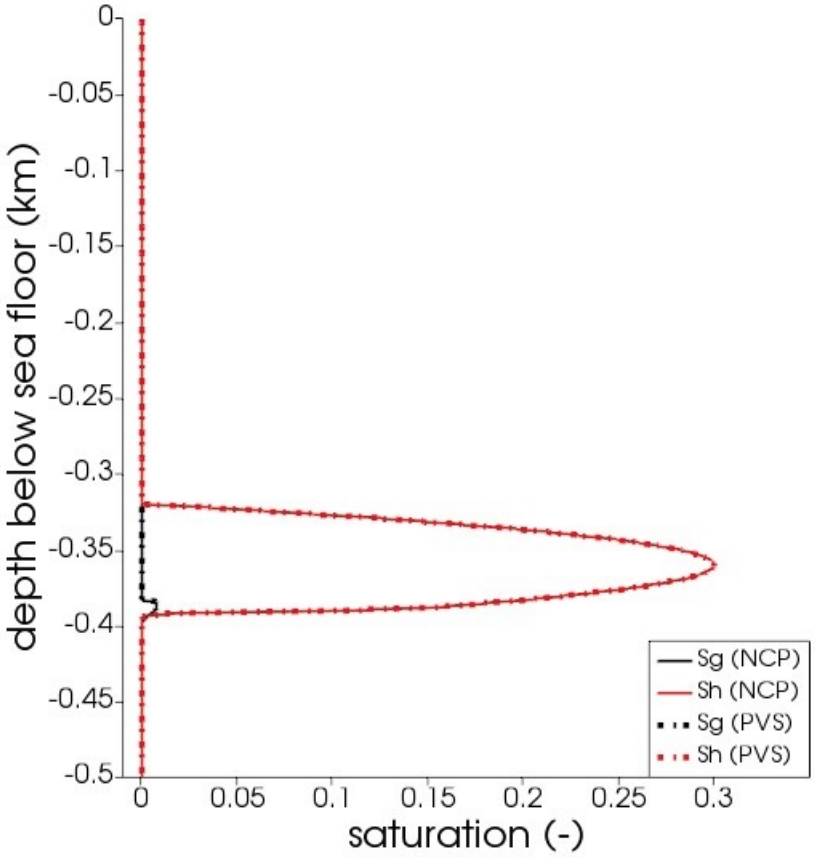
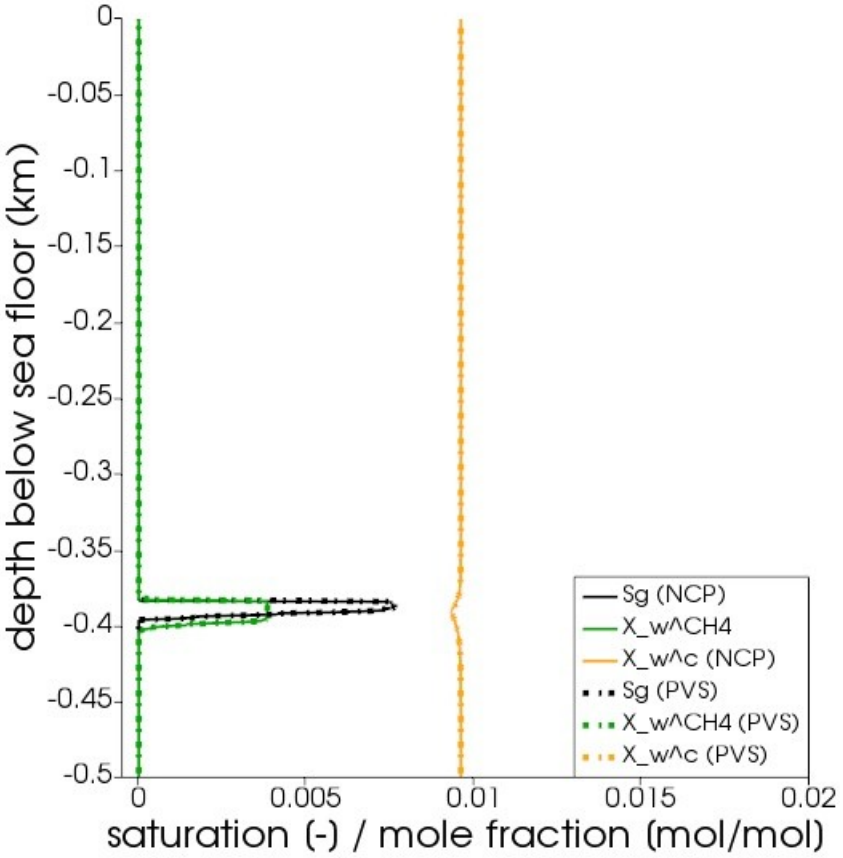
GEOMAR

Time = 30,000 years

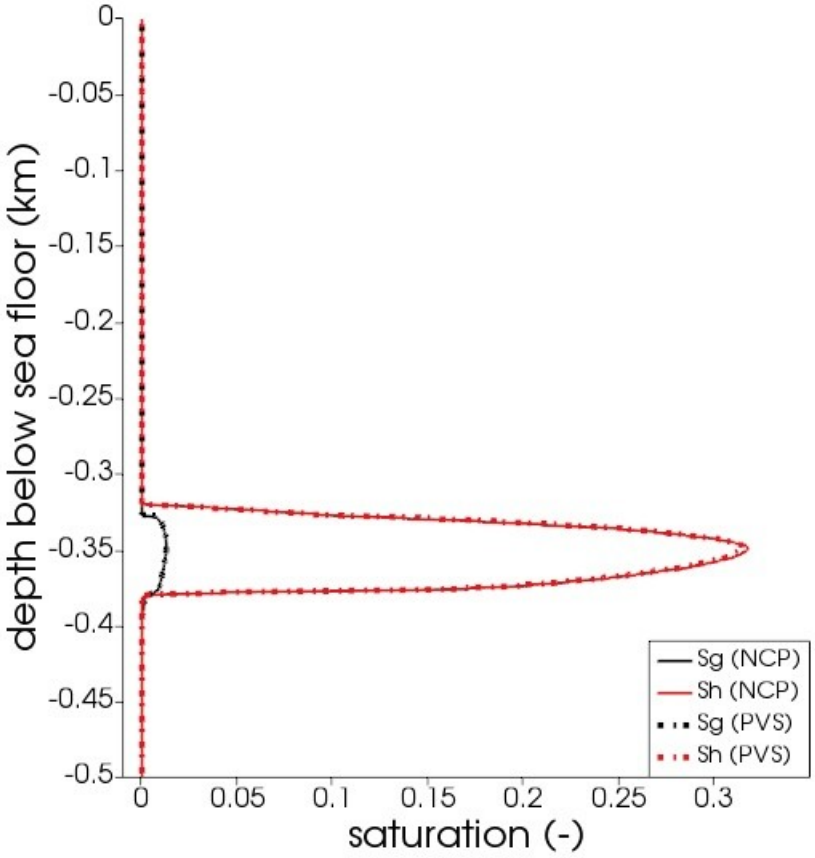


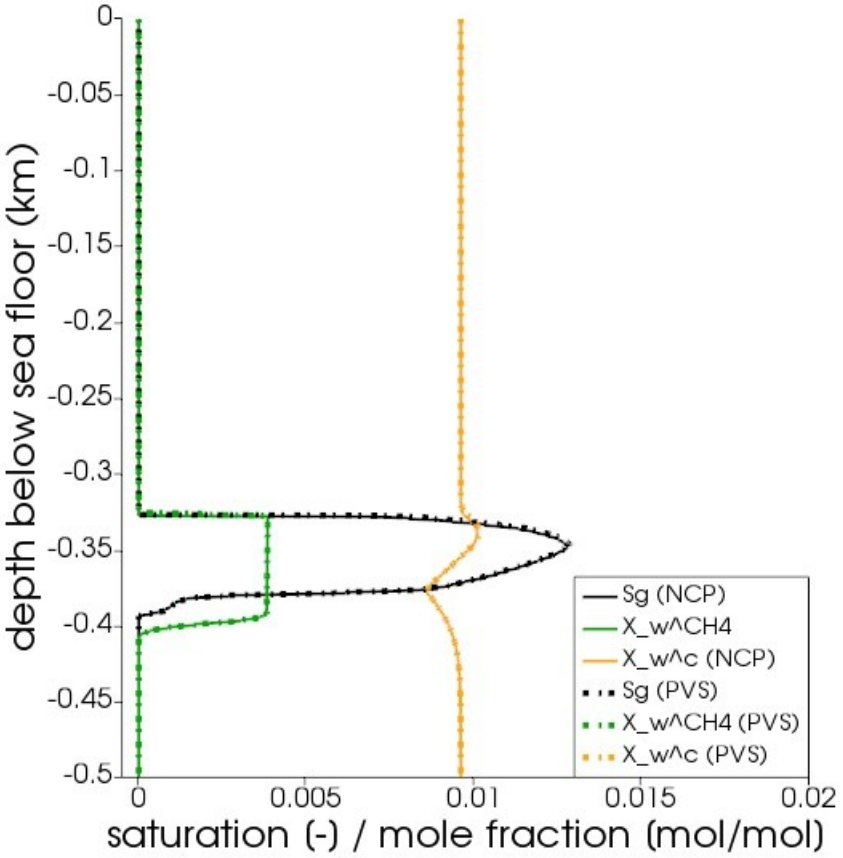


Field-scale Example
BCL System in Danube Paleo Delta

GEOMAR

Time = 60,000 years

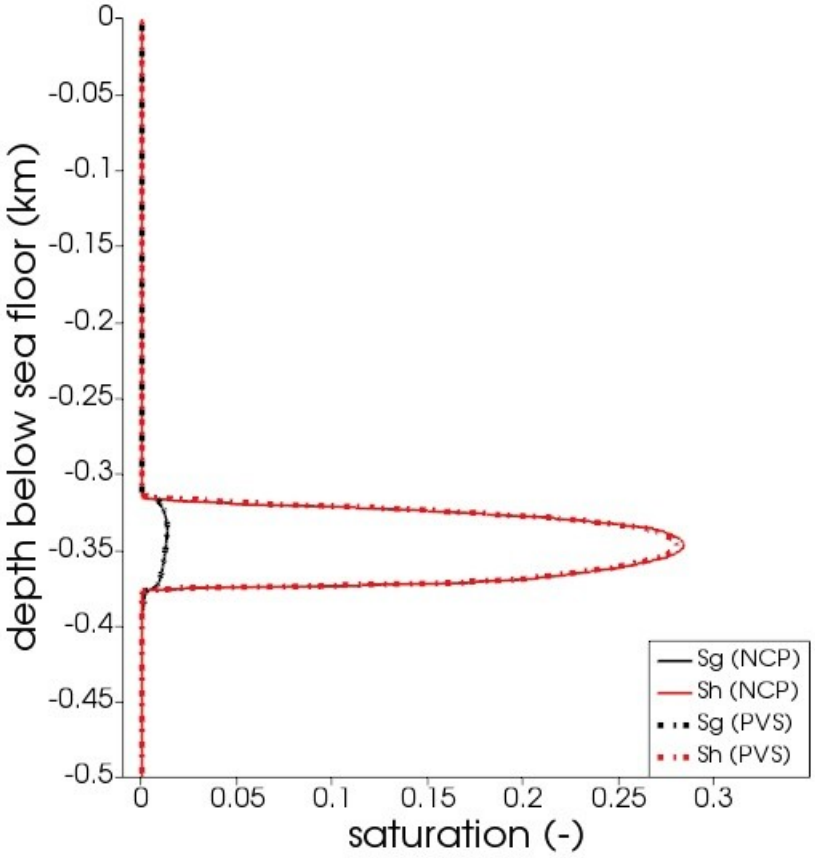


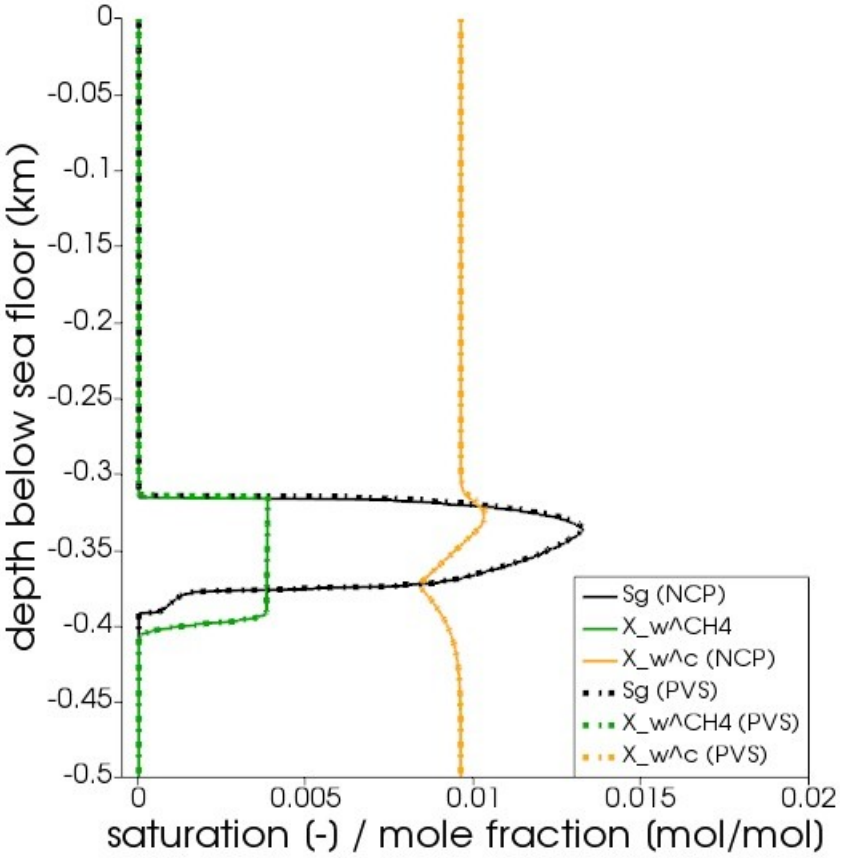


Field-scale Example
BCL System in Danube Paleo Delta

GEOMAR

Time = 67,500 years

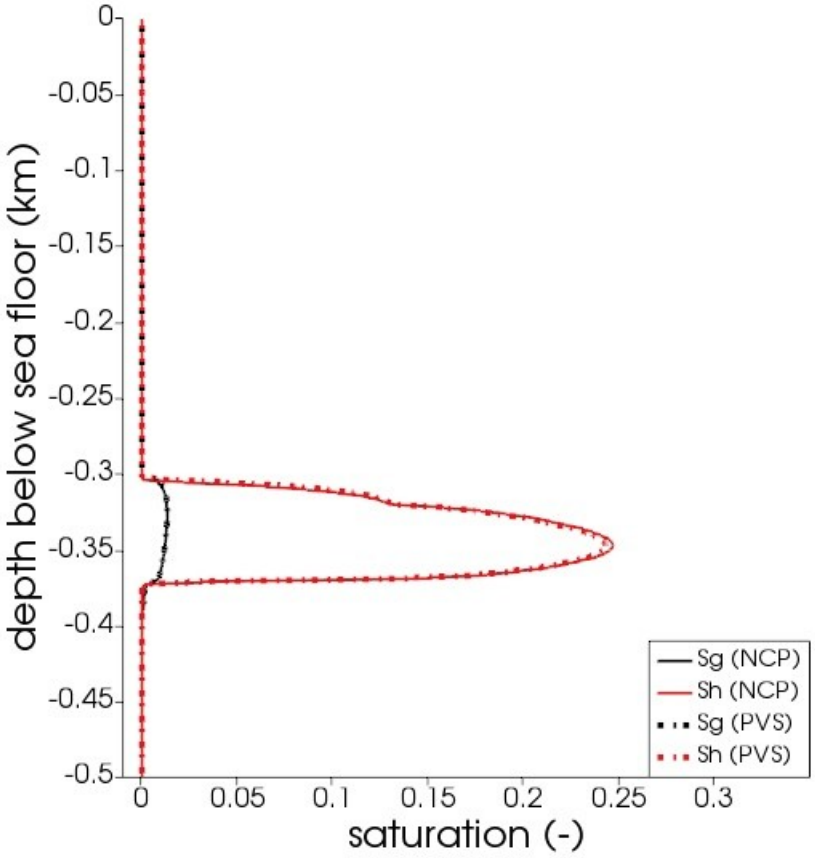


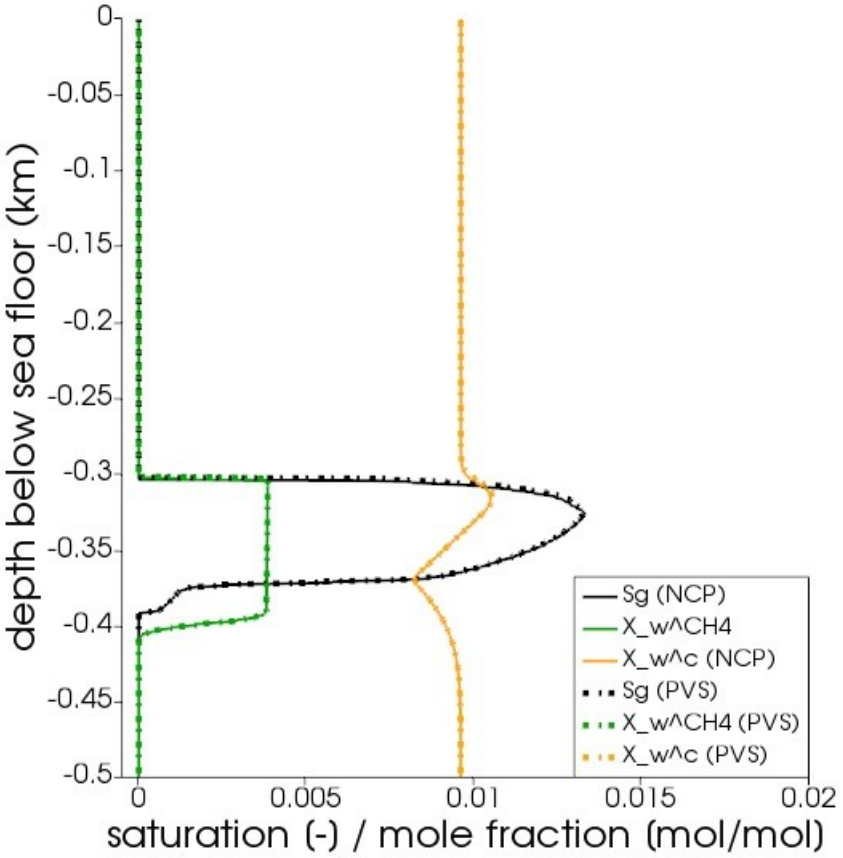


Field-scale Example
BCL System in Danube Paleo Delta

GEOMAR

Time = 75,000 years

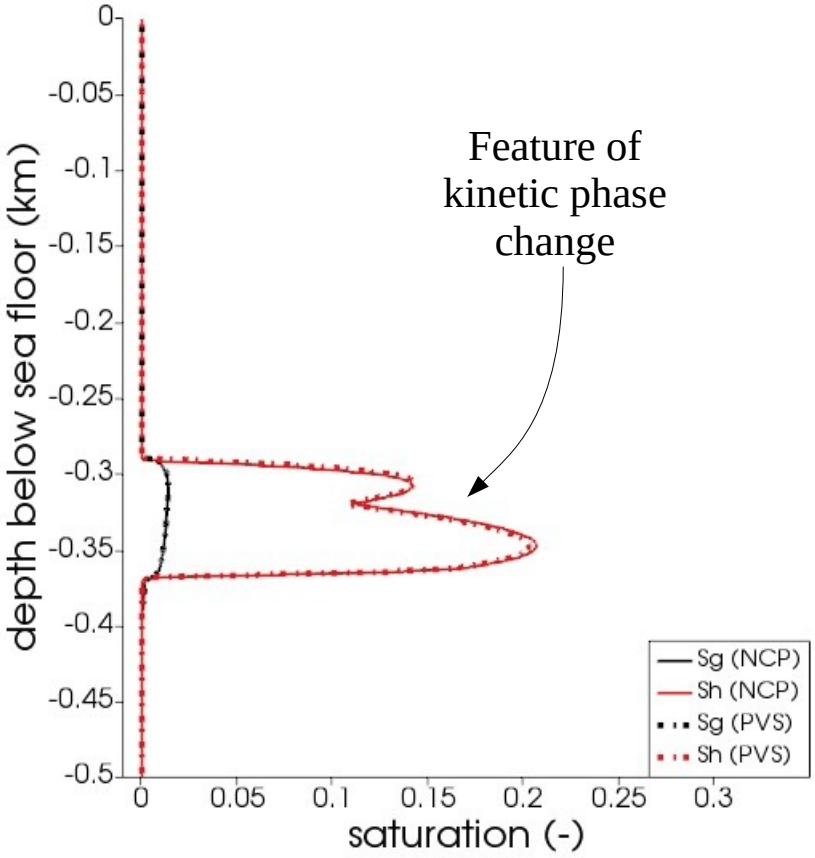


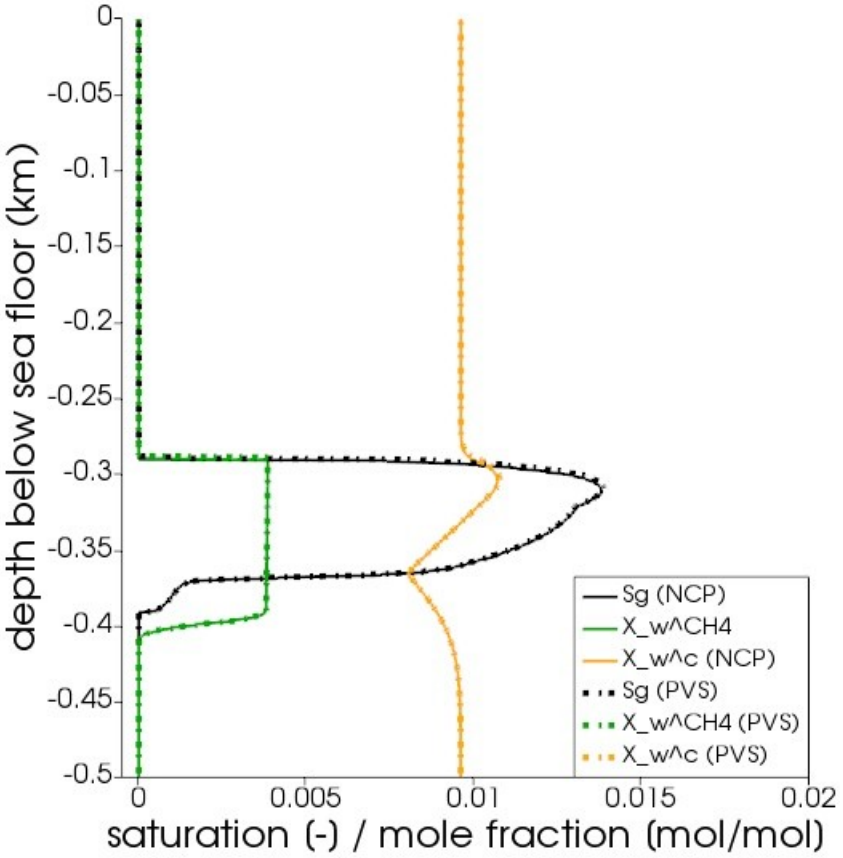


Field-scale Example
BCL System in Danube Paleo Delta

GEOMAR

Time = 82,500 years

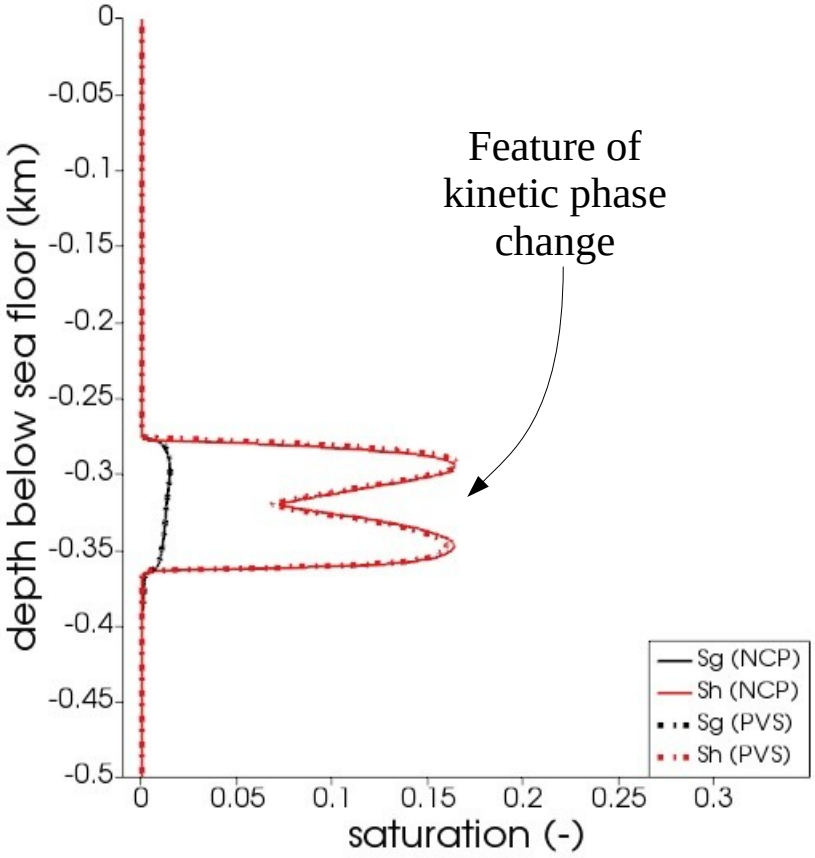


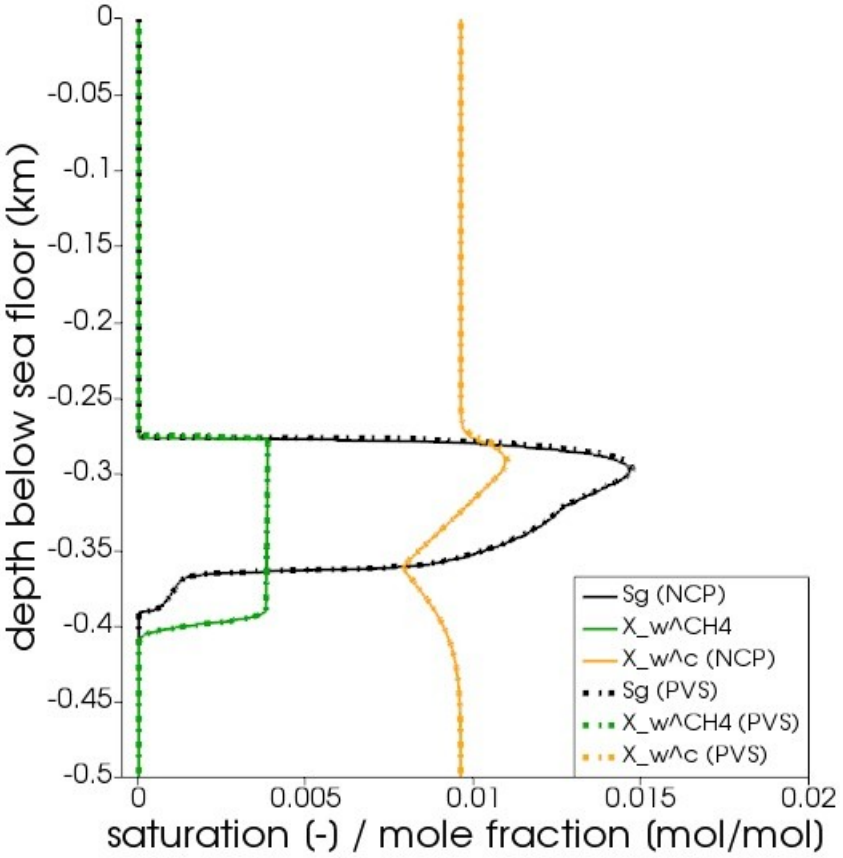


Field-scale Example
BCL System in Danube Paleo Delta

GEOMAR

Time = 90,000 years

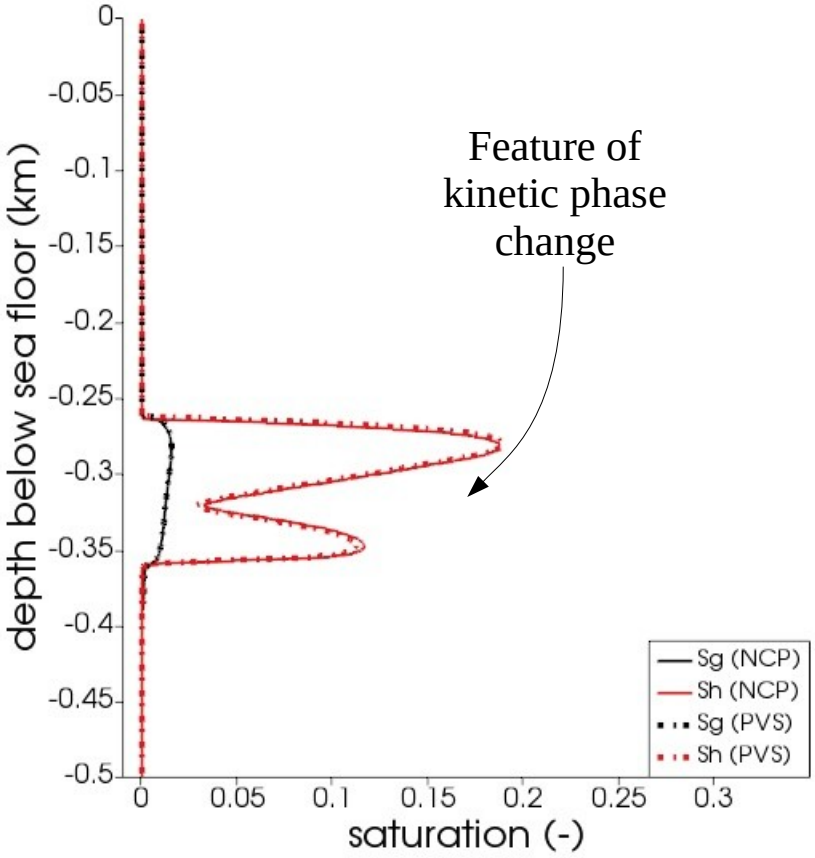


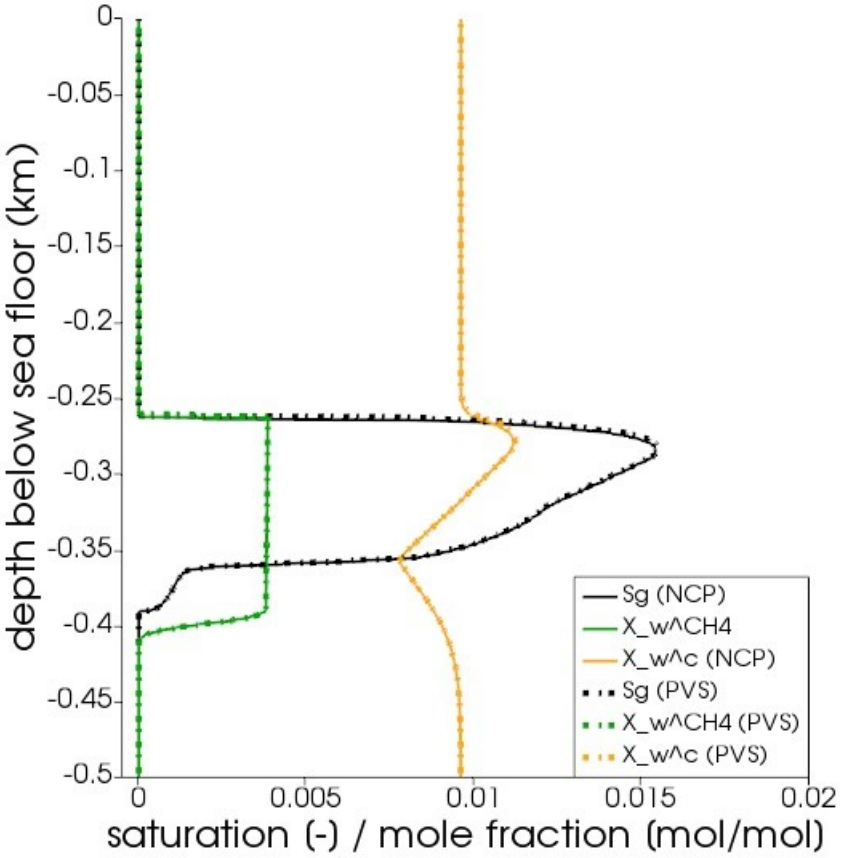


Field-scale Example
BCL System in Danube Paleo Delta

GEOMAR

Time =97,500 years

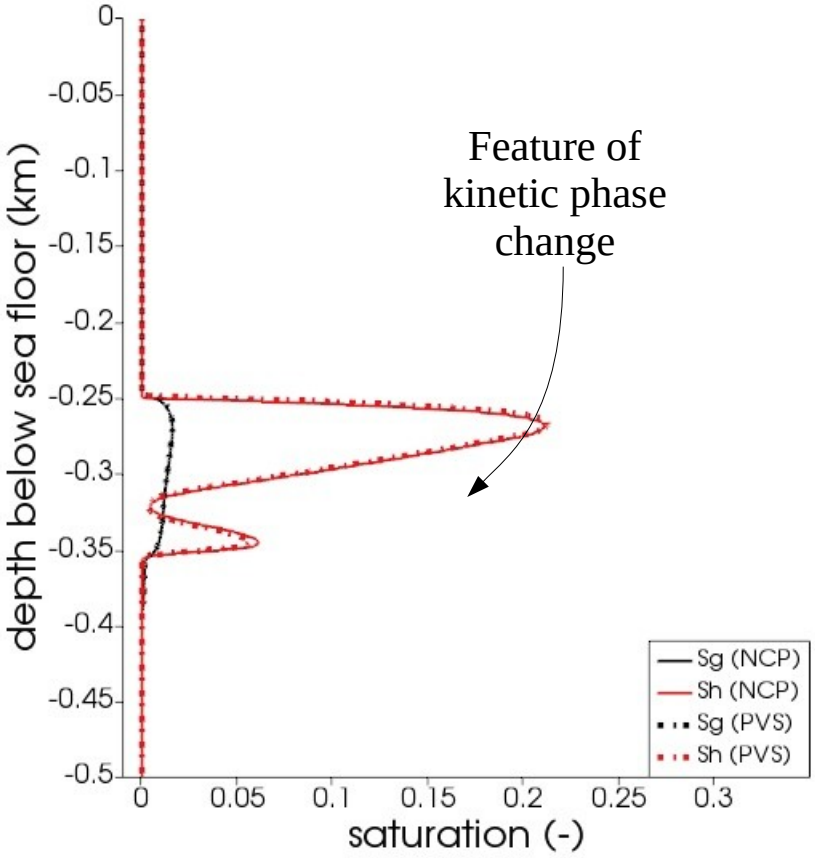


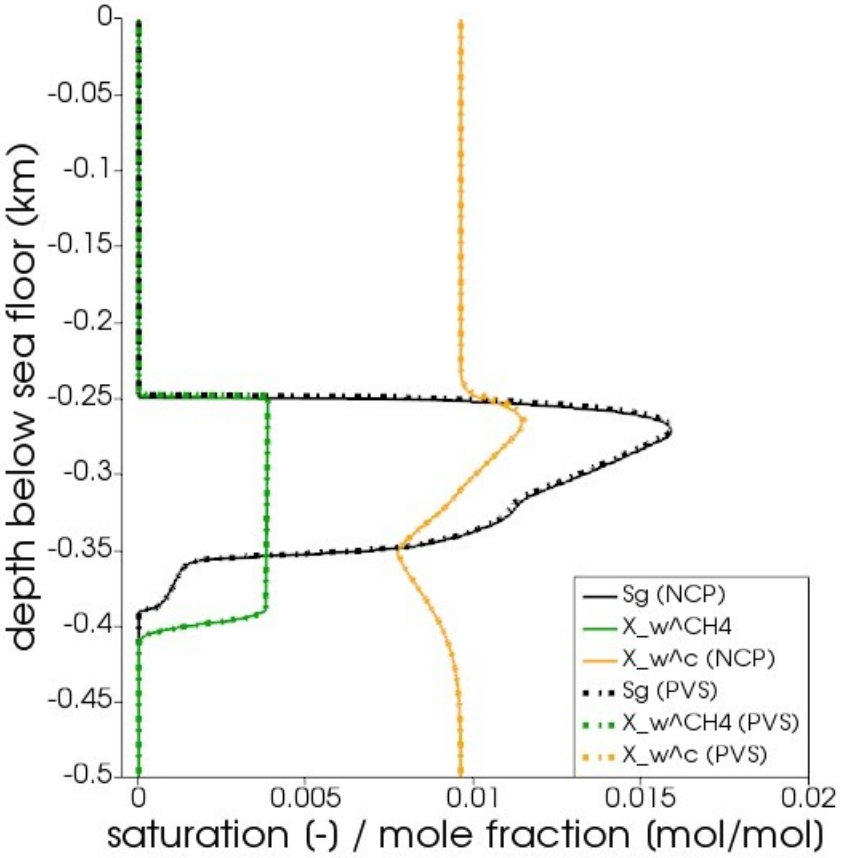


Field-scale Example
BCL System in Danube Paleo Delta

GEOMAR

Time = 105,000 years

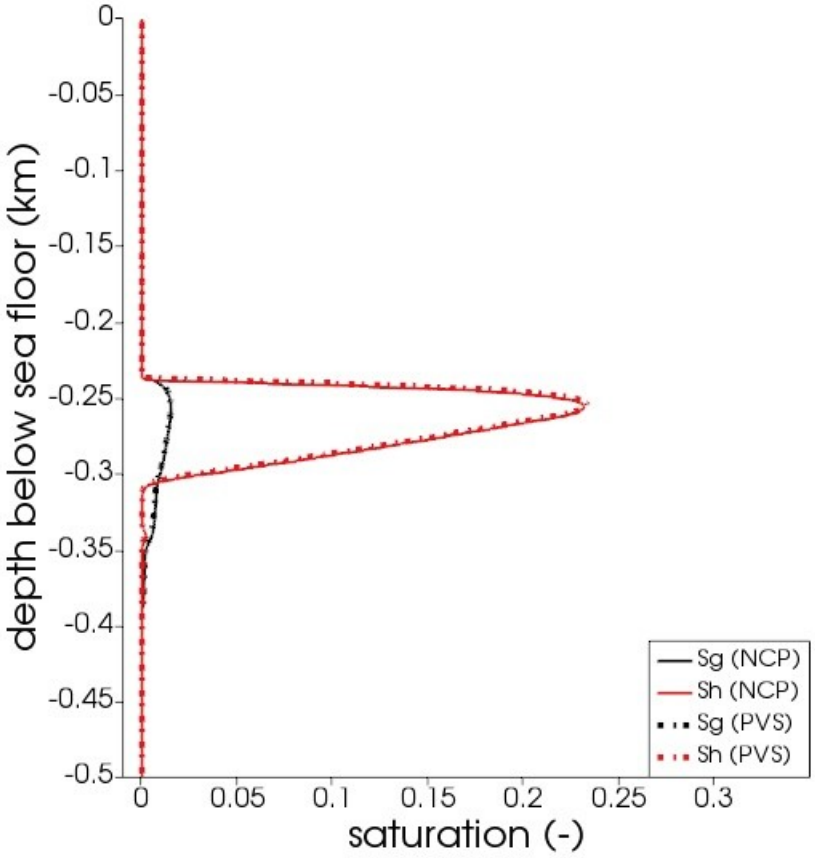


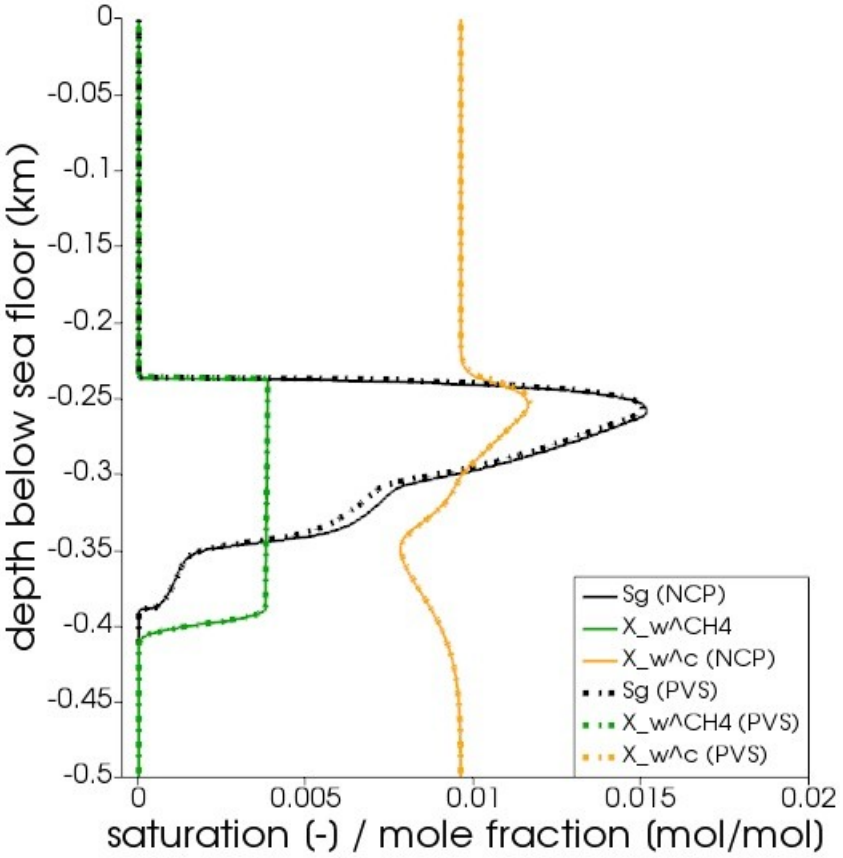


Field-scale Example
BCL System in Danube Paleo Delta

GEOMAR

Time = 112,500 years

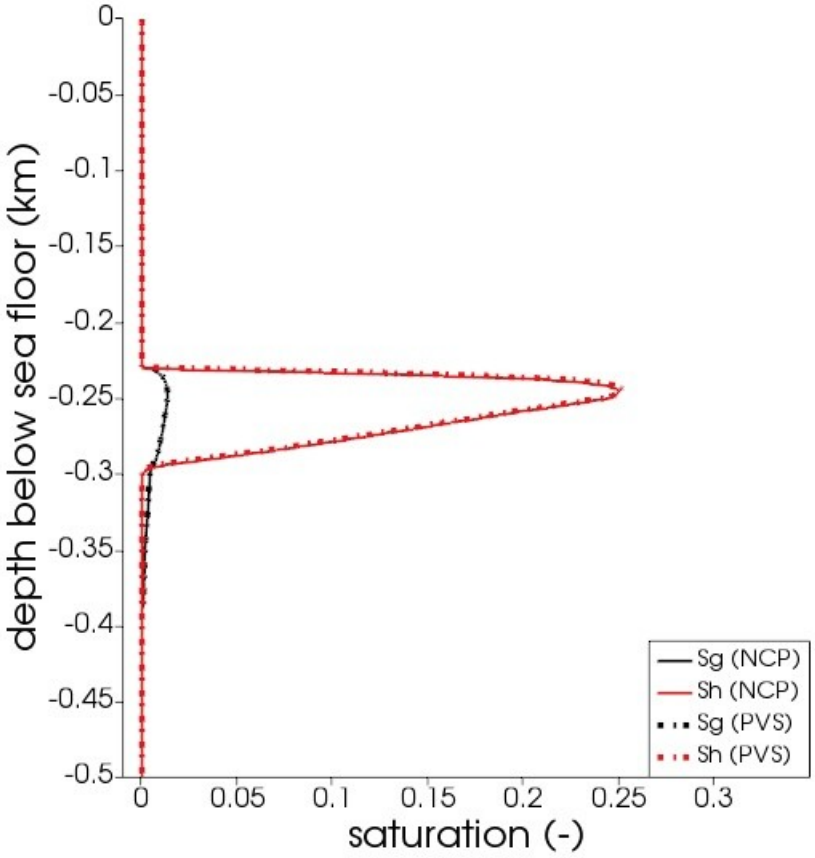


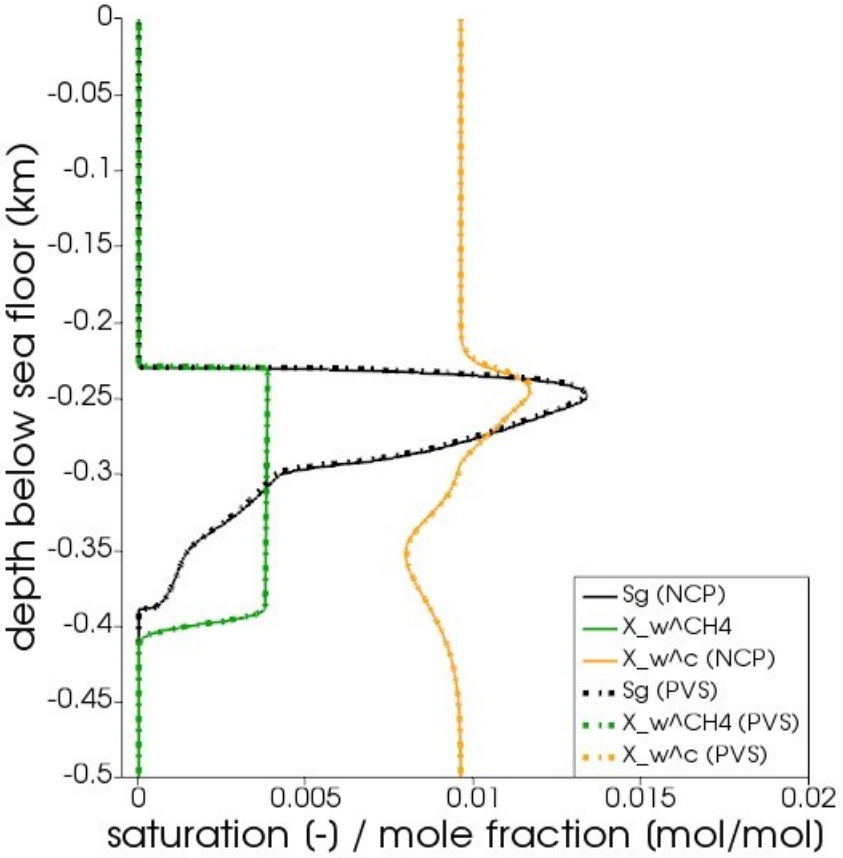


Field-scale Example
BCL System in Danube Paleo Delta

GEOMAR

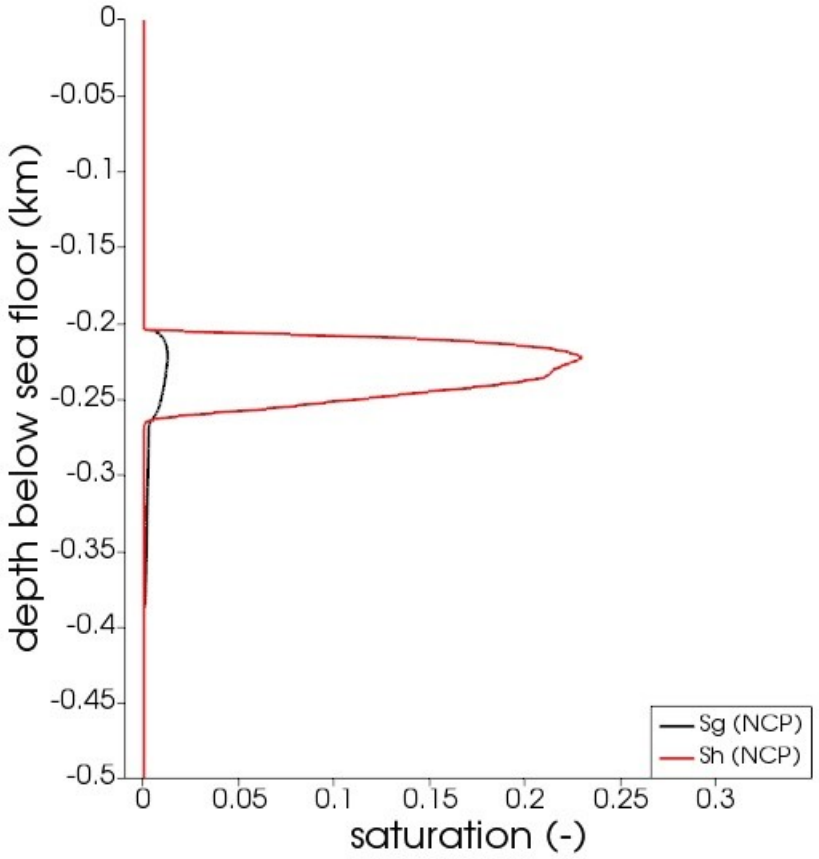
Time = 120,000 years

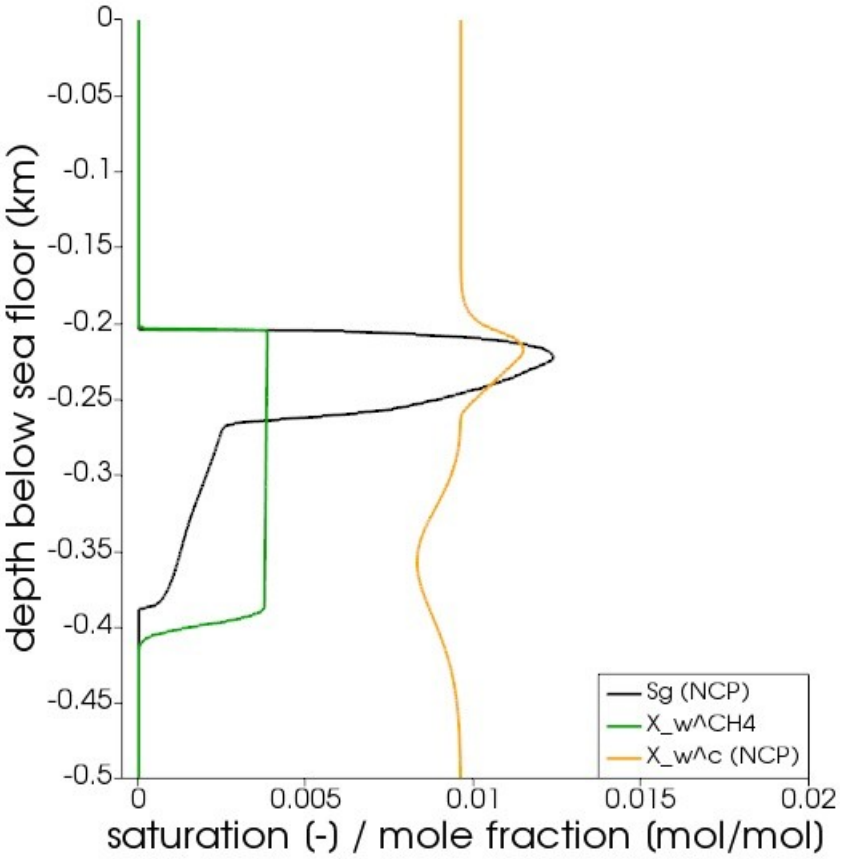




Field-scale Example
BCL System in Danube Paleo Delta

Time = 150,000 years

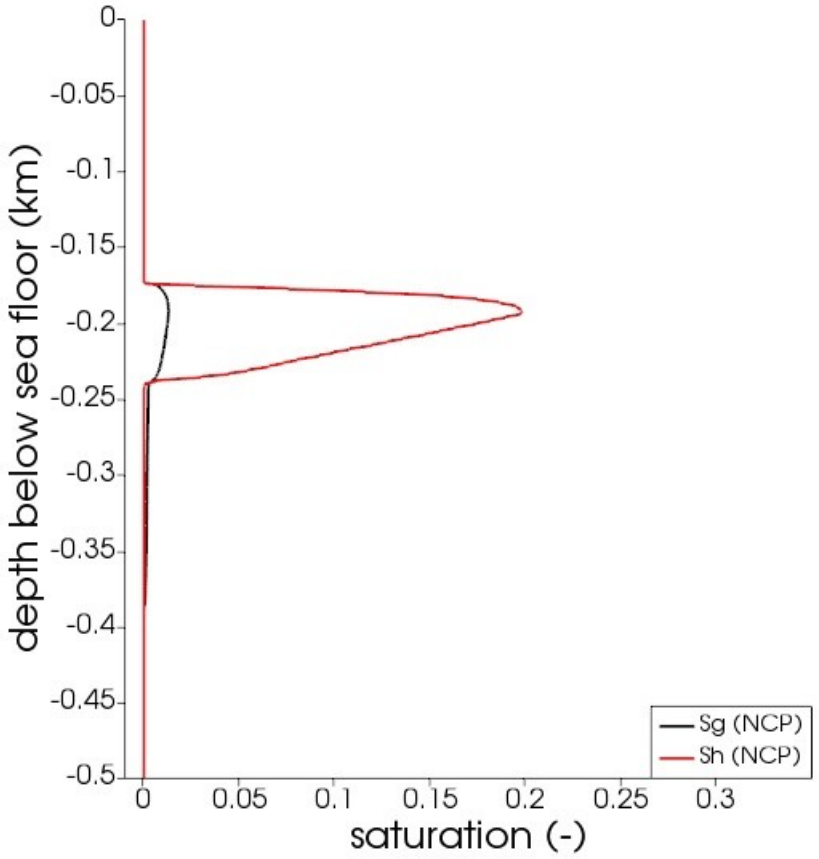


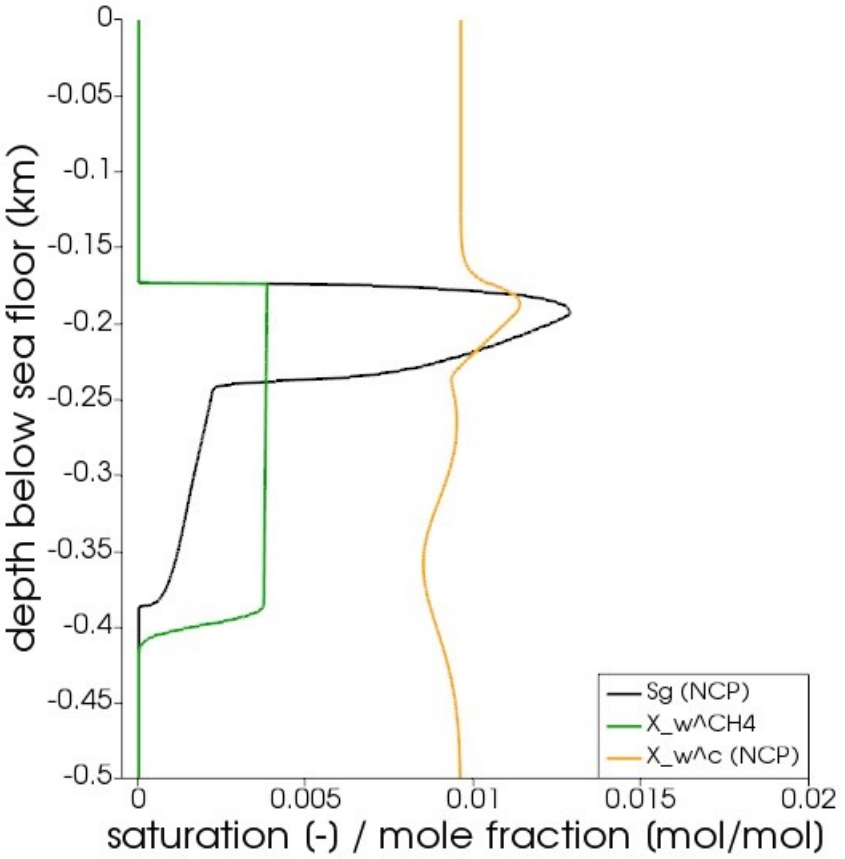


Field-scale Example
BCL System in Danube Paleo Delta

GEOMAR

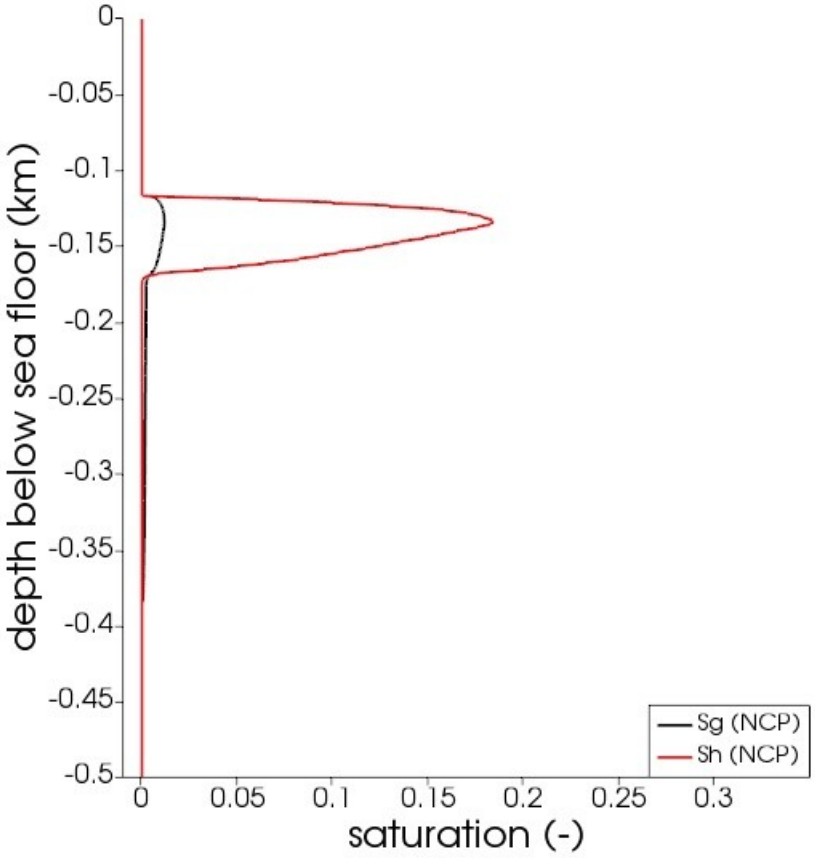
Time = 180,000 years

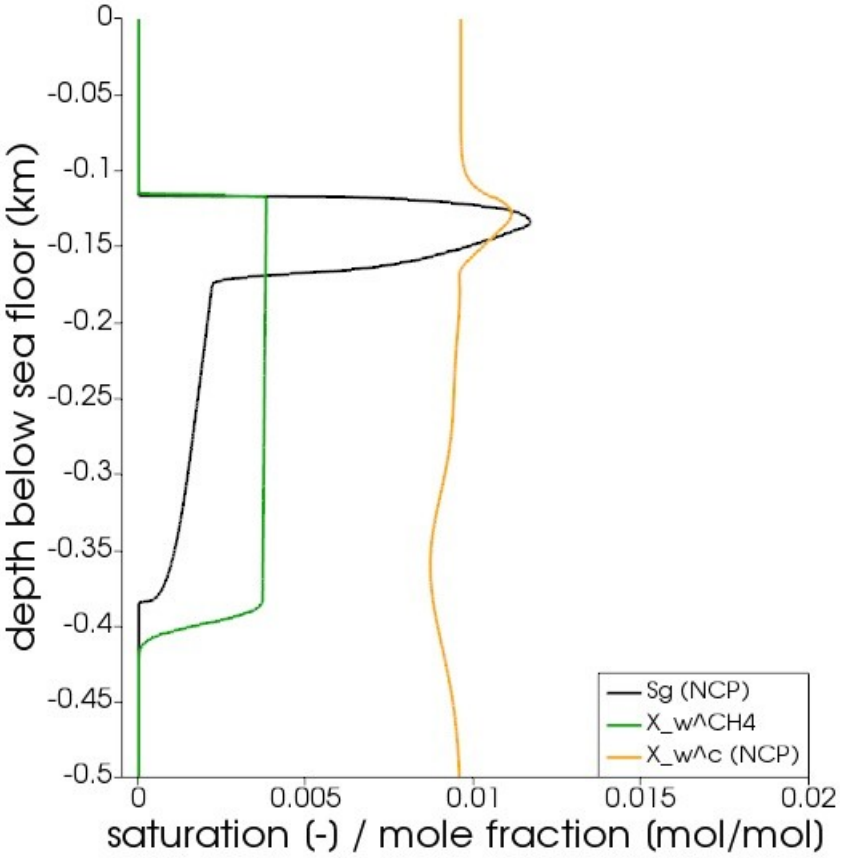




Field-scale Example
BCL System in Danube Paleo Delta

Time = 240,000 years

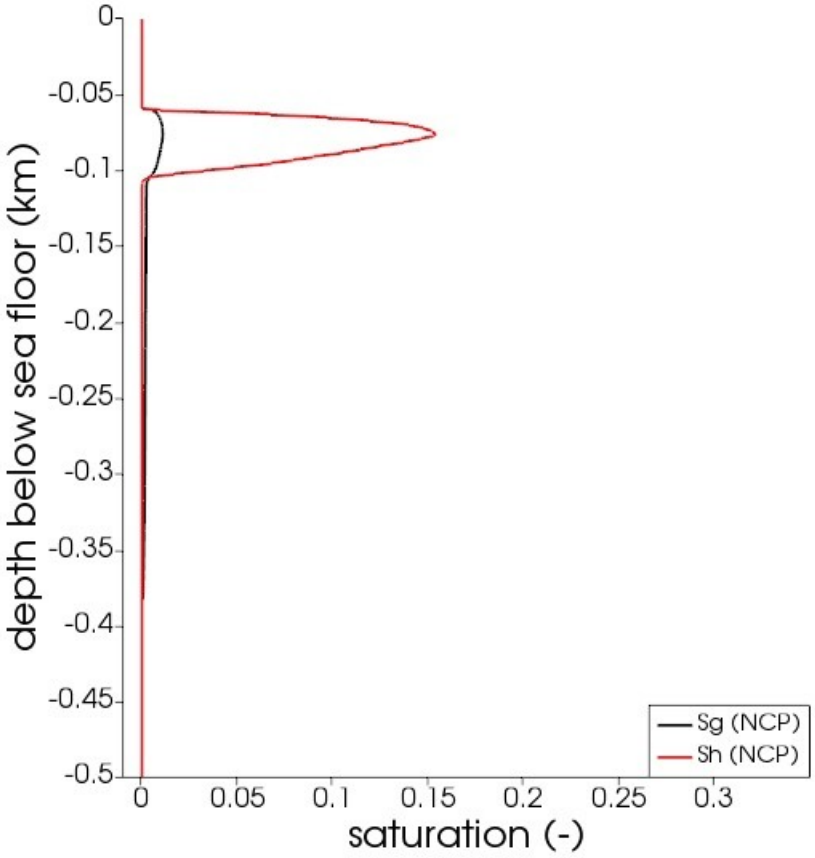


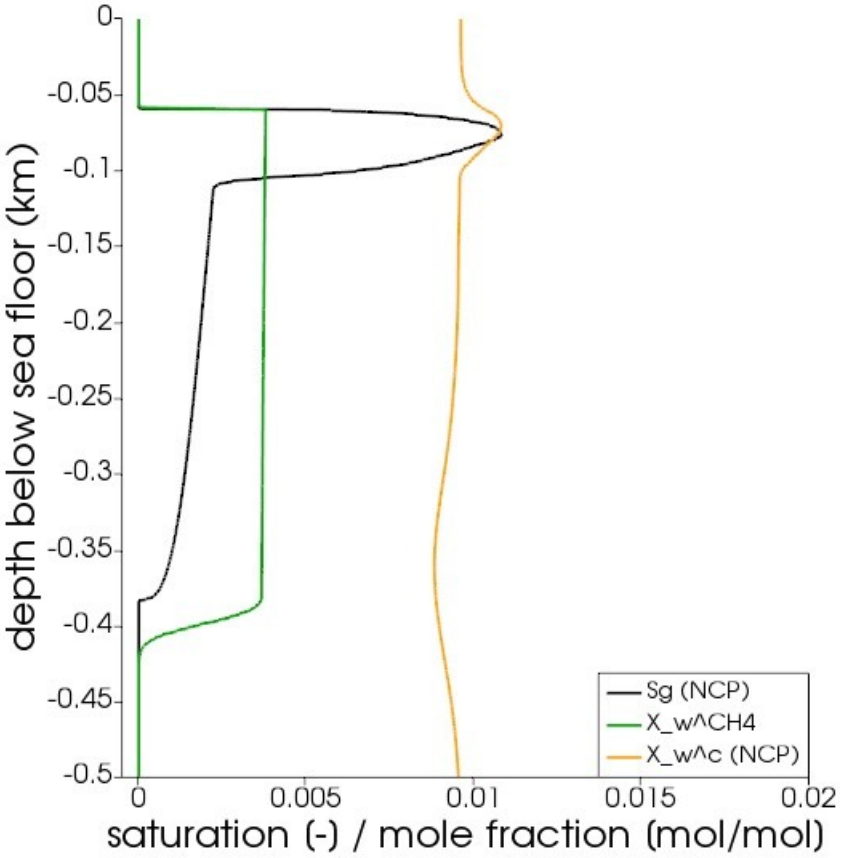


Field-scale Example
BCL System in Danube Paleo Delta

GEOMAR

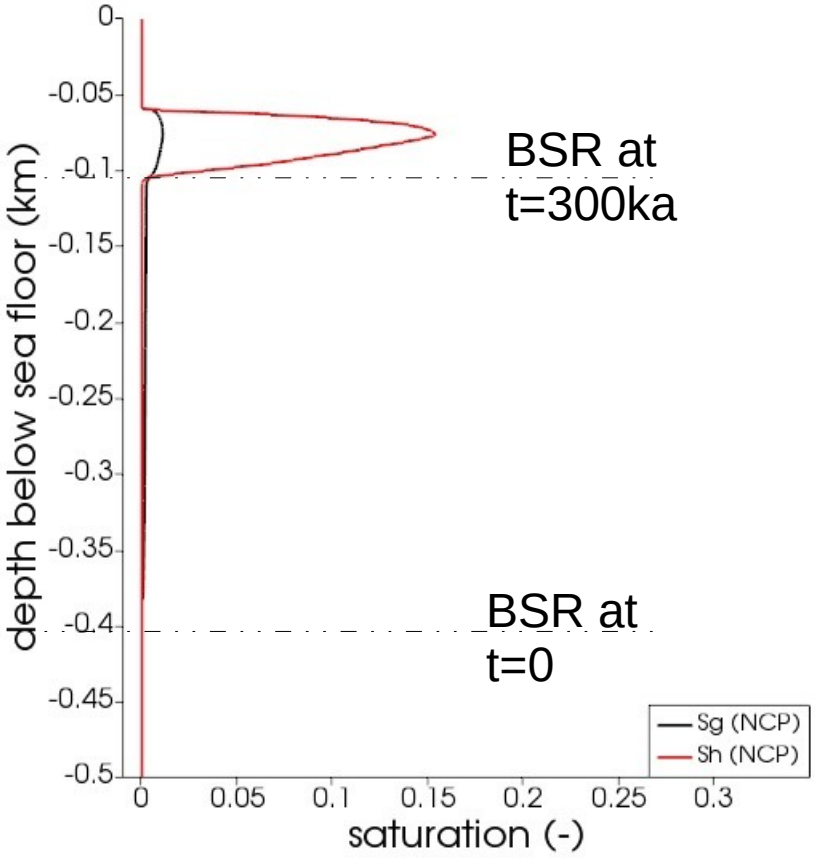
Time = 300,000 years

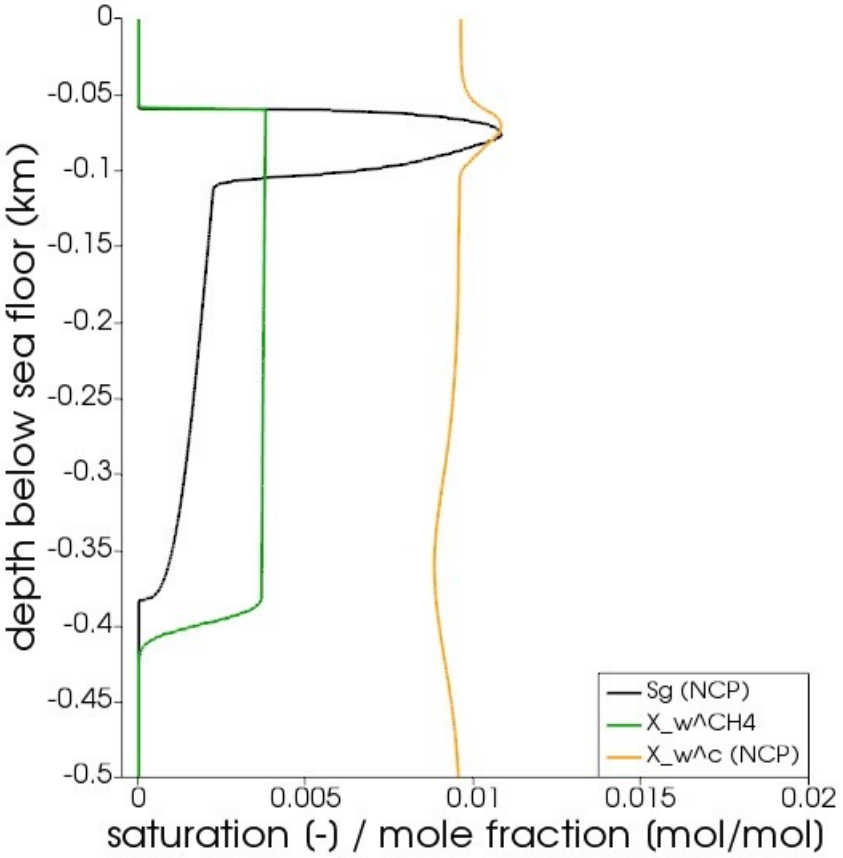




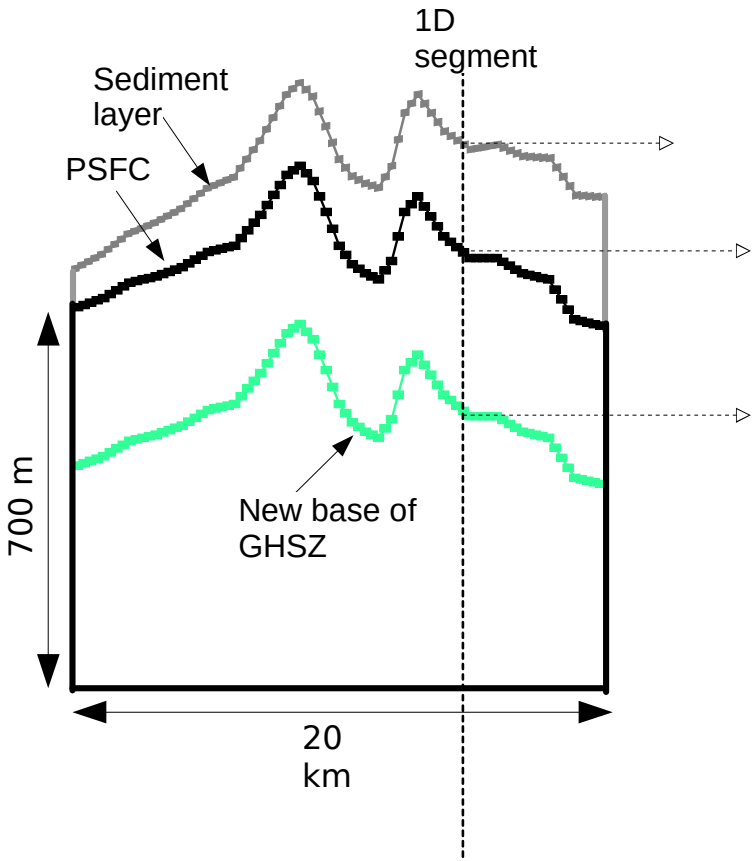
Field-scale Example
BCL System in Danube Paleo Delta

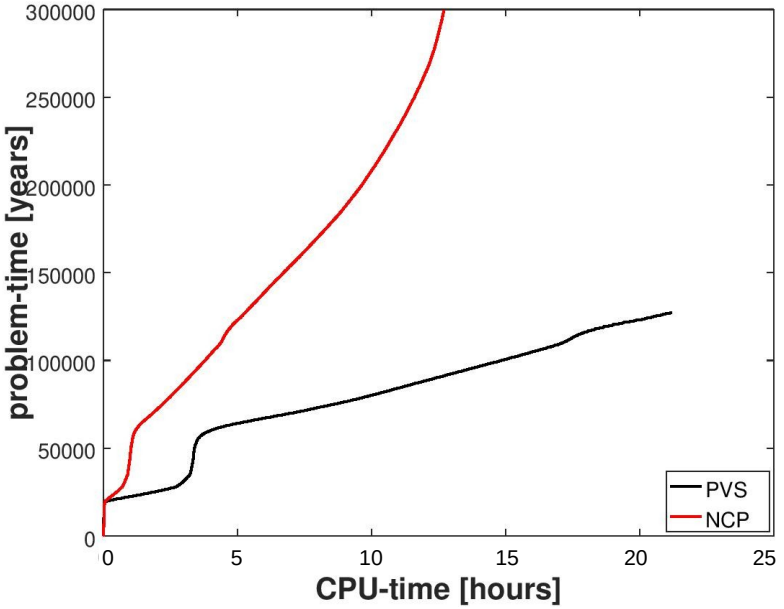
Time = 300,000 years

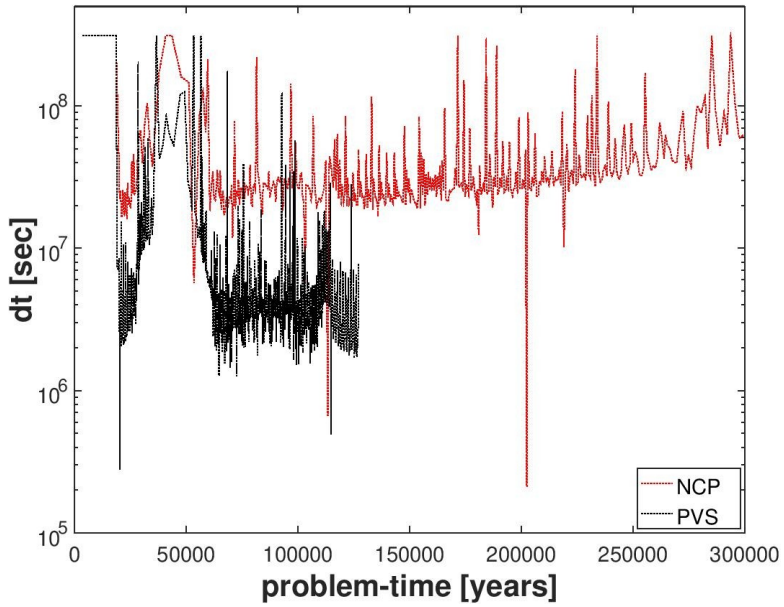




Field-scale Example
BCL System in Danube Paleo Delta





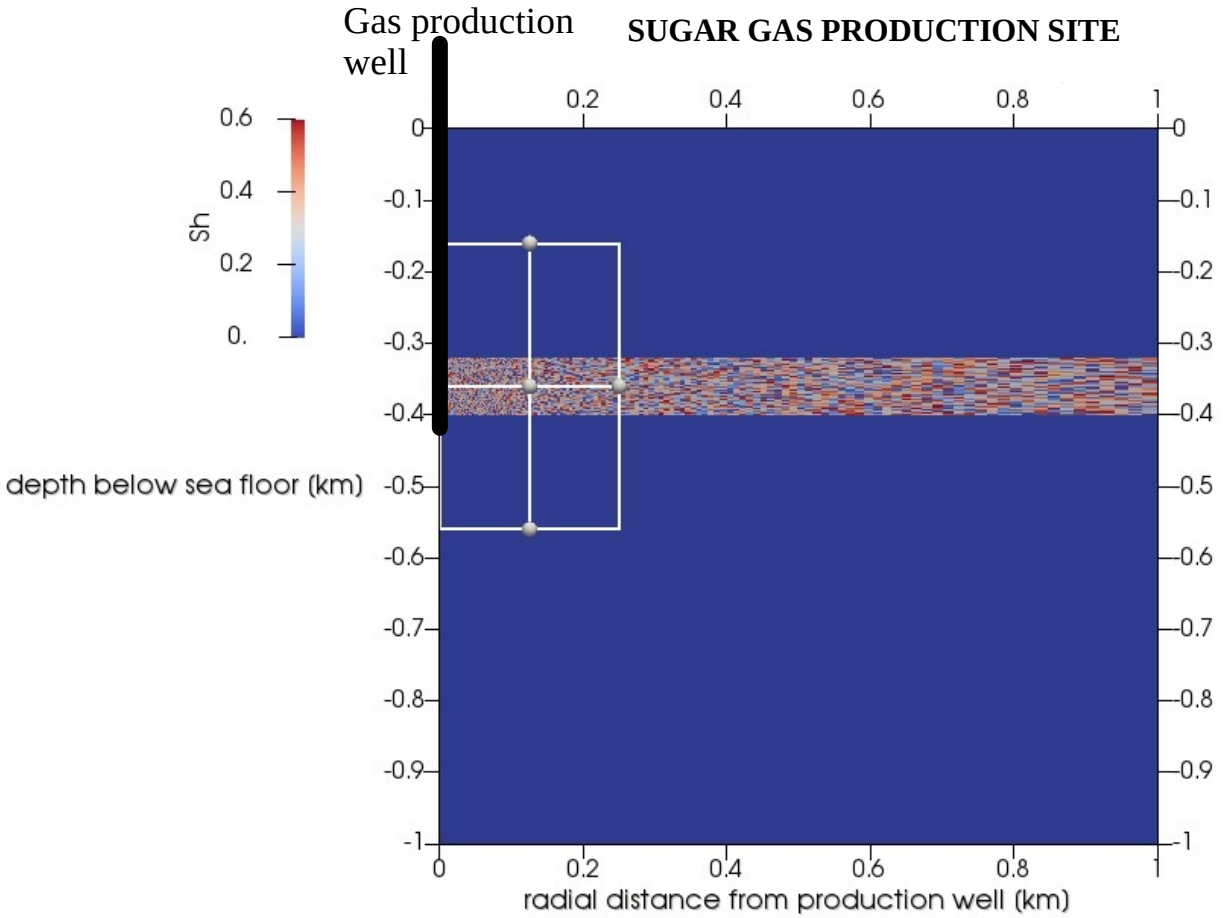


Gas Production Example

Single-well gas production scenario

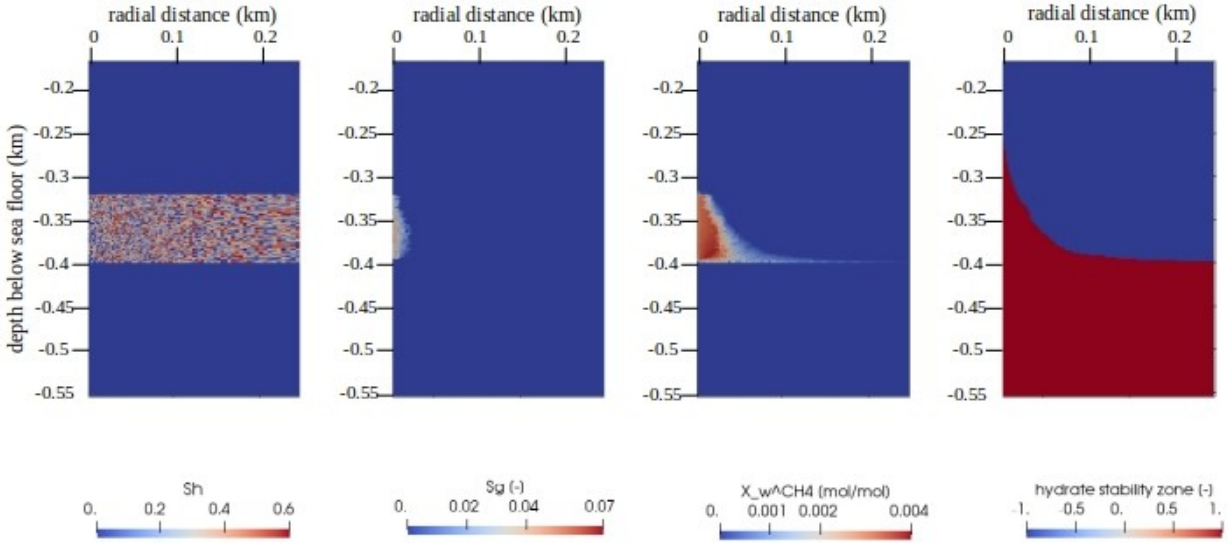
- Test setting based on the geological setting of the Black sea
- Random distribution of hydrate to test robustness of the scheme → Sh varies between **0 to 0.6**
- Corresponding abs. permeability ranges between **1.e-13 to 1.e-18** m^2

Results

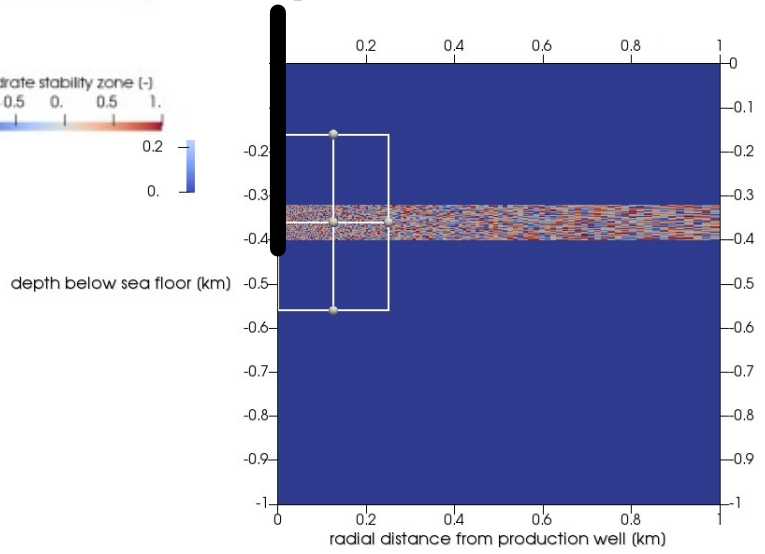


Gas Production Example

t = 10 days

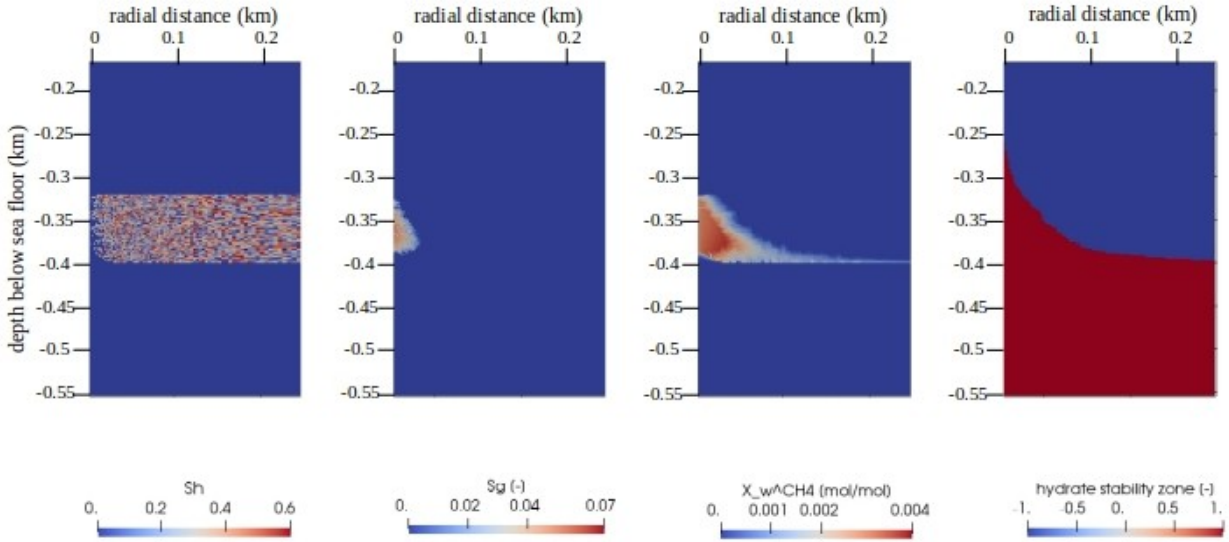


Gas production well

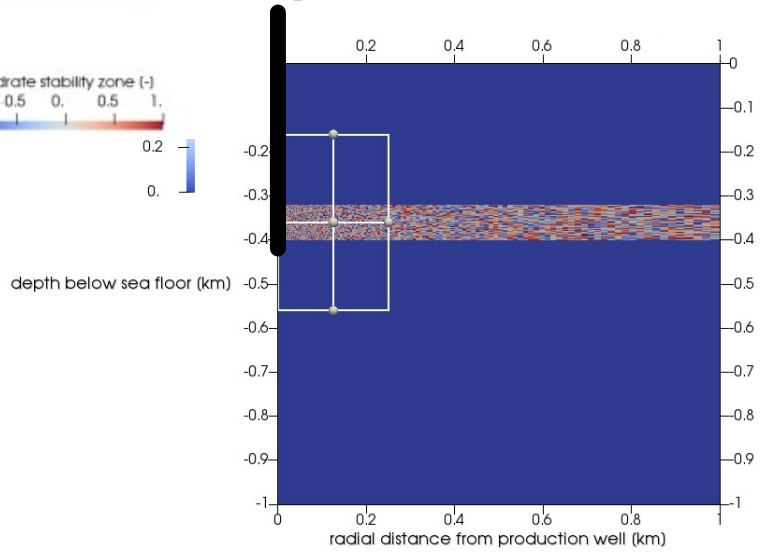


Gas Production Example

t = 90 days

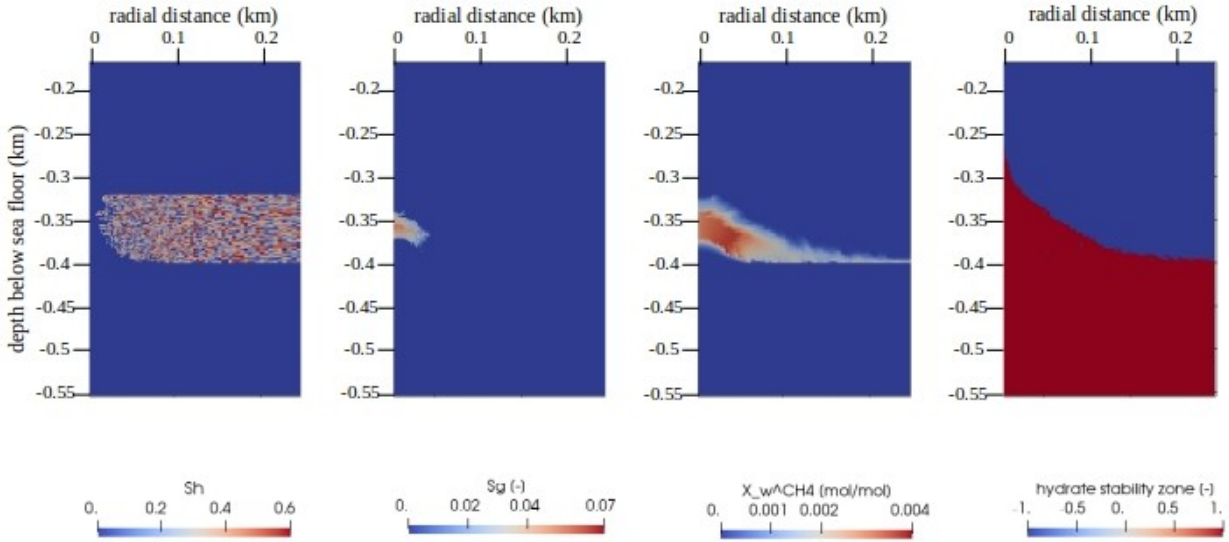


Gas production well

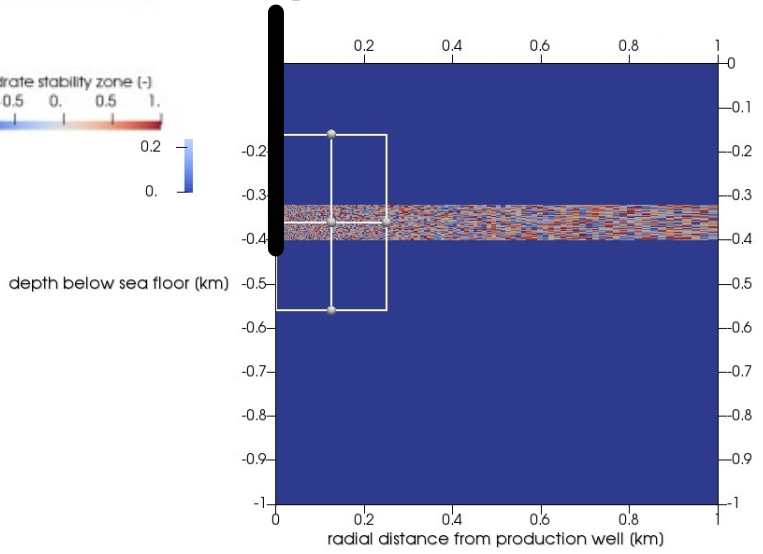


Gas Production Example

t = 360 days



Gas production well



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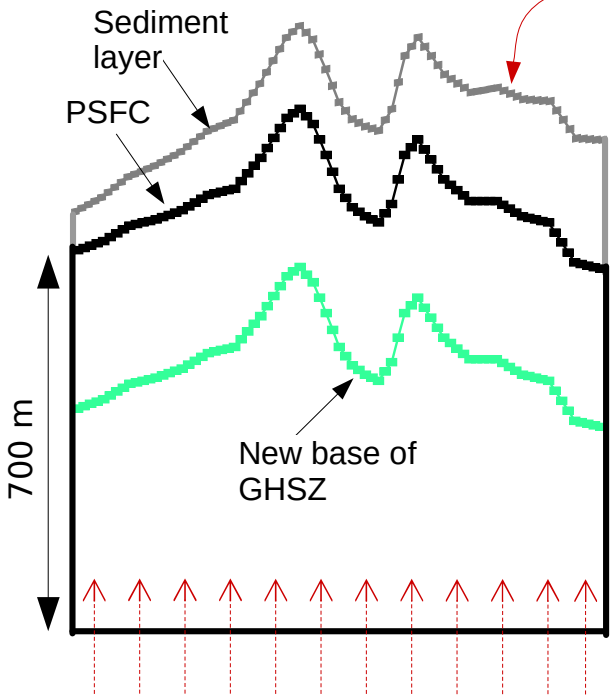
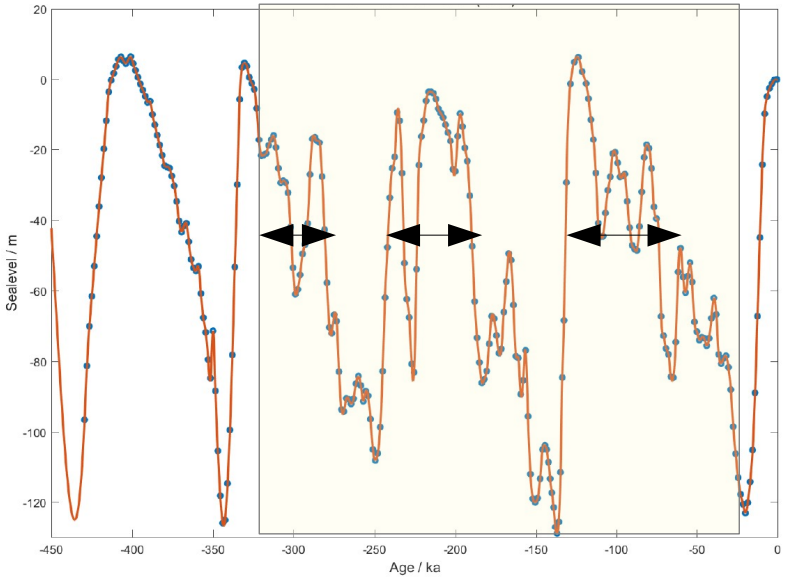
Thank you for your attention !

Further Field-Scale Studies



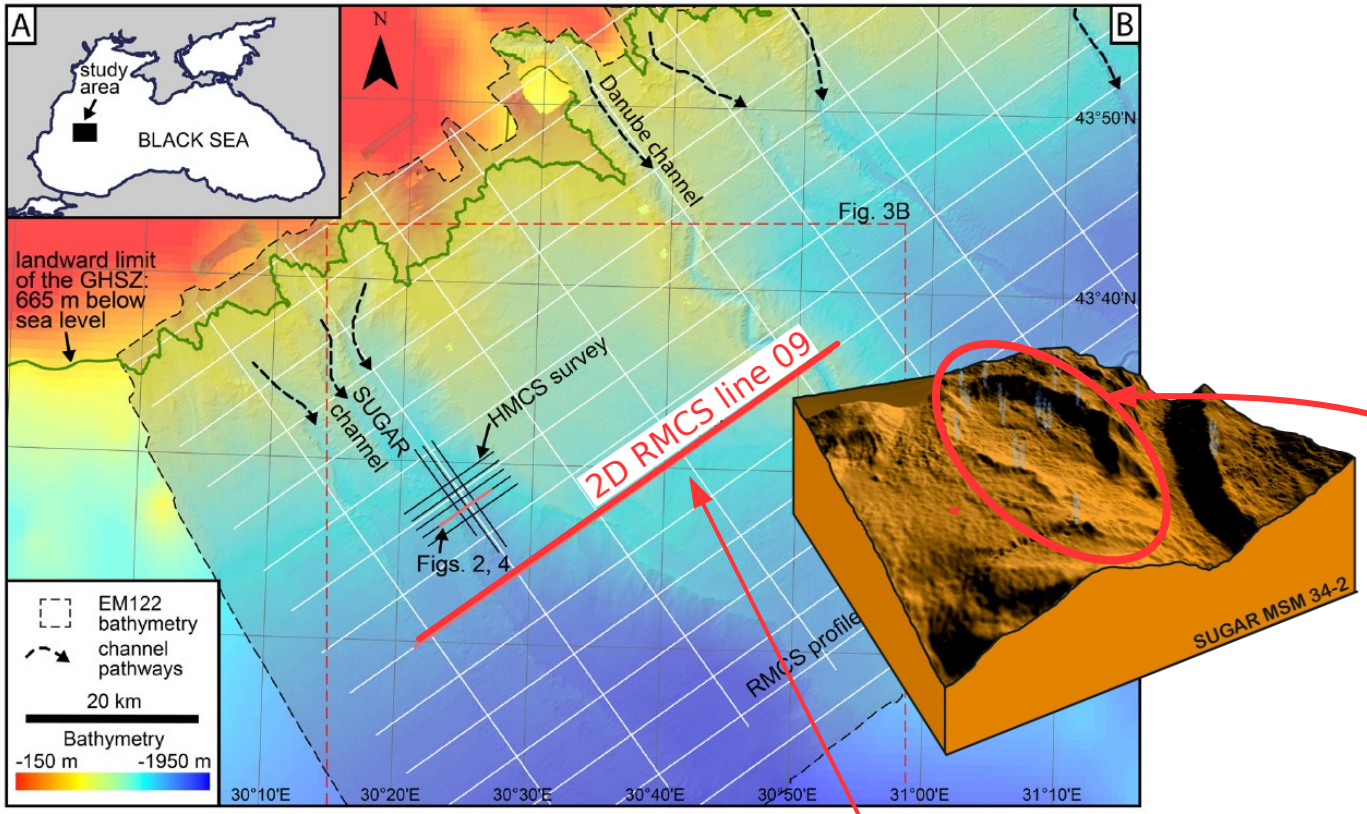
Thermogenic/biogenic methane gas sources

Depositional history [Waelbroek, 2002]



- Identify the marine and limnic stages
- Extrapolate deposition times and cut-off times from global water depths history

Further Field-Scale Studies



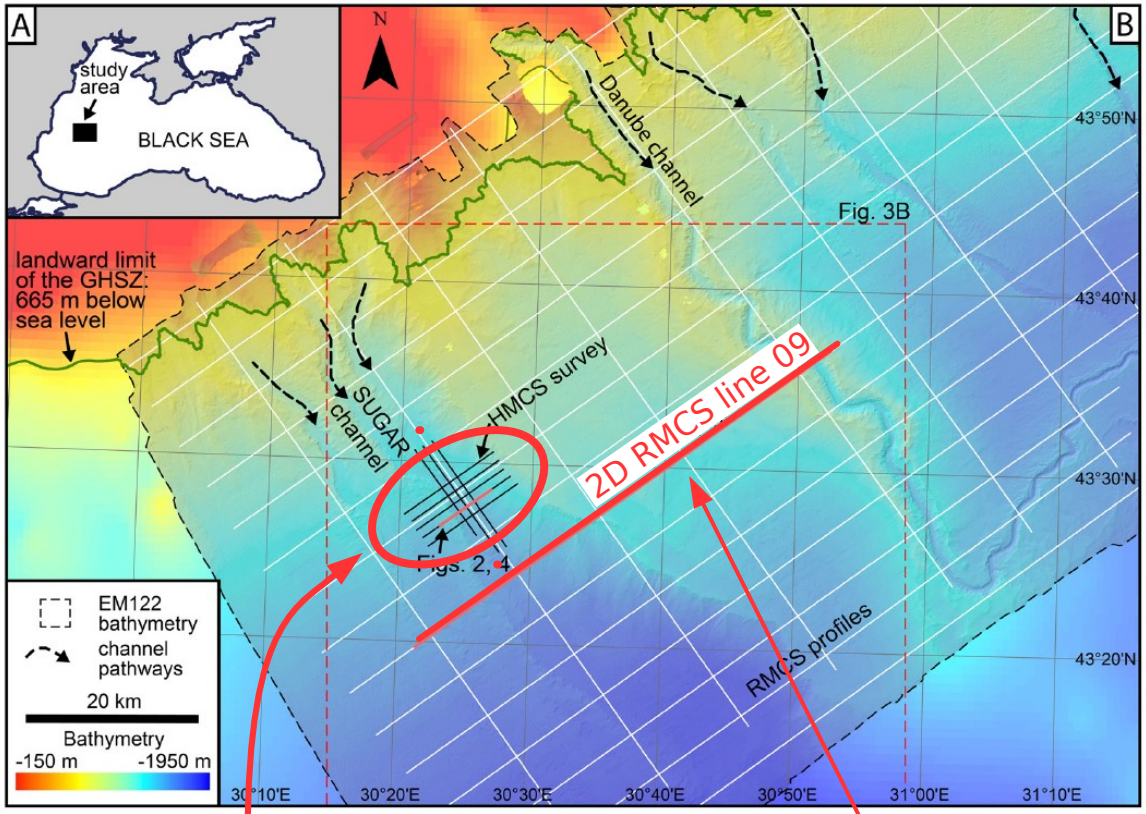
Gas seeps along the channel

cruise MSM34+35 in 2014

Further Field-Scale Studies

GEOMAR

SUGAR GAS PRODUCTION SITE



- simulate various *gas production scenarios* based on the geological setting of the gas hydrate reservoirs in the *paleo Danube deep-sea fan* in the Bulgarian sector of the Black Sea.
- slope stability/risk analyses.

research cruise M142 Dec. 2017

cruise MSM34+35 in 2014

Mathematical Model

TRANSPORT BLOCK

Governing equations

Mass balance for fluid phases $\alpha = g, w$:

$$\partial_t \phi \rho_\alpha S_\alpha + \nabla \cdot \phi \rho_\alpha S_\alpha \boldsymbol{v}_{\alpha,t} = \dot{g}_\alpha$$

where, $\dot{\phi} S_\alpha \boldsymbol{v}_{\alpha,t} = \boldsymbol{K} \frac{k_{r,\alpha}}{\mu_\alpha} (\nabla P_\alpha - \rho_\alpha \boldsymbol{g}) + \phi S_\alpha \dot{\boldsymbol{u}}$

Mass balance for hydrate phase:

$$\partial_t \phi \rho_h S_h + \nabla \cdot \phi \rho_h S_h \dot{\boldsymbol{u}} = \dot{g}_h$$

Energy balance:

$$\partial_t [(1-\phi)\rho_s u_s + \Sigma_\beta \phi \rho_\beta S_\beta u_\beta] + \Sigma_\beta \nabla \cdot (\phi \rho_\beta S_\beta \boldsymbol{v}_{\beta,t} h_\beta) = \nabla \cdot k_{eff}^{th} \nabla T + \Sigma_\beta \dot{g}_\beta$$

Closure relations

summation condition for $\beta = g, w, h$: $\Sigma_\beta S_\beta = 1$

and, relation between fluid pressures:

$$P_g - P_w = P_c(S_w, S_h, \phi \ldots)$$

Hydraulic properties

$$K = K_0 \cdot f^K_{S_h}(S_h) \cdot f^K_\phi(\phi) \quad , \quad P_c = P_c^{BC}(S_{we}) \cdot f^{P_c}_{S_h}(S_h) \cdot f^{P_c}_\phi(\phi)$$

Hydrate phase change kinetics

$$\dot{g}_g = k_{reac} A_{rs} (P_g - P_{eqb})$$

where, $P_{eqb} = A_1 \exp\left(A_2 - \frac{A_3}{T}\right)$,

$k_{reac} = k^0_{reac} \exp\left(-\frac{\Delta E_a}{T}\right)$, and

$A_{rs} = A_{rs}(S_h, \phi, K)$

TRANSFER VARIABLE

GEO-MECHANICS BLOCK OUTPUT

COUPLING BLOCK

ϕ

$\dot{\boldsymbol{u}}$

Governing equation

Mass balance for soil phase:

$$\partial_t (1-\phi) + \nabla \cdot (1-\phi) \rho_s \dot{\boldsymbol{u}} = 0$$

Ref.: Gupta, S., R. Helmig, and B. Wohlmuth, Non-isothermal, multi-phase, multi-component flows nthrough deformable methane hydrate reservoirs, Computational Geo-sciences, 1–26,2015

TRANSPORT BLOCK OUTPUTS S_w S_h P_g T

GEOMECHANICS BLOCK

Governing equation

Momentum balance for composite hydrate-soil phase:

$$\nabla \cdot (\Delta \tilde{\sigma} + \Delta P_{eff} \tilde{I}) + \Delta \rho_{sh} \boldsymbol{g} = 0$$

Constitutive law

Elastic properties:

$$E_{sh} = E_s + S_h^m E_h$$

$$\nu_{sh} = constant$$

non-associated $I_1 - J_2$ plasticity:

Yield curve:

$$F := I_1 + \alpha(S_h, \lambda, \dot{\lambda}) \sqrt{J_2} - c(S_h)$$

Plastic flow potential:

$$Q := I_1 + \beta(S_h, \lambda) \sqrt{J_2}$$

strain rates:

$$\dot{\tilde{\epsilon}} = \dot{\tilde{\epsilon}}_e + \dot{\tilde{\epsilon}}_p$$

where, $\dot{\tilde{\epsilon}}_p = \dot{\lambda} \frac{\partial Q}{\partial \tilde{\sigma}}$

and, $\dot{\tilde{\epsilon}} = \frac{1}{2}(\nabla \dot{\boldsymbol{u}} + \nabla^T \dot{\boldsymbol{u}})$

loading-unloading conditions:

$$\dot{\lambda} \geq 0 \quad , \quad F \leq 0 \quad , \quad \dot{\lambda} F = 0$$

Evolution of frictional resistance α

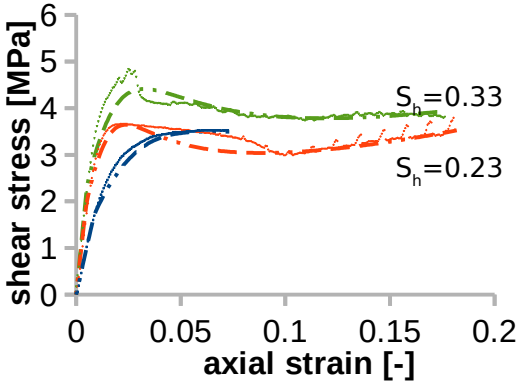
[Andrade et al. (2012)]

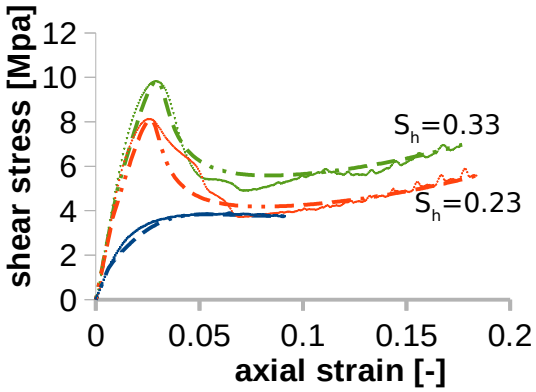
$$\alpha(S_h, \dot{\lambda}, \lambda) = \alpha_{res}(S_h, \dot{\lambda}) + \beta(S_h, \lambda)$$

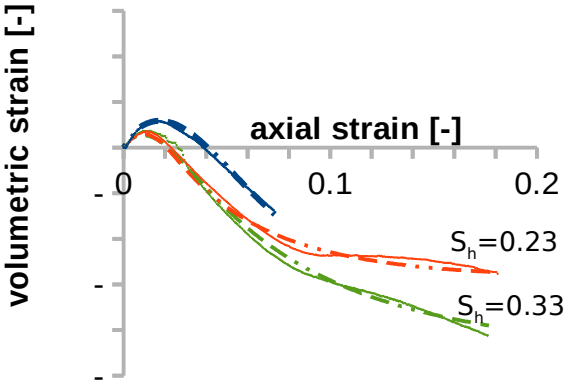
Further Testing

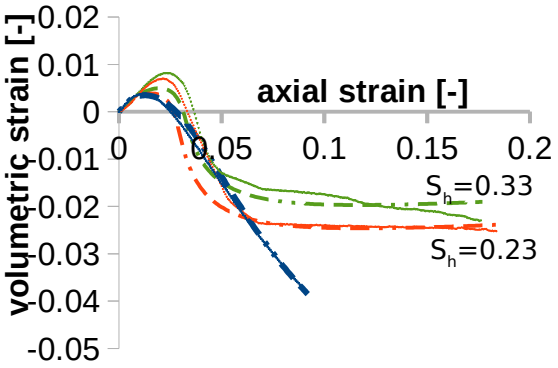
Drained triaxial experiments for calibration of plasticity model

- homogeneous gas hydrate distributions
- no hydrate phase change









A. Water saturated samples,
Hydrates are formed through excess gas method.

B. Gas saturated samples,
Hydrates are formed through excess gas method.

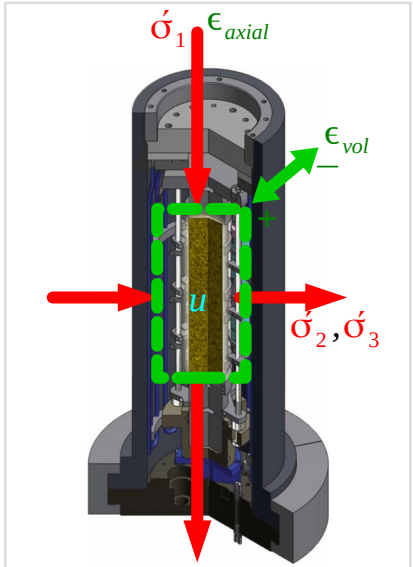
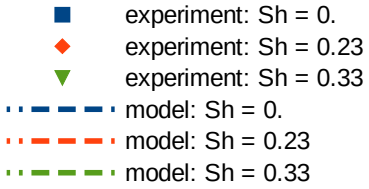


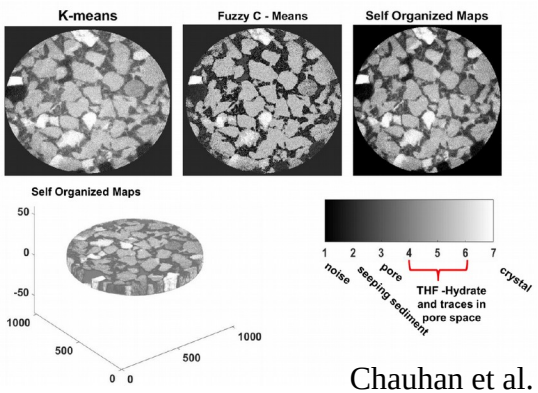
Fig.: Triaxial setup for flow-through expts up to 40 MPa, sample Ø 80 mm, height 160 mm



Further Testing

LAB-SCALE TEST

- advanced high-pressure flow-through triaxial set-up
- Heterogeneous gas hydrate distributions
- Coupled flow, hydrate phase change, and geomechanics



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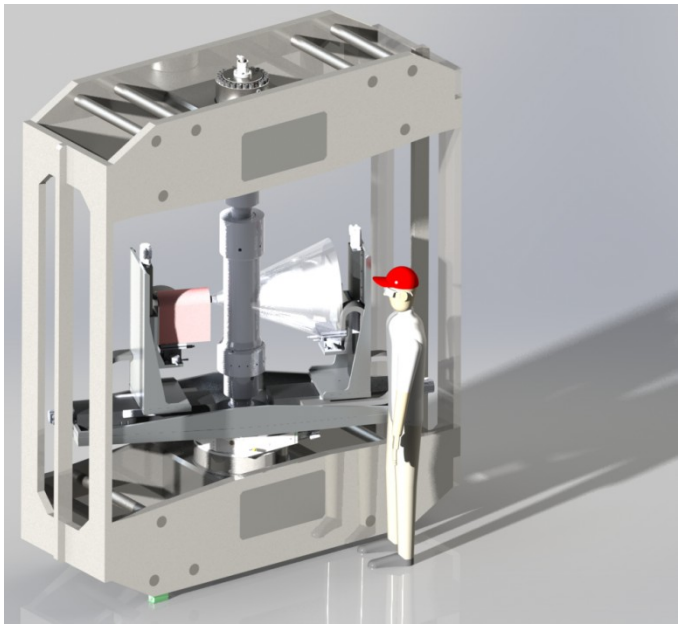

Fig.: XRAY-CT TRIAXIAL SET-UP