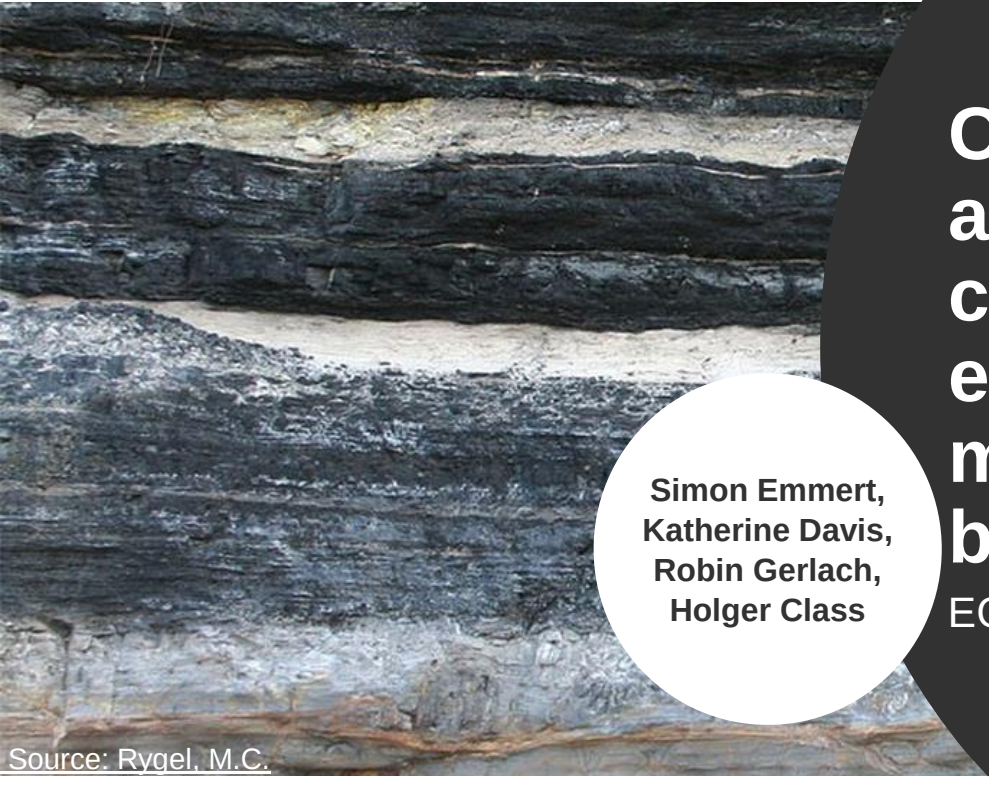
University of Stuttgart
Institute for Modelling Hydraulic and Environmental Systems
Department of Hydromechanics and Modelling of Hydrosystems



Source: Rygel, M.C.

Calibrating and validating a numerical model concept for microbially enhanced coal bed methane production with batch and column data

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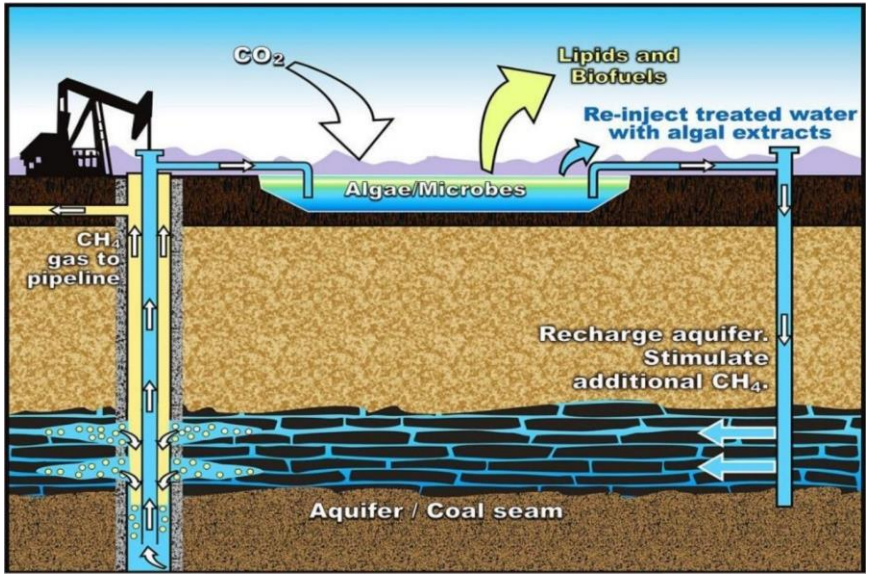
EGU 2020

Gefördert durch DFG Deutsche Forschungsgemeinschaft
MONTANA STATE UNIVERSITY
DuMu^x
SFB 1313 Interface-Driven Multi-Field Processes in Porous Media
CENTER FOR BIOFILM ENGINEERING
LH²

Motivation

Microbially enhanced coal-bed methane (MECBM) production

- Coal-bed methane (CBM) is an unconventional source of natural gas
- CBM can have **thermogenic** or **biogenic** origin
- **MECBM** follows the biogenic path by **restoring** the conditions for **microbial growth**
  - Microbes convert coal and nutrients to methane (anaerobic)
- **MECBM** could **enhance** methane **production,** reducing the need for new wells and hydraulic fracturing
- Interesting field-scale applications with e.g. lipids and biofuels production envisioned



Source: Barnhart, Elliott P., et al. "Enhanced coal-dependent methanogenesis coupled with algal biofuels: Potential water recycle and carbon capture." International Journal of Coal Geology 171 (2017): 69-75. https://doi.org/10.1016/j.coal.2017.01.001

MECBM model concept

1. Averaging to model efficiently
2. MECBM „food-web“ of methanogenesis
3. Balance equations

Averaging

Modelling & evaluation of all processes at REV scale

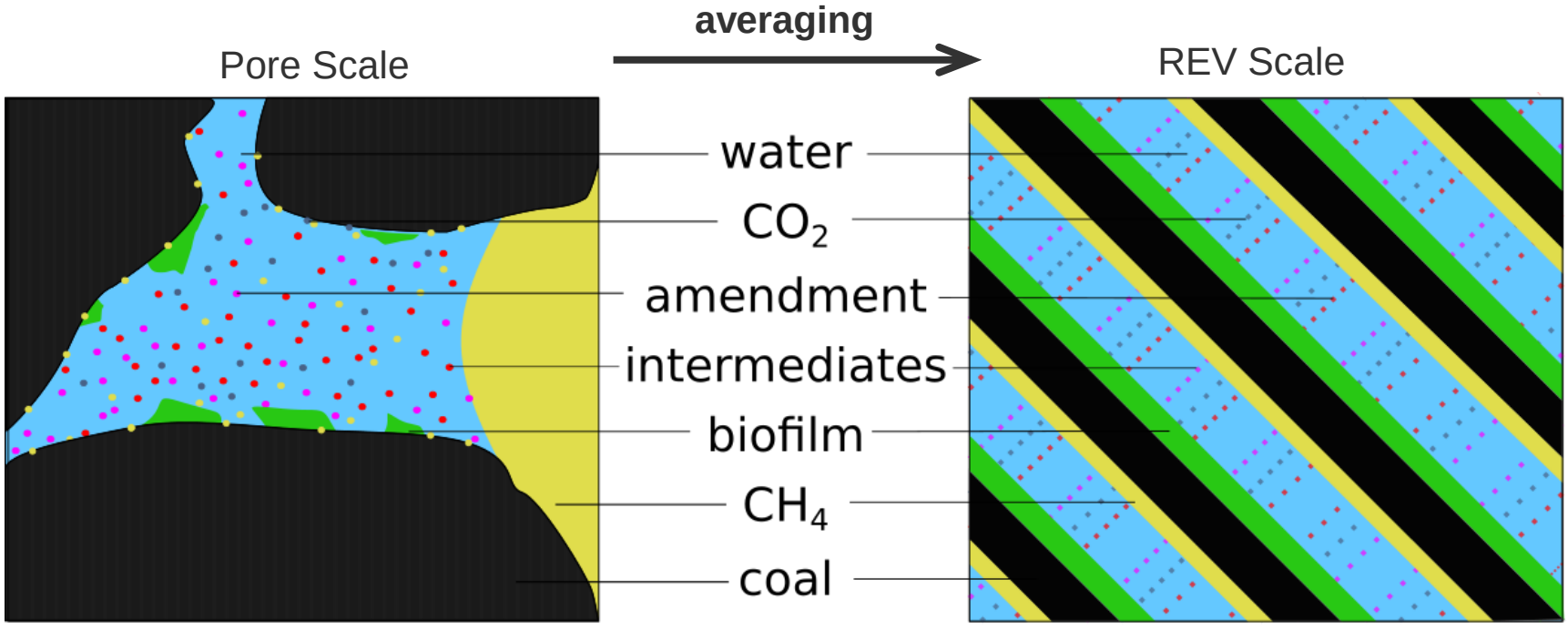


Figure 2: Processes occur on the pore scale but are treated in an averaged sense on the REV scale in the model.

From: Emmert, Simon et al., “Importance of Specific Substrate Utilization by Microbes in Microbially Enhanced Coal-Bed Methane Production: A Modelling Study”, International Journal of Coal Geology (2020), **submitted**

Coal-bed methane “food web”

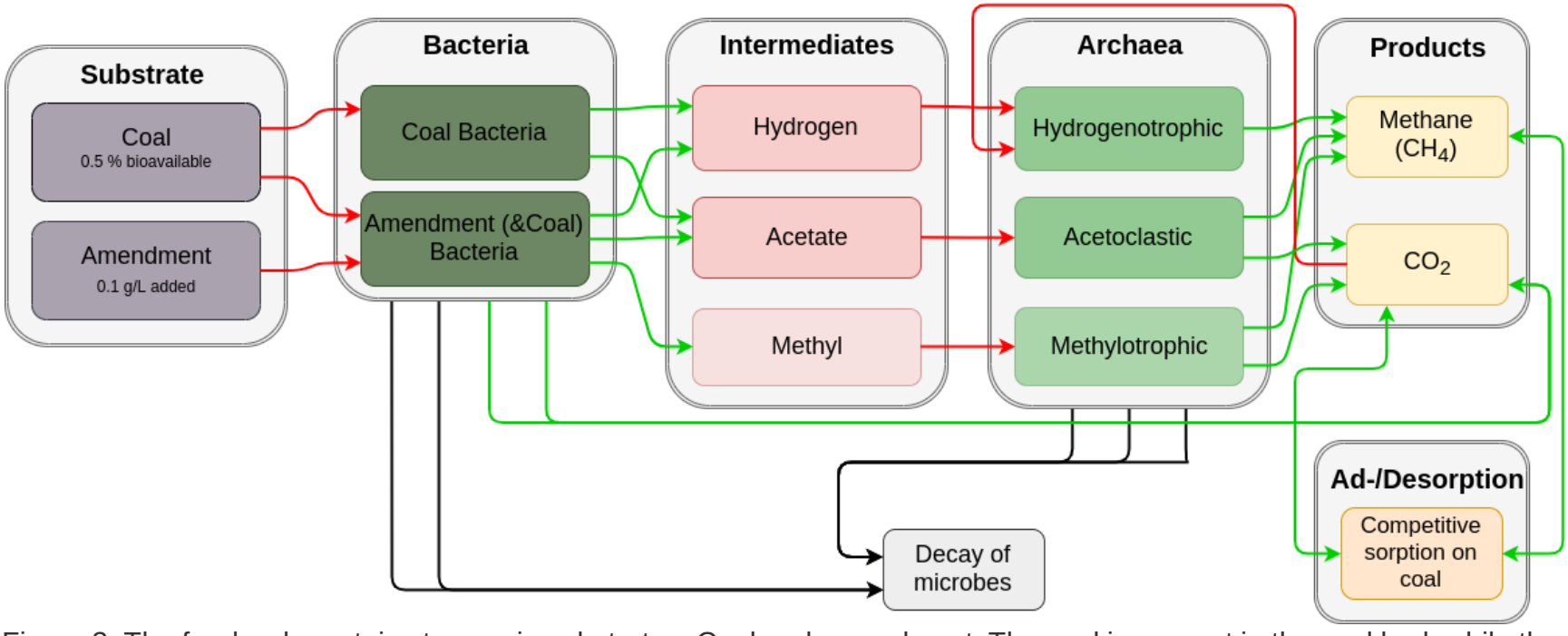


Figure 3: The food web contains two main substrates: Coal and amendment. The coal is present in the coal bed, while the amendment is possibly added to stimulate growth of bacteria. The bacteria convert coal and/or amendment to intermediates which are then converted to CH_4 and CO_2 via methanogenesis.

From: Emmert, Simon et al., “Importance of Specific Substrate Utilization by Microbes in Microbially Enhanced Coal-Bed Methane Production: A Modelling Study”, International Journal of Coal Geology (2020), **submitted**

Mass balance equations

Components, coal and biomass

- Mass balance equation for components κ:

$$\sum_{\alpha} \frac{\partial}{\partial t}\left(\phi \rho_{\alpha} x_{\alpha}^{\kappa} S_{\alpha}\right) + \nabla \cdot \left(\rho_{\alpha} x_{\alpha}^{\kappa} \mathbf{v}_{\alpha}\right) - \nabla \cdot \left(\rho_{\alpha} \mathbf{D}_{\alpha,\mathrm{pm}}^{\kappa} \nabla x_{\alpha}^{\kappa}\right) = q^{\kappa}$$

$$\kappa \in \{\mathrm{Water},\ \mathrm{CH_4},\ \mathrm{Acetate},\ \mathrm{Amendment},\ \mathrm{RMethyl},\ \mathrm{H_2},\ \mathrm{NaCl},\ \mathrm{CO_2}\}$$

$$\alpha \in \{\mathrm{w},\ \mathrm{n}\}$$

- Mass balance for solid phases (coal, bacteria and archaea):

$$\frac{\partial}{\partial t}\left(\phi_{\lambda} \rho_{\lambda}\right) = q^{\lambda} \qquad \lambda \in \{\mathrm{cBac},\ \mathrm{aBac},\ \mathrm{aArch},\ \mathrm{hArch},\ \mathrm{mArch},\ \mathrm{cCoal},\}$$

ϕ porosity, ρ density, x mole fraction of component κ in phase α, S saturation, v Darcy velocity, D diffusion tensor, q source sink term, ϕ_{λ}volume-fraction of solid λ

Mass balance equations

Biomass and component source/sink term

Source and sink term for **biomass**:

$$q^{\mathrm{cBac}} = r_{\mathrm{g,c}}^{\mathrm{cBac}} - r_{\mathrm{d}}^{\mathrm{cBac}}$$

Growth rate (Monod) kinetics exemplary for the coal consuming **bacteria** on coal:

$$r_{\mathrm{g,c}}^{\mathrm{cBac}} = \mu_{\mathrm{cBac}} \left(\frac{\rho_{\mathrm{c}} \phi_{\mathrm{c}}}{K_{\mathrm{c}} + \rho_{\mathrm{c}} \phi_{\mathrm{c}}} \right) \cdot \rho_{\mathrm{cBac}} \phi_{\mathrm{cBac}}$$

Decay rate for the coal consuming **bacteria**:

$$r_{d}^{cBac} = k_{\mathrm{b0}} \cdot \rho_{\mathrm{cBac}} \phi_{\mathrm{cBac}}$$

Source and sink term for one **component** (exemplary for hydrogen):

$$q^{\mathrm{H_2}} = \left(r_{g,c}^{cBac} \cdot \frac{Y_{H_2,c}}{Y_{cBac,c}} + r_{g,c}^{aBac} \cdot \frac{Y_{H_2,c}}{Y_{aBac,c}} + r_{g,Am}^{aBac} \cdot \frac{Y_{H_2,Am}}{Y_{aBac,Am}} - \frac{r_g^{hArch}}{Y_{hArch,H_2}} \right)$$

$r_{g,c}$ growth rate, r_d decay rate, μ_{cBac} max growth rate, K_c half saturation , ρ_c density, $\phi_c$volume-fraction,

$Y_{H2,c}$ Yield of hydrogen from coal, $Y_{cBac,c}$ Yield of coal bacteria from coal, …

Similar reactions for the coal & amendment consuming bacteria and all three types of archaea.

DuMu^x model:

Calibration with batch experiments

Separate calibration to glass beads (GB) and coal experimental data

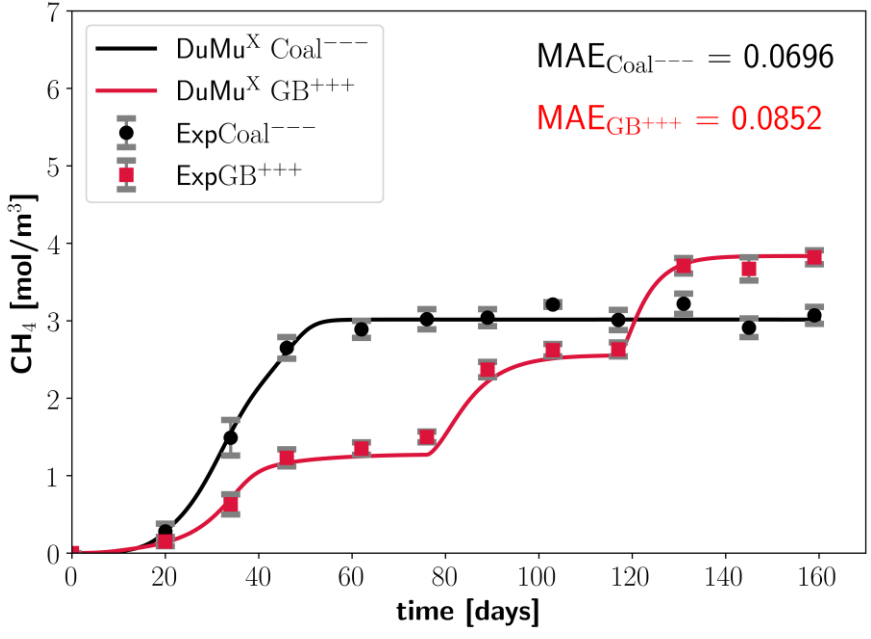


Figure 4: Glass beads with three amendment stimulations (GB+++) and coal only (coal---) setups are used for calibration.
The glass beads cases consist of glass beads as porous medium, formation water and amendment additions at three possible addition times (indicated by “+”). They are used to calibrate the amendment-dependent parameters.
The coal only setup consists of coal and formation water and is used to calibrate the coal dependent parameters. No amendment is added (indicated by “-”) at any of three possible addition times.

Experimental Data:
Davis, Katherine J., et al. **"Biogenic coal-to-methane conversion efficiency decreases after repeated organic amendment."** Energy & Fuels 32.3 (2018): 2916-2925.
Simulation:
Emmert, Simon et al., “Importance of Specific Substrate Utilization by Microbes in Microbially Enhanced Coal-Bed Methane Production: A Modelling Study”, International Journal of Coal Geology (2020), **submitted**

DuMu^x model:

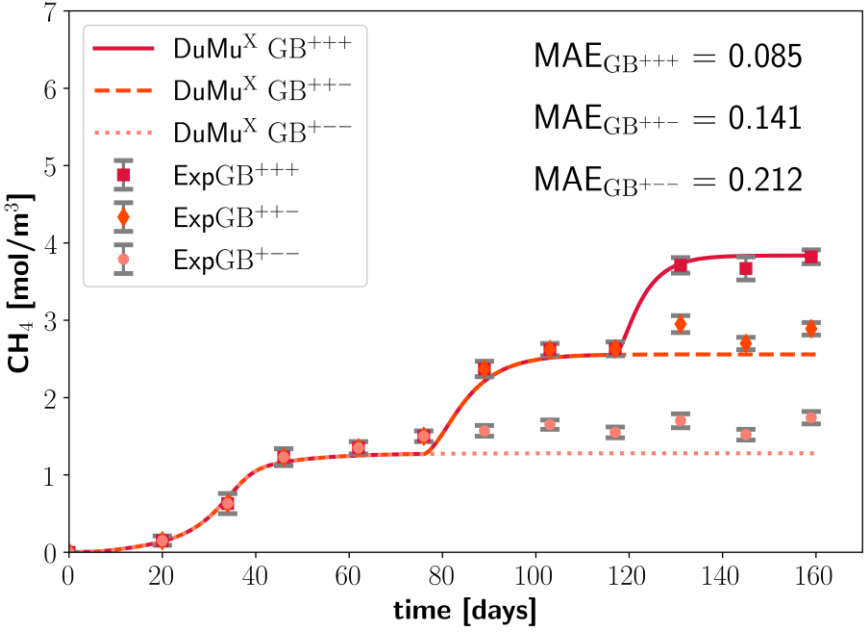
Validation with batch experiments

More variations with coal and amendment additions at different times are investigated and compared against experimental results for validation.

Validation of the GB+++ and coal--- fits with other data sets

Amendment simulations using GB+++ and coal--- fit

AMENDMENT ONLY SYSTEMS



- Amendment only system
- One to three amendment additions
- Overall good fit for CH_4 production increases
- Underestimation of CH_4 production by the model towards the end, resulting in larger MAE

Experimental Data:
Davis, Katherine J., et al. **"Biogenic coal-to-methane conversion efficiency decreases after repeated organic amendment."** Energy & Fuels 32.3 (2018): 2916-2925.
Simulation:
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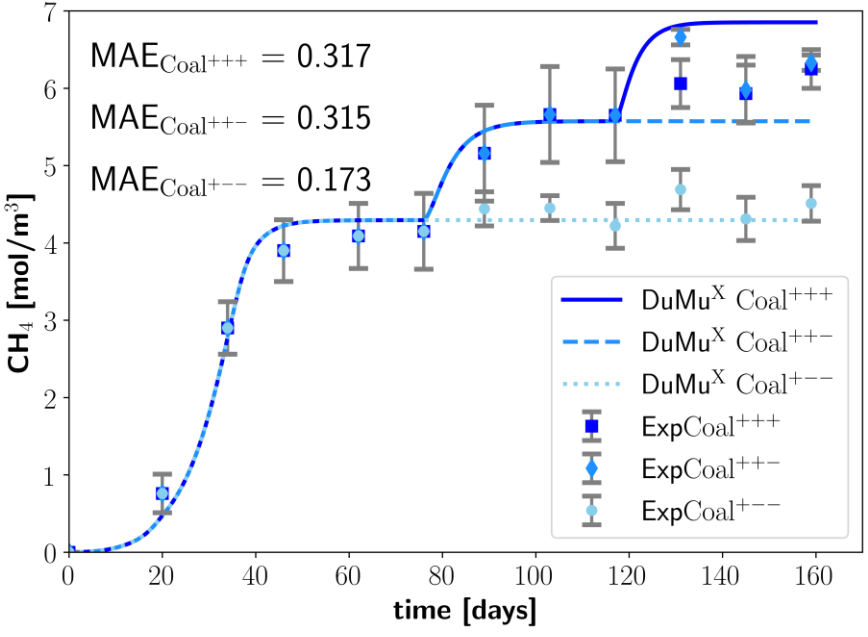
Validation of the GB+++ and coal--- fits with other data sets

Coal and amendment simulations using GB+++ and coal--- fit

COAL WITH AMENDMENT SYSTEMS



- Coal with amendment additions
- Up to three amendment additions
- Overall good fit for CH_4 production increases
- Overestimation of CH_4 production by the model during increases
- Model output shows systematic increase for Coal^{+++} and Coal^{++-} after day 120, while experimental studies deviate

Experimental Data:
Davis, Katherine J., et al. **"Biogenic coal-to-methane conversion efficiency decreases after repeated organic amendment."** Energy & Fuels 32.3 (2018): 2916-2925.
Simulation:
Emmert, Simon et al., “Importance of Specific Substrate Utilization by Microbes in Microbially Enhanced Coal-Bed Methane Production: A Modelling Study”, International Journal of Coal Geology (2020), **submitted**

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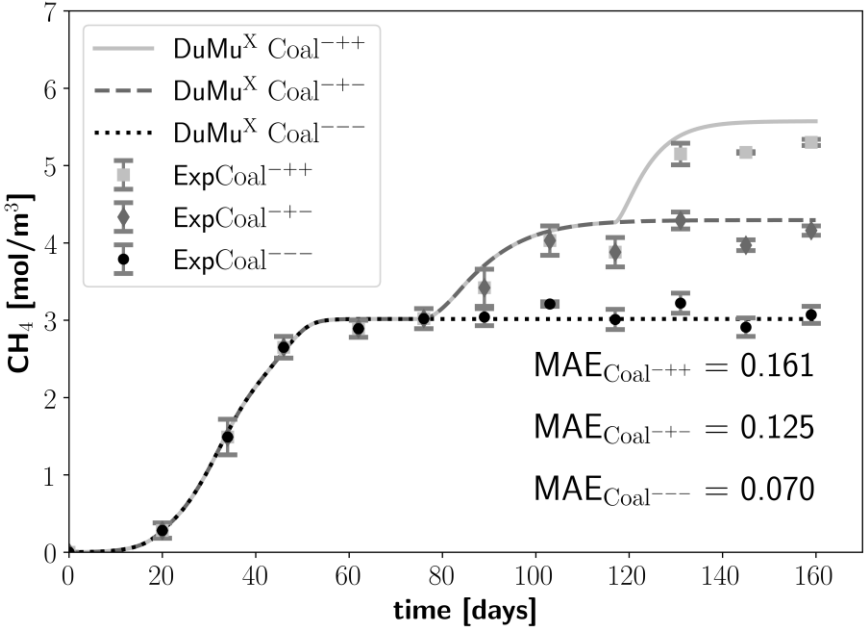
COAL WITH AMENDMENT SYSTEMS



- Coal with amendment additions after day 76
- Two possible amendment additions
- Overall very good fit for CH_4 production increases
- Increases of CH_4 production as well as overall production match the experiments

Experimental Data:
Davis, Katherine J., et al. **"Biogenic coal-to-methane conversion efficiency decreases after repeated organic amendment."** Energy & Fuels 32.3 (2018): 2916-2925.
Simulation:
Emmert, Simon et al., “Importance of Specific Substrate Utilization by Microbes in Microbially Enhanced Coal-Bed Methane Production: A Modelling Study”, International Journal of Coal Geology (2020), **submitted**

DuMu^X model:

Column study

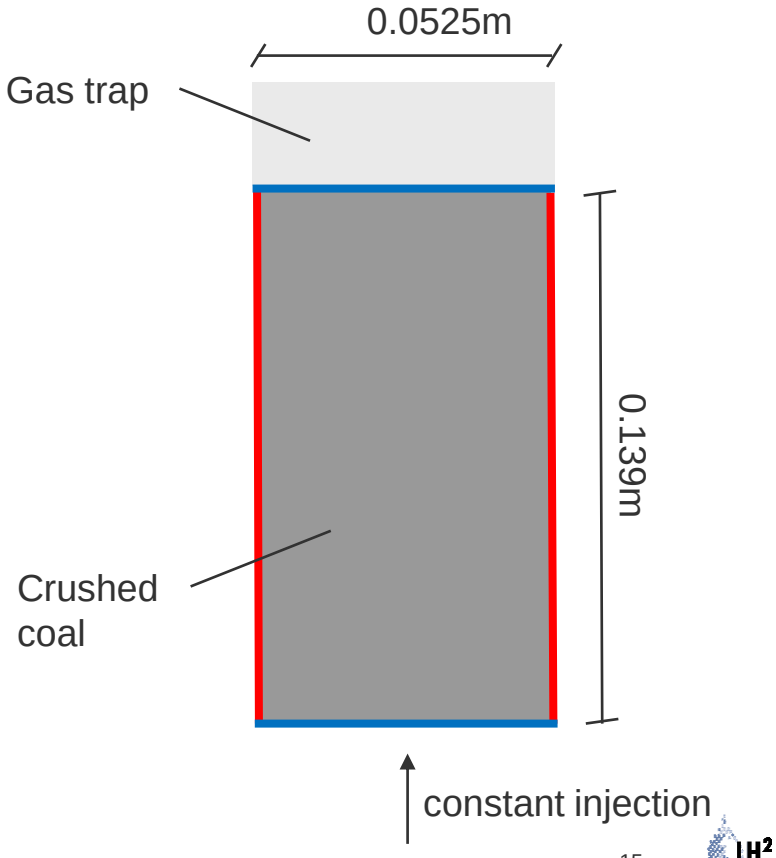
Not described in detail and not as many results as envisioned, as the publication is still in preparation.

MECBM column study + experiment

Column setup in the experiment and the model

- **Experiment:**
  - 300 mL with 190 g coal

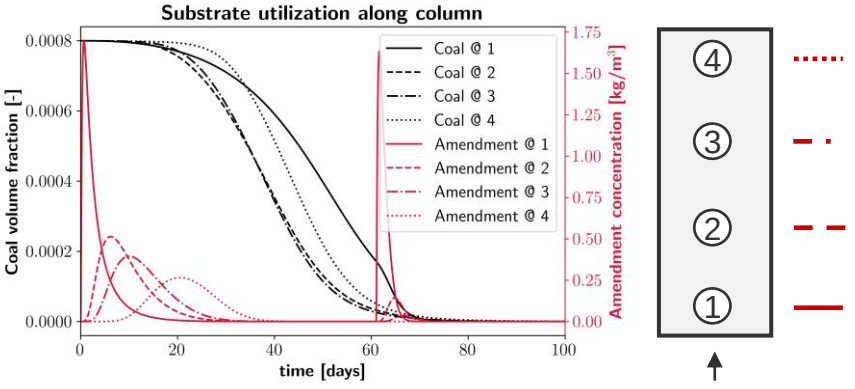
    → Porosity 0.48
  - 2 amendment injections
    - Day 0 + Day 61
  - **Gas trap** on top
- **Model:**
  - Neumann no-flow on sides
  - In-/outflow on top/bottom
  - Fixed pressure at top

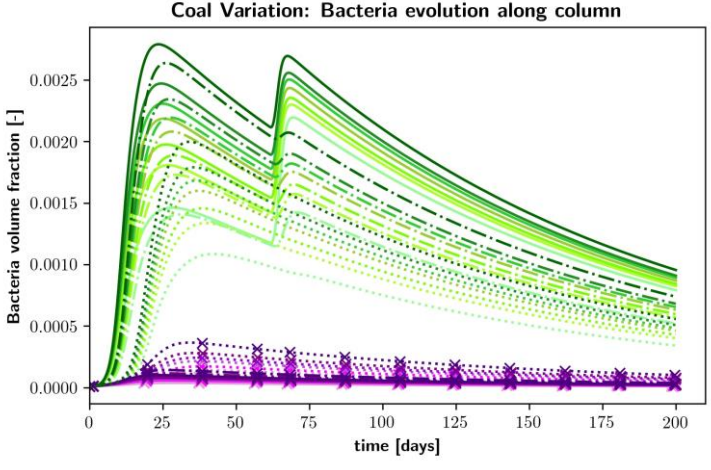


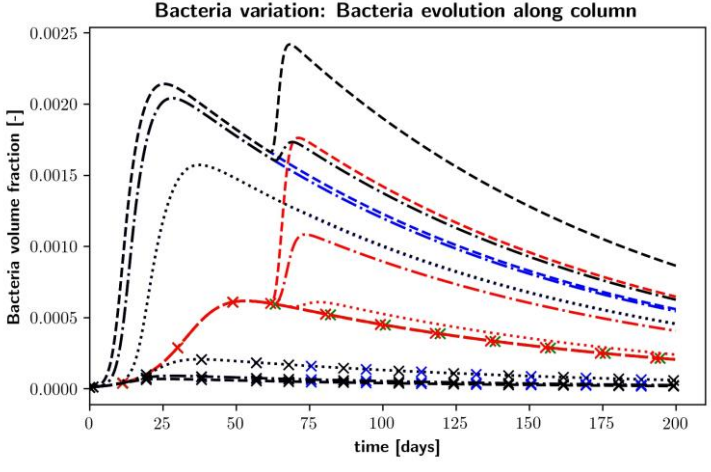
DuMu^x results: MECBM column variations – saved for later

Substrate utilization, coal and biofilm variations

- Preliminary results here:
  - Right top: Substrate (red: amendment, black: coal) along the column
  - Right bottom: Different initial conditions and assumptions regarding bacteria
  - Bottom: Variations of coal bioavailability results in different bacteria evolution along the along







Summary

From a validated batch model to column scale

- Model reproduces the observations from **batch experiments**
  - Methane production via all metabolic pathways can be calculated
  - **Successful calibration** and **validation**

- Flow in **columns** matches expectations of growth and decay of biofilm
  - Growth, decay of biofilm and transport of components as expected
  - **Hydraulic** and **biofilm** parameters **are under investigation**

→ Model can be used to **test further hypotheses** and **guide future experiments,** but still needs to be **enhanced** regarding the overall **CH_4 production**

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Thank you!

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Gefördert durch DFG Deutsche Forschungsgemeinschaft

MONTANA STATE UNIVERSITY

DuMu^x

SFB 1313 Interface-Driven Multi-Field Processes in Porous Media

CENTER FOR BIOFILM ENGINEERING

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Main sources

- Experimental studies:
  - [1] Davis, Katherine J., et al. **"Biogenic coal-to-methane conversion efficiency decreases after repeated organic amendment."** *Energy & Fuels* 32.3 (2018): 2916-2925.
  - [2] Davis, Katherine J., et al. "**Type and amount of organic amendments affect enhanced biogenic methane production from coal and microbial community structure."** *Fuel* 211 (2018): 600-608.
  - [3] Davis, Katherine J., and Robin Gerlach. **"Transition of biogenic coal-to-methane conversion from the laboratory to the field: A review of important parameters and studies."** *International Journal of Coal Geology* (2017).
- MECBM:
  - [4] Barnhart, Elliott P., et al. "**Hydrogeochemistry and coal-associated bacterial populations from a methanogenic coal bed."** *International Journal of Coal Geology* 162 (2016): 14-26.
- Graphs:
  - Title-Picture by: Rygel, M.C. access via (https://commons.wikimedia.org/wiki/File:Tongarra_Coal_ashbeds.JPG)
- Publication (in preparation):
  - Emmert, Simon et al., “Importance of Specific Substrate Utilization by Microbes in Microbially Enhanced Coal-Bed Methane Production: A Modelling Study”, International Journal of Coal Geology (2020), **submitted**