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Supplement of

Two-phase reactive transport modeling of heterogeneous gas production in a low- and intermediate-level waste repository

Falko Vehling and Haibing Shao

Correspondence to: Falko Vehling (falko.vehling@ufz.de)

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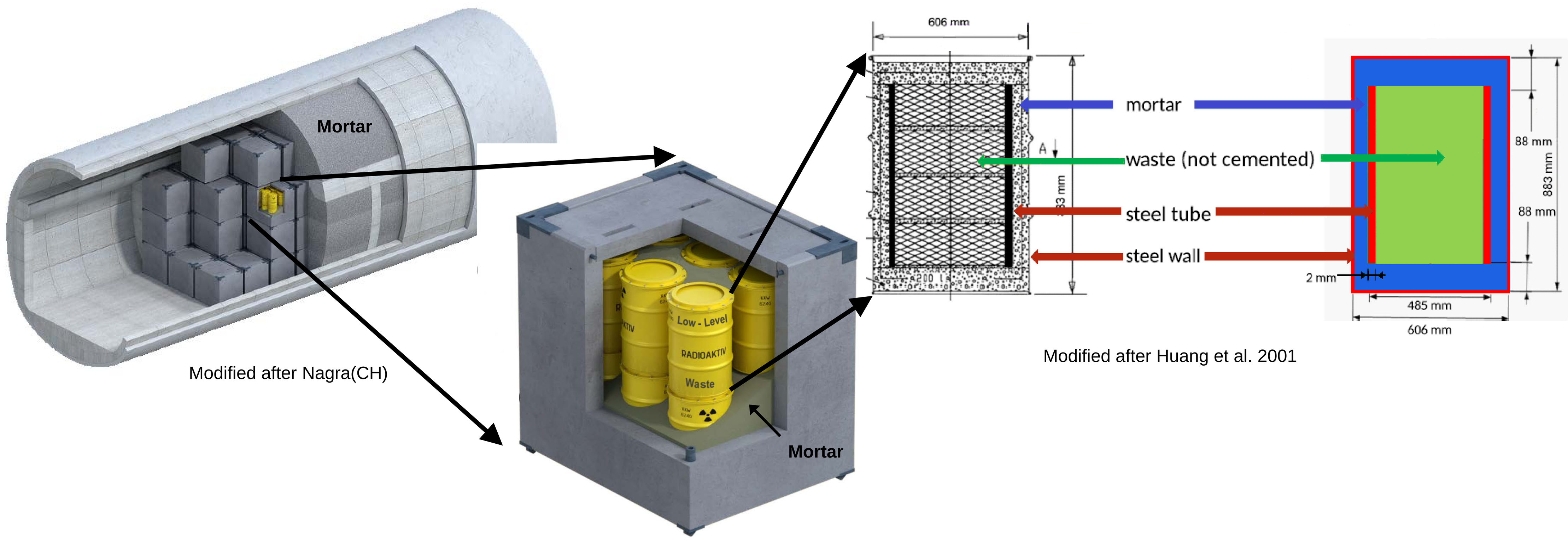
Falko Vehling and Haibing Shao

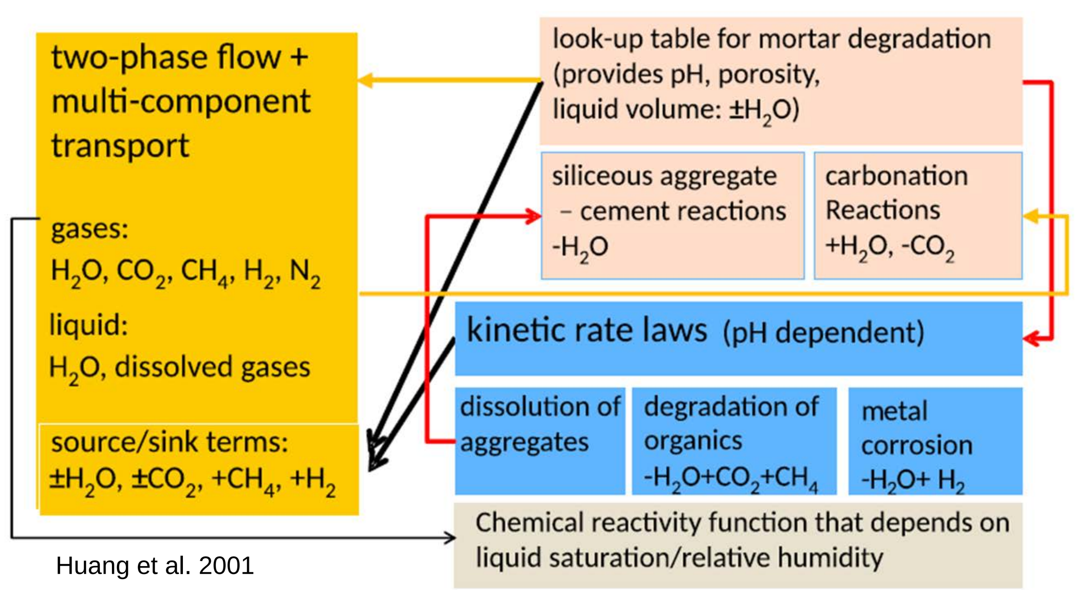
Helmholtz Centre for Environmental Research - UFZ,
Department of Environmental Informatics, 04318 Leipzig, Germany

Introduction

- **Study case:** Underground repository for low- and intermediate-level radioactive waste
- **Multiple barrier concept:** Gallery stacked with concrete containers filled with cemented waste drums
- **Chemical reactions:** Waste and mortar degradation
- **Two-phase transport problem:** Water consuming reactions with gas generation and pressure build up



Model Coupling



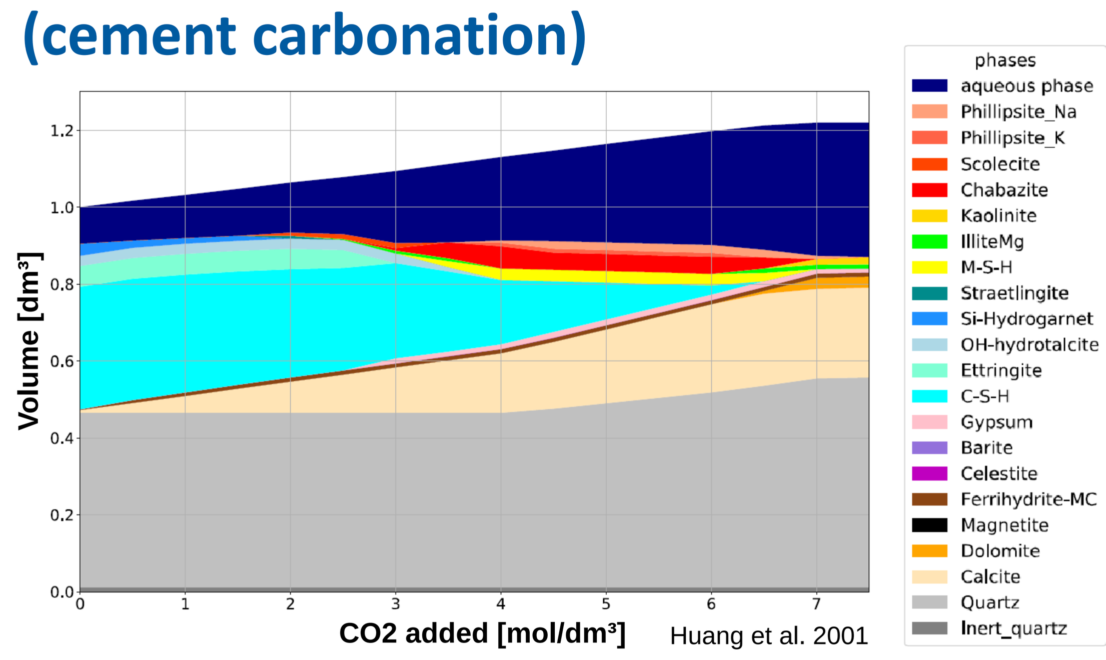
Chemical Reactions

Cellulose degradation: k_D = 0.07 mol/(kg a)
$C_6H_{10}O_5 + H_2O \rightarrow 3\ CO_2 + 3\ CH_4$

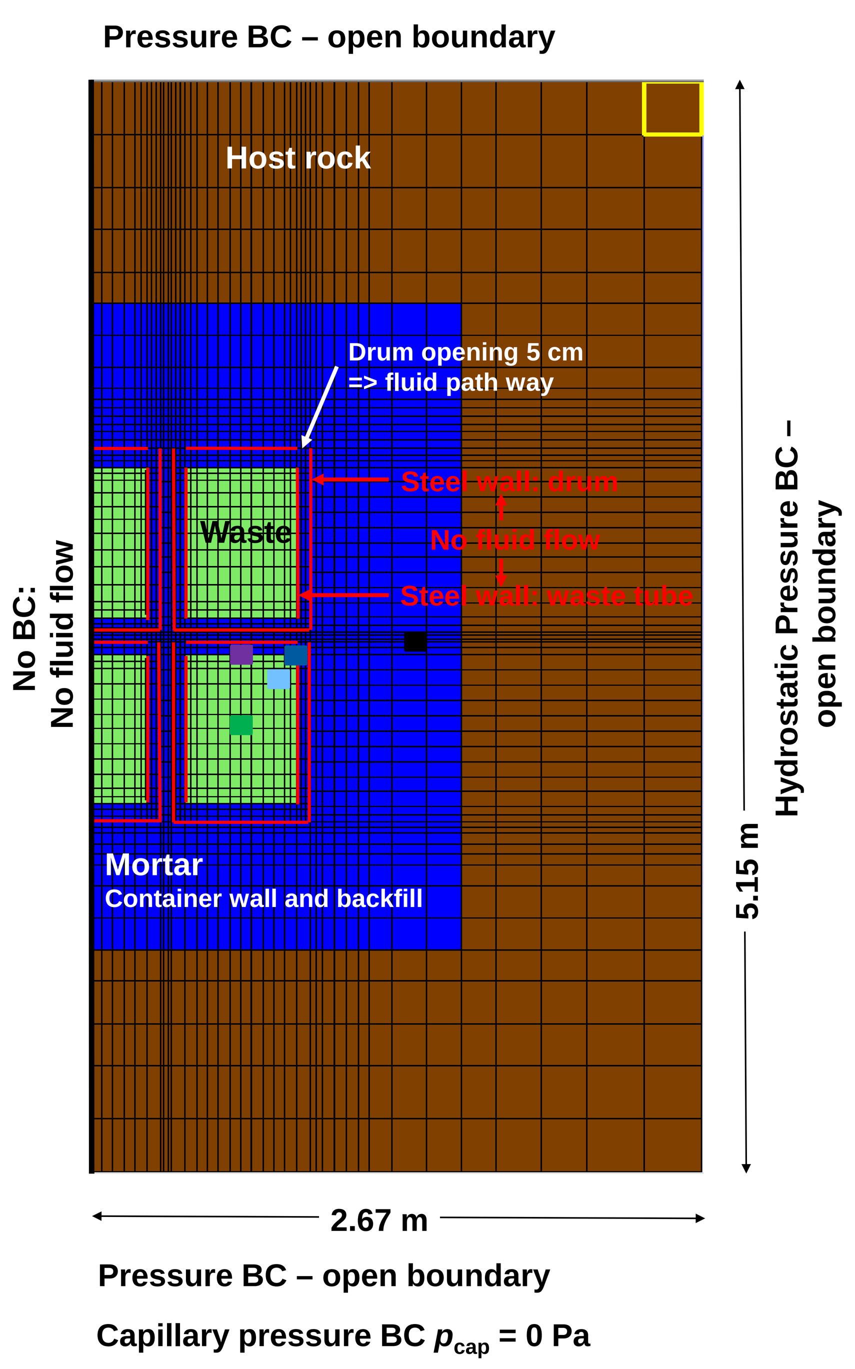
Plastic and **Polystyrene** degradation:
k_D = 0.005 mol/(kg a)
$C_8H_8 + 6\ H_2O \rightarrow 3\ CO_2 + 5\ CH_4$

Anoxic corrosion of **Iron:** $Fe + 4\ H_2O \rightarrow Fe_3O_4 + 4\ H_2$
Cor. rate: 2 µm/a for pH < 10.5 & 0.02 µm/a for pH > 10.5

Mineralogical changes of phase volumes in mortar for added CO_2 (cement carbonation)



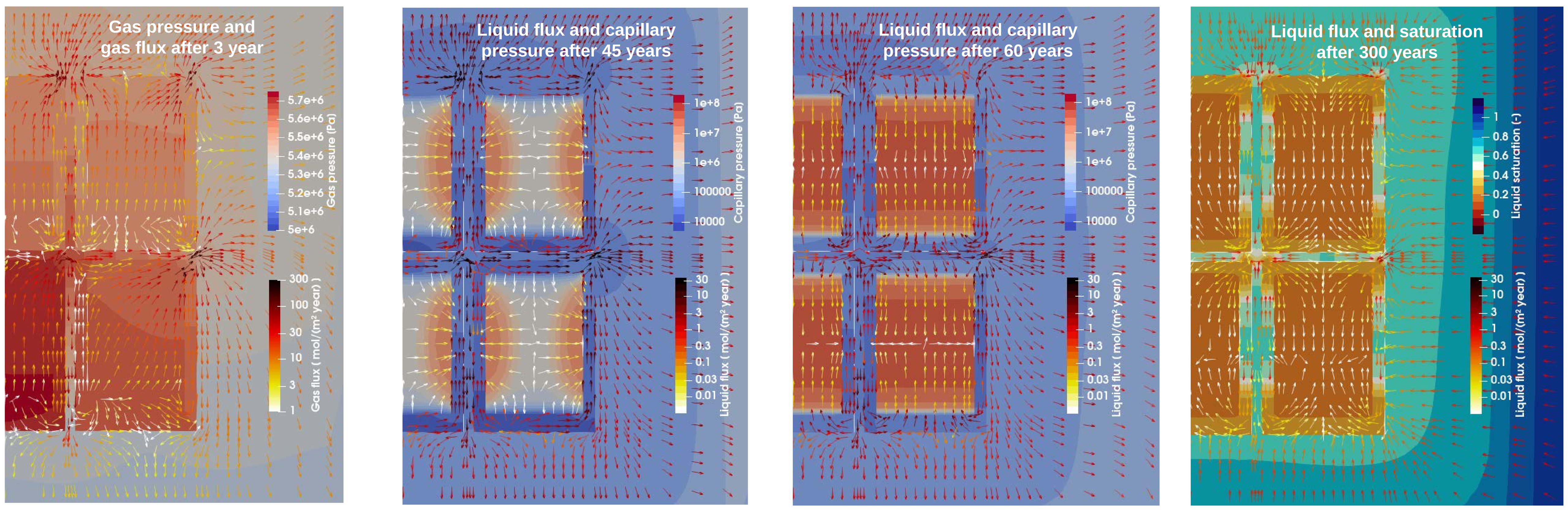
Domain and Mesh



Model Parameters

Material Parameter	Mortar (Croisé et al 2011)	Waste matrix	Host rock (Granite)	Unit
Porosity	0.0952	0.2	0.005	-
Intrinsic permeability k	1e-19 variable	1e-16	8.7e-19	m²
Residual saturation S_L^{rel}	0.2	0.2	0.2	-
Van Genuchten pseudo gas entry pressure p_d	1e5 variable	1e4	1e6	Pa
Van Genuchten parameter m	0.36	0.5	0.36	-

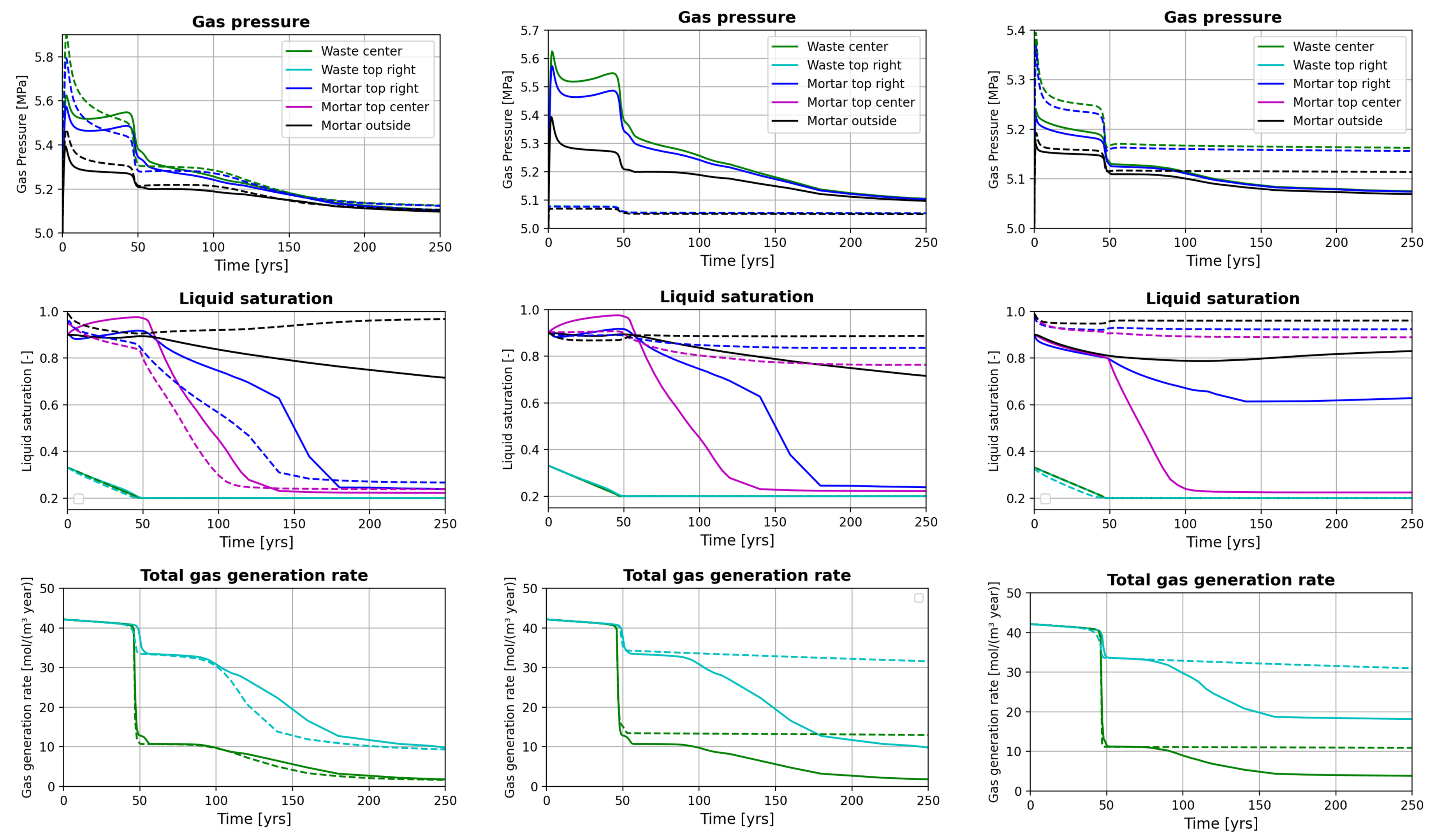
Modelling Results



Effect of **cement carbonation** and **siliceous aggregate-cement reaction**
k = 1e -19 m², p_d = 1e5 Pa
— : with cement reactions

Effect of mortar **permeability**,
p_d = 1e5 Pa
— : k = 1e-19 m² - - : k = 2.5e-18 m²

Effect of **gas entry pressure**,
k = 5e -19 m²
— : p_d = 1e5 Pa - - : p_d = 5e5 Pa
Without cement reactions



Key findings

- Fast gas generation at the beginning but slows down after 50 years
- Cement carbonation (CO_2 uptake) reduces initial gas pressure
- Both, k and p_d, are key parameters controlling water supply for waste degradation
- Cement chemistry is more important for low k and p_d

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[1] Huang, Y., Shao, H., Wieland, E ., Kolditz, O. & Kosakowski, G. *Two-phase transport in a cemented waste package considering the spatio-temporal evolution of chemical conditions*. Npj Materials Degradation (2021)

Contact:

falko.vehling@ufz.de

www.ufz.de