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Hydro-Mechanical-Chemical modelling of Brucite – Periclase (de)hydration reactions

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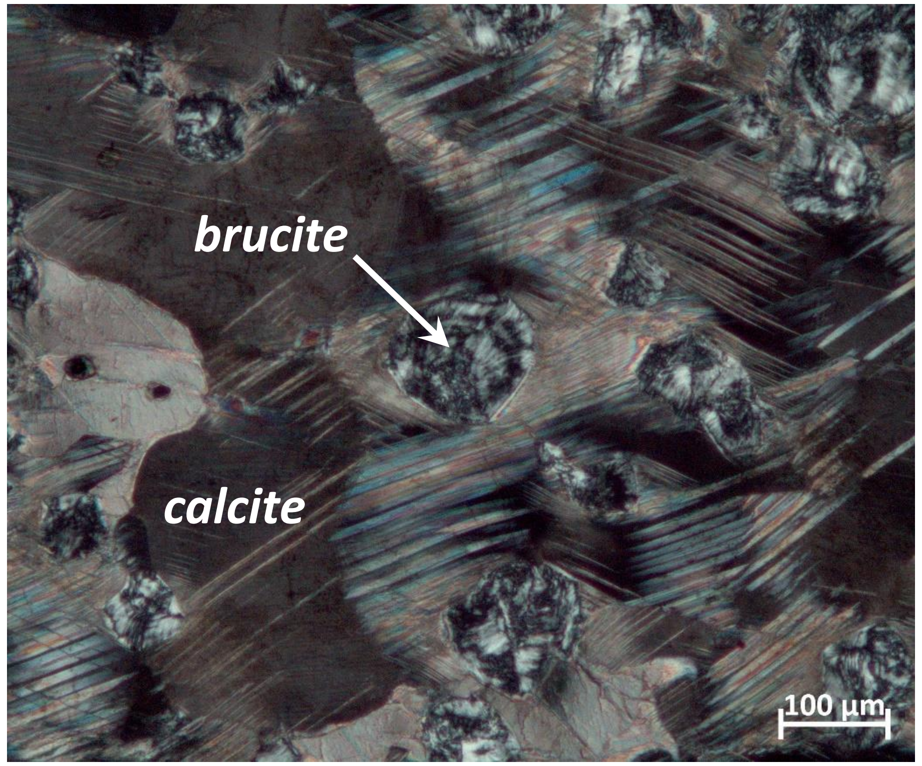
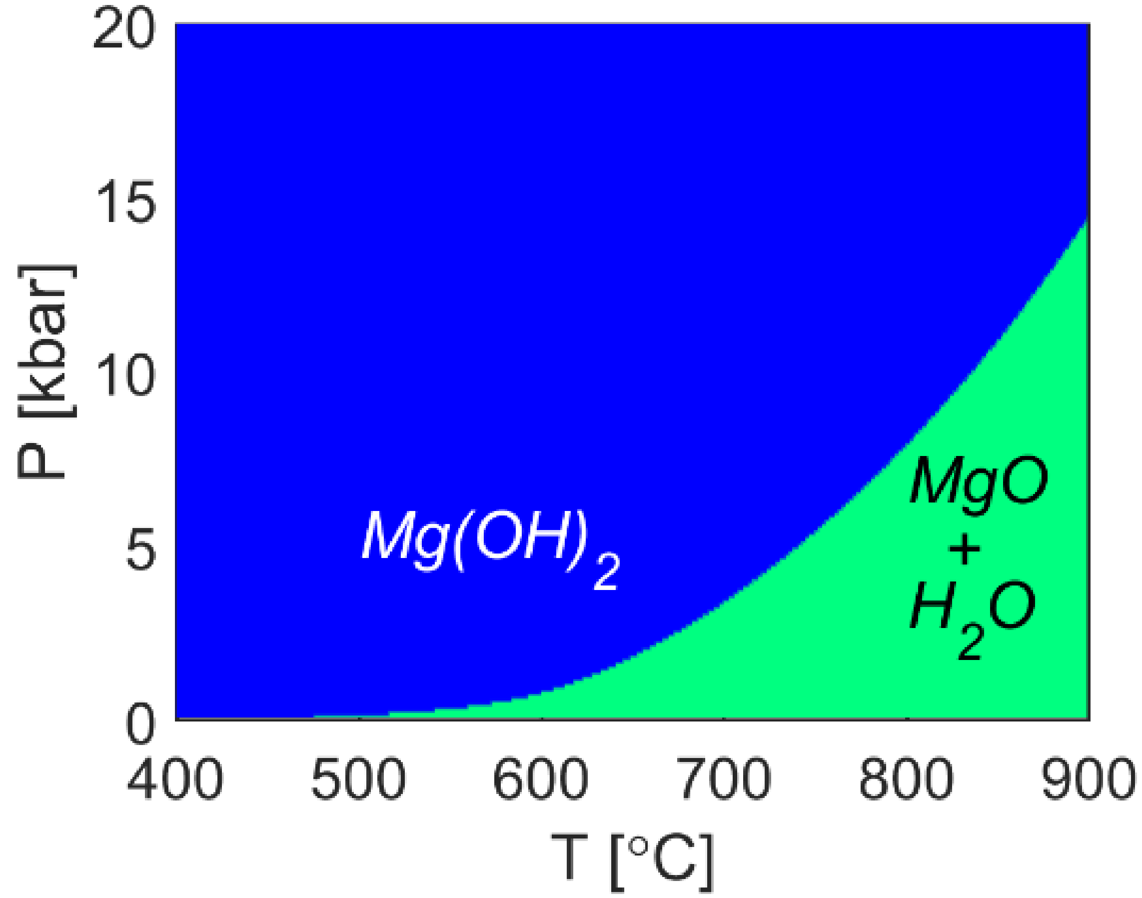
Aim and scientific questions

Brucite in natural rock





Periclase + Water = Brucite

$MgO + H_2O = Mg(OH)_2$

Aim

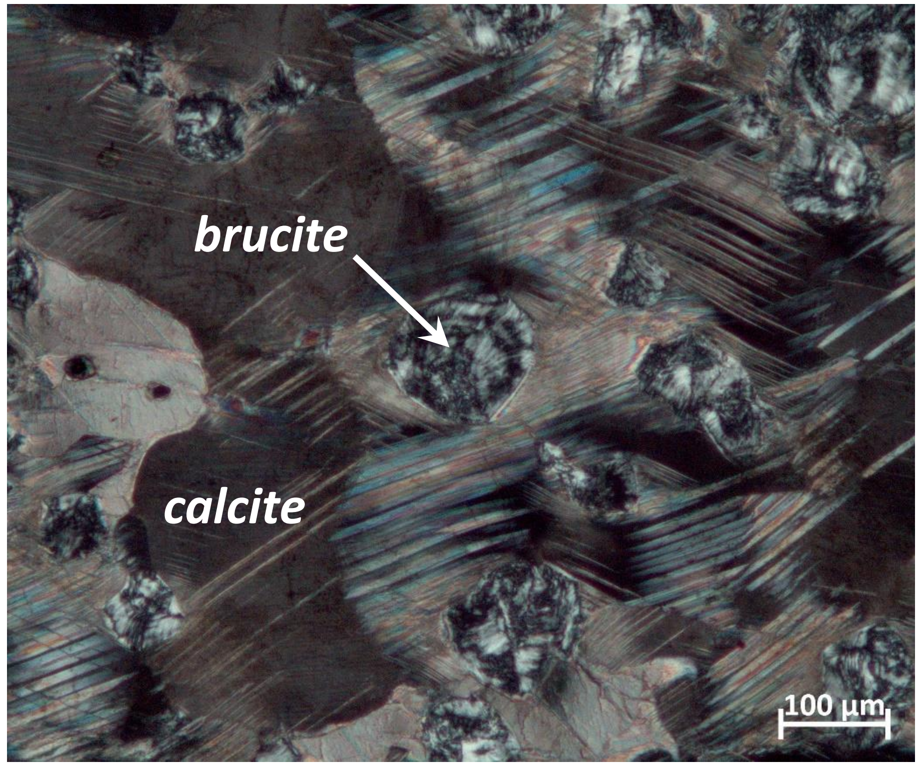
Develop a mathematical model, which describes the hydro-chemical process of the (de)hydration reaction and the coupled two-dimensional deformation in a compressible poro-viscous rock.

Scientific questions

- How does the deformation of a poro-viscous rock affect the (de)hydration reaction?
- How does far-field compression affect the reaction?

The (de)hydration reaction

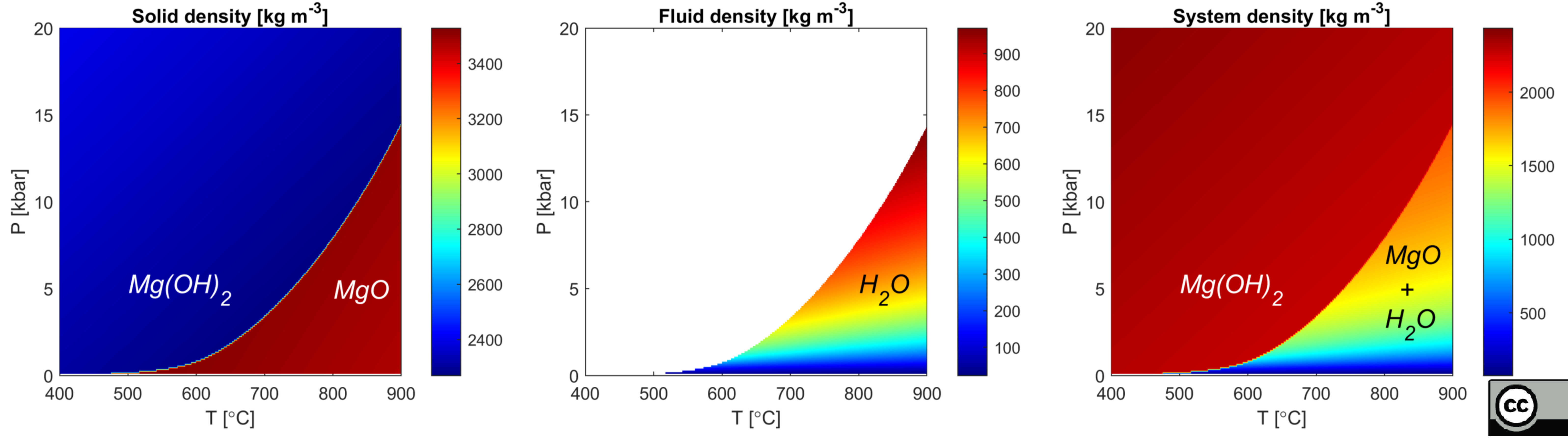
Brucite in natural rock



Periclase + Water = Brucite

$MgO + H_2O = Mg(OH)_2$

Required solid and fluid densities are calculated from minimization of Gibbs energy (see density maps below). The reaction has a positive Clapeyron slope. For completeness, also the system density is shown.

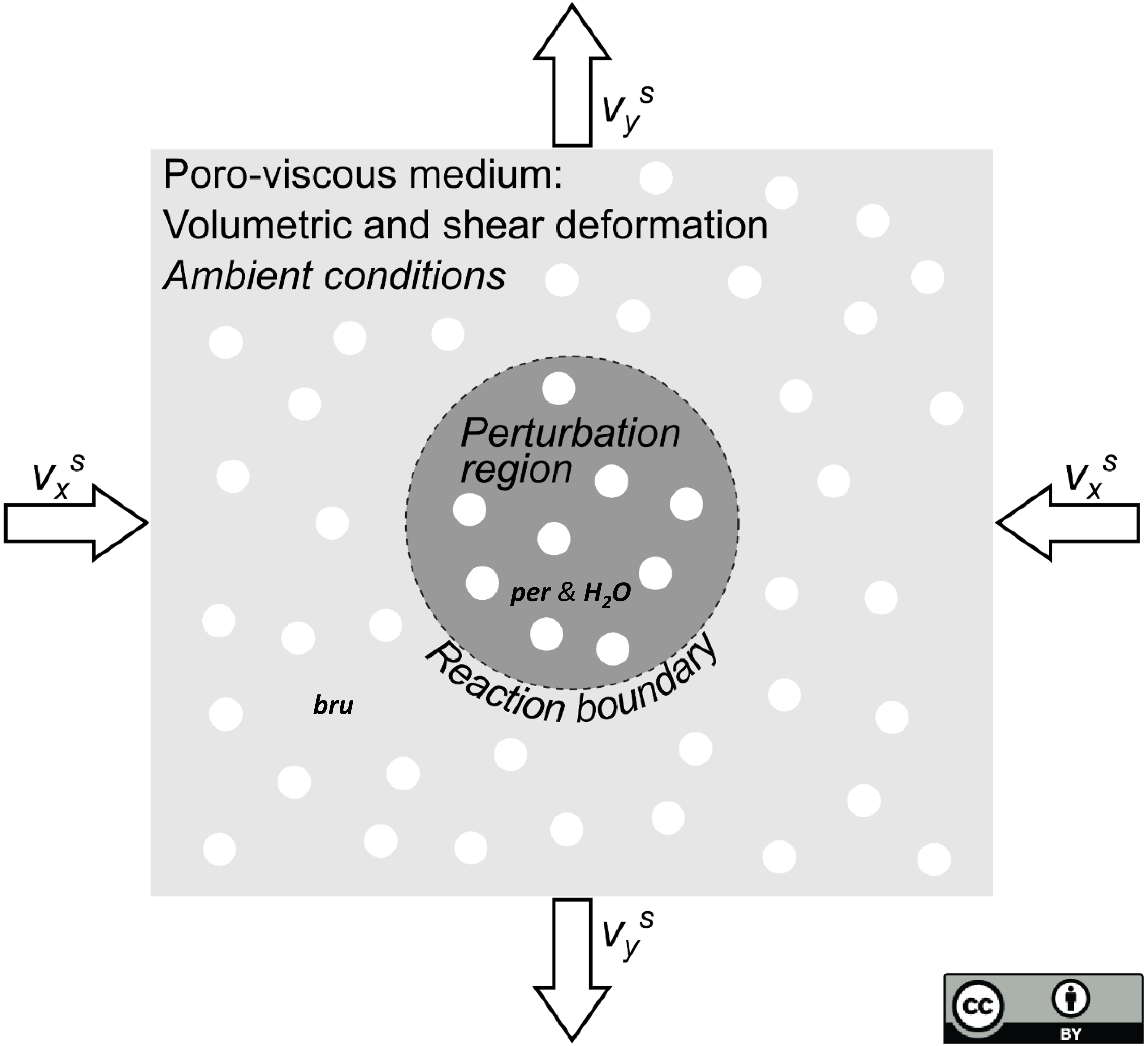


Model

Model
- 2D compressible poro-viscous medium
- Power-law flow law for shear deformation
- Thermodynamic equilibrium
- Closed system (all required H_2O in system)
- Application of Darcy law
- Constant temperature

A circular region has initially either smaller or larger pressure than the surrounding medium to initially have either brucite in the inclusion and periclase and water in the surrounding or vice versa.

Solution of system of equations with pseudo-transient finite difference method; see
Duretz et al., GJI, 2019
Räss et al., GJI, 2019



Governing equations in 2D

Derivation of the system of equations is based on
Yarushina & Podladchikov, JGR, 2015
and
Malvoisin et al., G-cubed, 2015

Viscous bulk and shear deformation.

Symbol	Name	Units
p_f	Fluid pressure	$[Pa]$
φ	Porosity	$[\ ]$
ρ_s	Solid density	$[kg\cdot m^{-3}]$
ρ_f	Fluid density	$[kg\cdot m^{-3}]$
X_s	Mass fraction MgO	$[\ ]$
p	Total pressure	$[Pa]$
v_x^s, v_y^s	Solid velocities	$[m\cdot s^{-1}]$
$\tau_{xx}, \tau_{yy}, \tau_{xy}$	Deviatoric stresses	$[Pa]$
τ_{ref}	Reference stress	$[Pa]$
k	Permeability	$[m^2]$
η_f	Fluid viscosity	$[Pa\cdot s]$
η^s	Shear viscosity solid	$[Pa\cdot s]$
λ	Bulk viscosity solid	$[Pa\cdot s]$
n	Stress exponent	$[\ ]$

$$\rho_T = \rho_f\varphi + \rho_s(1-\varphi) \qquad \rho_X = \rho_s X_s$$

Conservation of total mass

$$\frac{\partial\rho_T}{\partial t} - \frac{\partial}{\partial x}\left[\frac{\rho_f k\varphi^3}{\eta_f}\frac{\partial p_f}{\partial x}\right] - \frac{\partial}{\partial y}\left[\frac{\rho_f k\varphi^3}{\eta_f}\frac{\partial p_f}{\partial y}\right] + \frac{\partial\rho_T v_x^s}{\partial x} + \frac{\partial\rho_T v_y^s}{\partial y} = 0$$

Conservation of MgO in solid

$$\frac{\partial\left[\rho_X(1-\varphi)\right]}{\partial t} + \frac{\partial\left[\rho_X(1-\varphi)v_x^s\right]}{\partial x} + \frac{\partial\left[\rho_X(1-\varphi)v_y^s\right]}{\partial y} = 0$$

Densities and MgO fraction

$$\rho_f = \rho_f(p_f); \qquad \rho_s = \rho_s(p_f); \qquad X_s = X_s(p_f)$$

Force balance equations

$$-\frac{\partial p}{\partial x} + \frac{\partial\tau_{xx}}{\partial x} + \frac{\partial\tau_{xy}}{\partial y} = 0; \qquad -\frac{\partial p}{\partial y} + \frac{\partial\tau_{yy}}{\partial y} + \frac{\partial\tau_{xy}}{\partial x} = 0$$

Volumetric rheology

$$p = p_f - (1-\varphi)\lambda\left(\frac{\partial v_x^s}{\partial x} + \frac{\partial v_y^s}{\partial y}\right)$$

Power-law viscous behaviour only

Shear rheology

$$\tau_{xx} = 2\eta^s\left(\frac{\tau_{II}}{\tau_{ref}}\right)^{1-n}\left[\frac{\partial v_x^s}{\partial x} - \frac{1}{3}\left(\frac{\partial v_x^s}{\partial x} + \frac{\partial v_y^s}{\partial y}\right)\right]$$

$$\tau_{yy} = 2\eta^s\left(\frac{\tau_{II}}{\tau_{ref}}\right)^{1-n}\left[\frac{\partial v_y^s}{\partial y} - \frac{1}{3}\left(\frac{\partial v_x^s}{\partial x} + \frac{\partial v_y^s}{\partial y}\right)\right]$$

$$\tau_{xy} = \eta^s\left(\frac{\tau_{II}}{\tau_{ref}}\right)^{1-n}\left(\frac{\partial v_x^s}{\partial y} + \frac{\partial v_y^s}{\partial x}\right)$$

Governing equations in 2D

Conservation of total mass

$$\frac{\partial \rho_T}{\partial t} - \frac{\partial}{\partial x}\left[\frac{\rho_f k \varphi^3}{\eta_f}\frac{\partial p_f}{\partial x}\right] - \frac{\partial}{\partial y}\left[\frac{\rho_f k \varphi^3}{\eta_f}\frac{\partial p_f}{\partial y}\right] + \frac{\partial \rho_T v_x^s}{\partial x} + \frac{\partial \rho_T v_y^s}{\partial y} = 0$$

Conservation of MgO in solid

$$\frac{\partial\left[\rho_X (1-\varphi)\right]}{\partial t} + \frac{\partial\left[\rho_X (1-\varphi) v_x^s\right]}{\partial x} + \frac{\partial\left[\rho_X (1-\varphi) v_y^s\right]}{\partial y} = 0$$

Densities and MgO fraction

$$\rho_f = \rho_f\left(p_f\right); \qquad \rho_s = \rho_s\left(p_f\right); \qquad X_s = X_s\left(p_f\right)$$

$$-\frac{\partial p}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} = 0; \qquad -\frac{\partial p}{\partial y} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{xy}}{\partial x} = 0$$

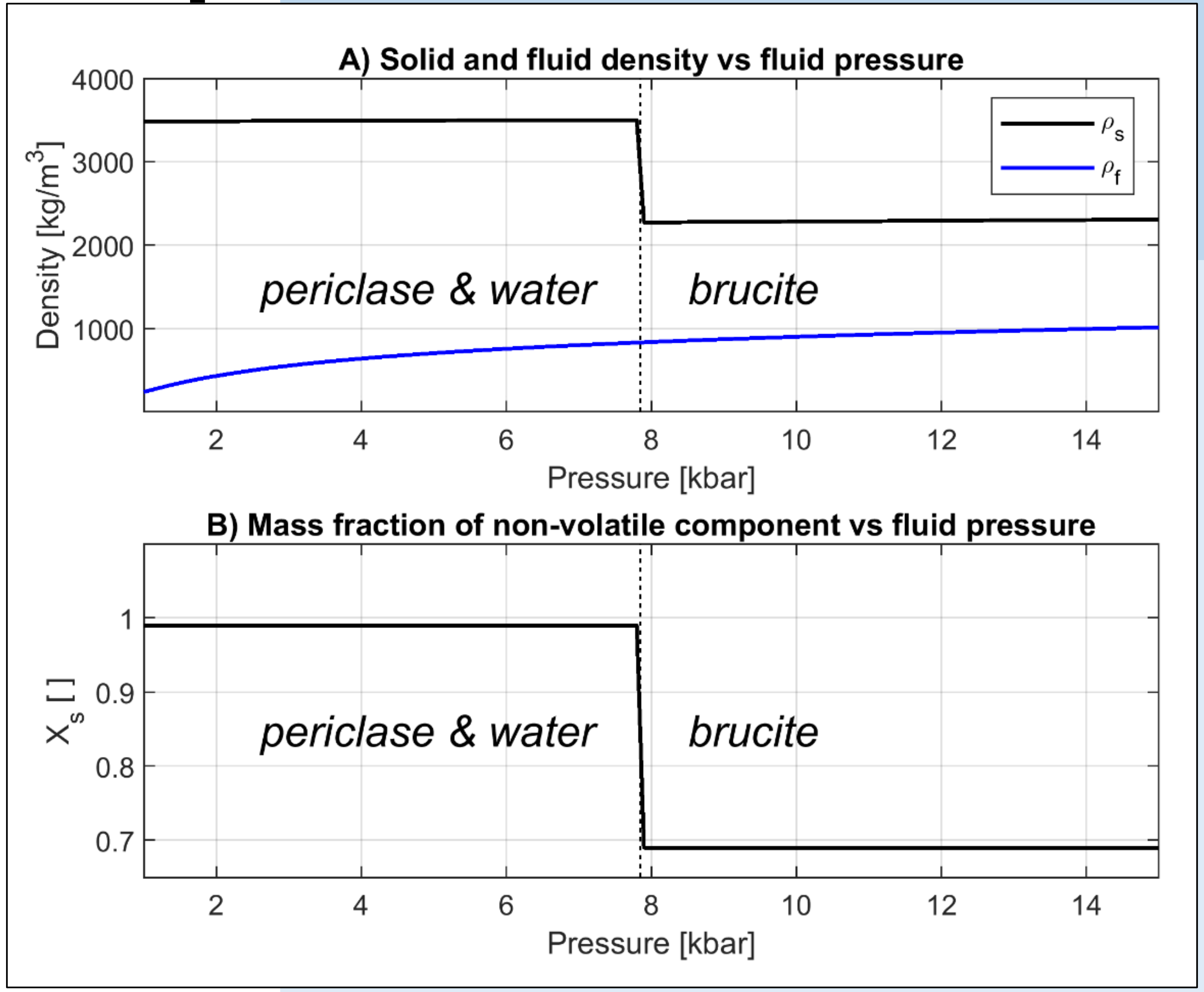
$$p = p_f - (1-\varphi)\lambda\left(\frac{\partial v_x^s}{\partial x} + \frac{\partial v_y^s}{\partial y}\right)$$

$$\tau_{xx} = 2\eta^s\left(\frac{\tau_{II}}{\tau_{ref}}\right)^{1-n}\left[\frac{\partial v_x^s}{\partial x} - \frac{1}{3}\left(\frac{\partial v_x^s}{\partial x} + \frac{\partial v_y^s}{\partial y}\right)\right]$$

$$\tau_{yy} = 2\eta^s\left(\frac{\tau_{II}}{\tau_{ref}}\right)^{1-n}\left[\frac{\partial v_y^s}{\partial y} - \frac{1}{3}\left(\frac{\partial v_x^s}{\partial x} + \frac{\partial v_y^s}{\partial y}\right)\right]$$

$$\tau_{xy} = \eta^s\left(\frac{\tau_{II}}{\tau_{ref}}\right)^{1-n}\left(\frac{\partial v_x^s}{\partial y} + \frac{\partial v_y^s}{\partial x}\right)$$

Three look-up tables from equilibrium thermodynamics

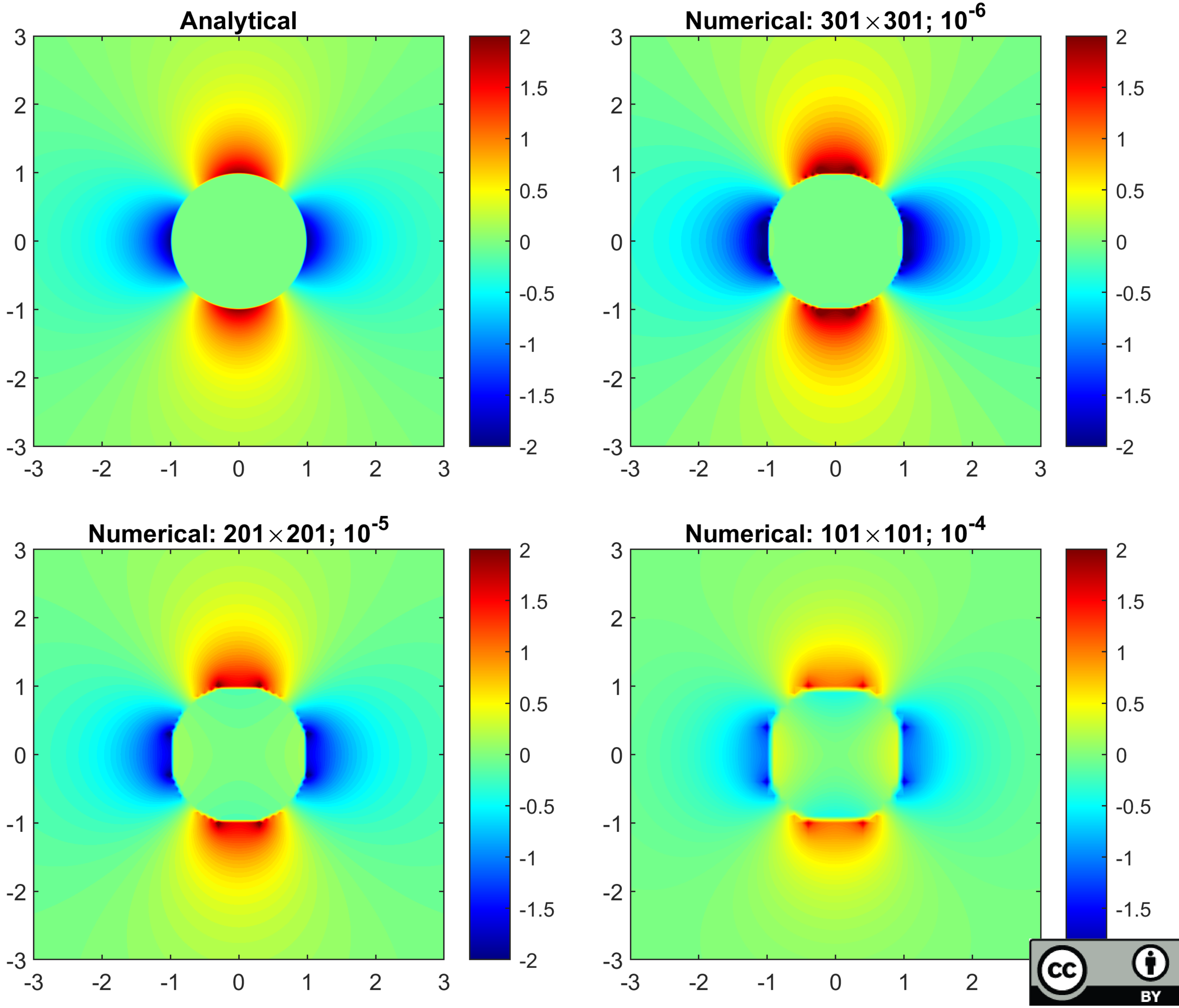


Test: Mechanical

Model:
Only mechanical process.
Circular inclusion has shear viscosity 1000 times smaller than surrounding. Pure shear background deformation with horizontal shortening. Bulk viscous compressibility with bulk viscosity equal to shear viscosity.
Analytical solution from
Moulas et al., Tectonophysics, 2014; based on Schmid & Podladchikov, GJI, 2003

The panels show colorplots of the dimensionless pressure field. Title of panels indicates numerical resolution (e.g. 101×101) and tolerance for iterative solver (e.g. 10^{-4}).

The code can reproduce pressure variations due to weak inclusions under far-field deformation.

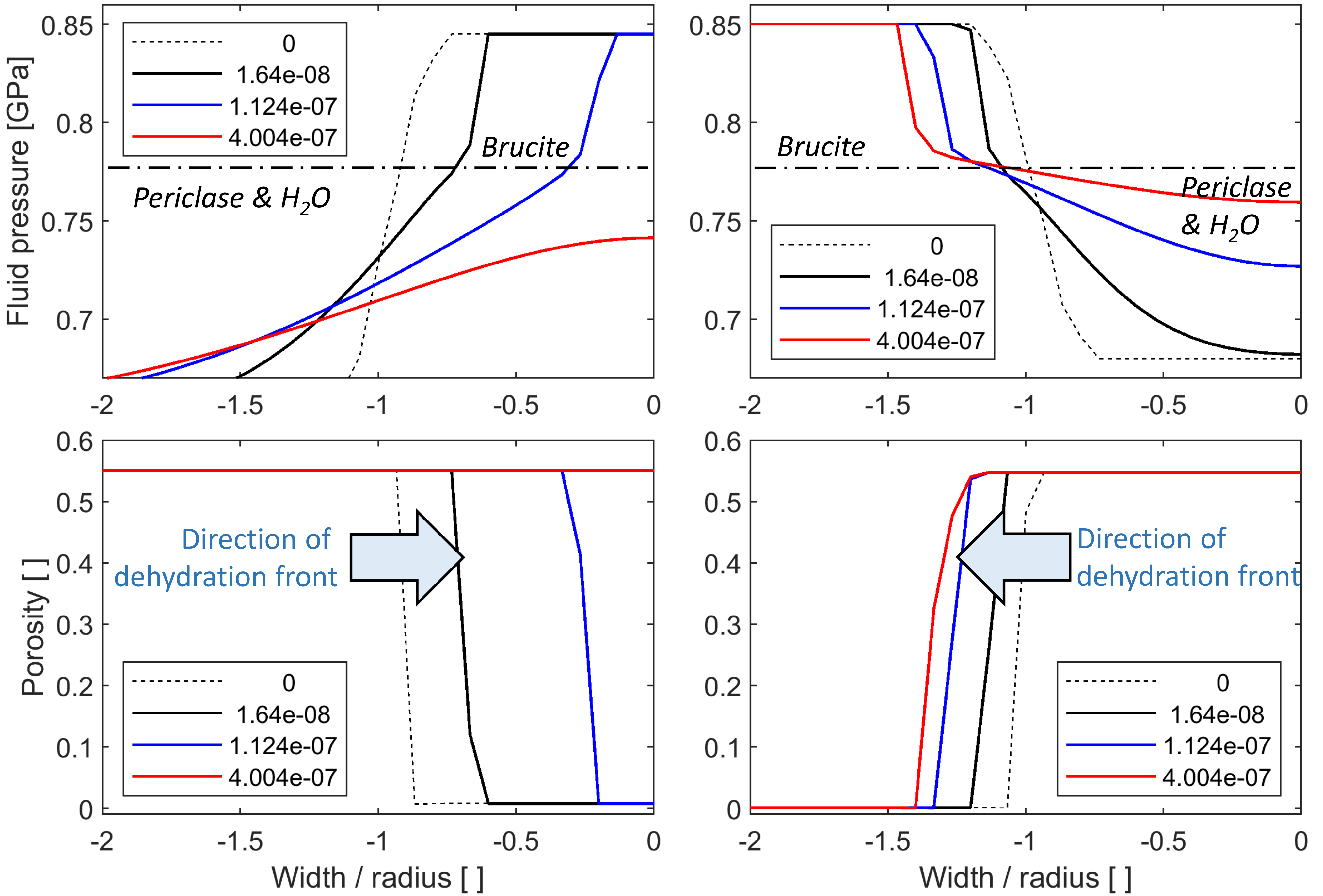


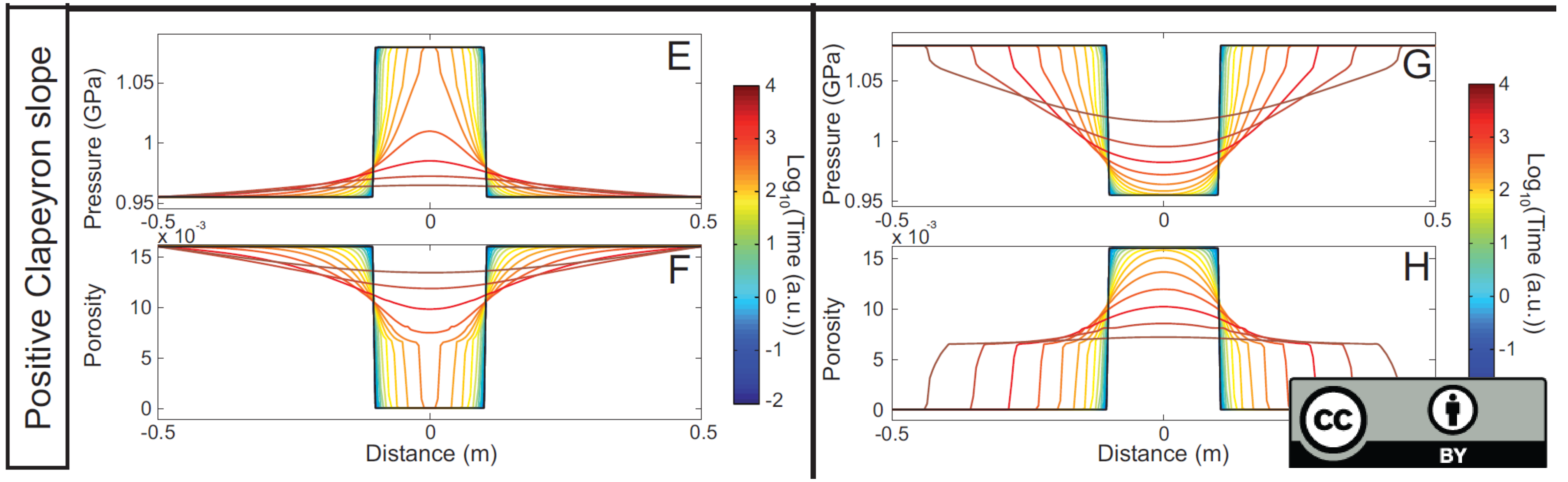
Test: Hydro-chemical

Model:

Only hydro-chemical process, no mechanical deformation, i.e. solid velocities are zero.
Circular inclusion has initially higher or smaller fluid pressure than surrounding. The pressure controlling the reaction is between the pressure of the inclusion and the surrounding.
Temperature is constant and 800 °C.
Legend indicates dimensonless time.

The model reproduces the general behaviour of the evolution of fluid pressure and porosity as reported in Malvoisin et al., G-cubed, 2015 (see bottom figure).
Left column: Larger pressure in inclusion
Right column: Smaller pressure in inclusion

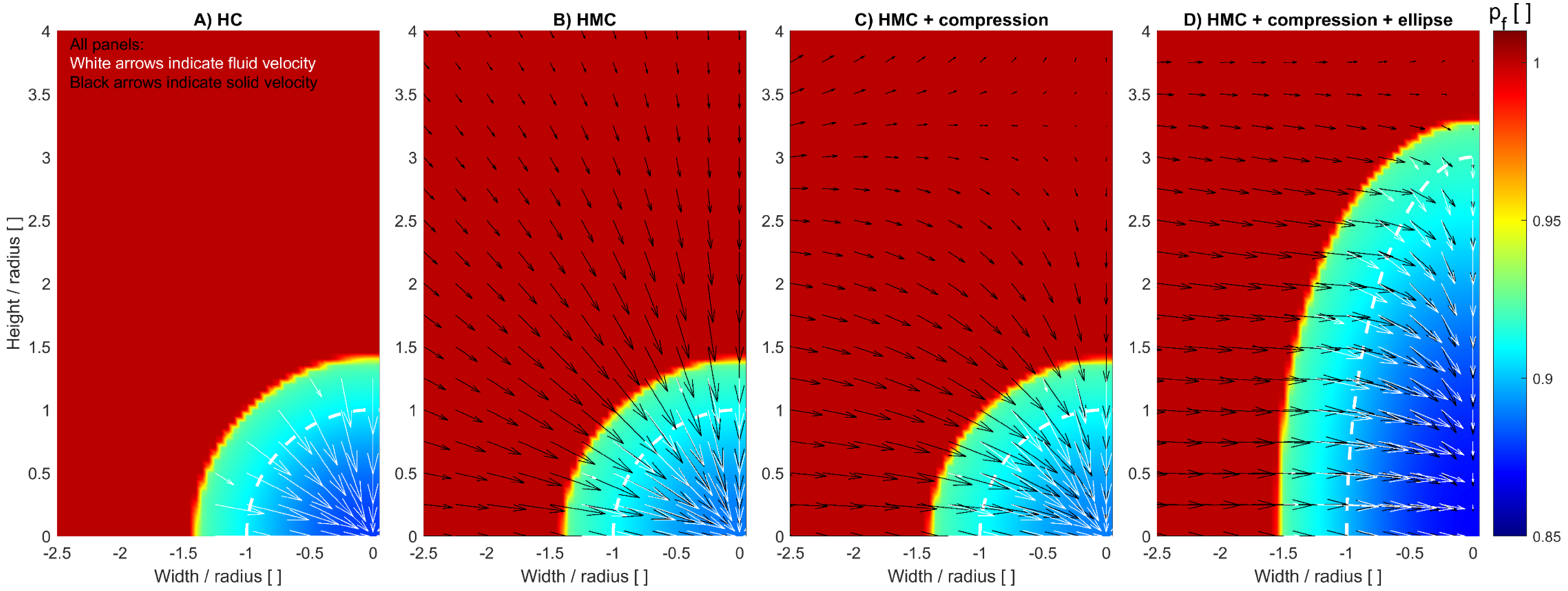




Malvoisin et al., G-cubed, 2015; their figure 10.

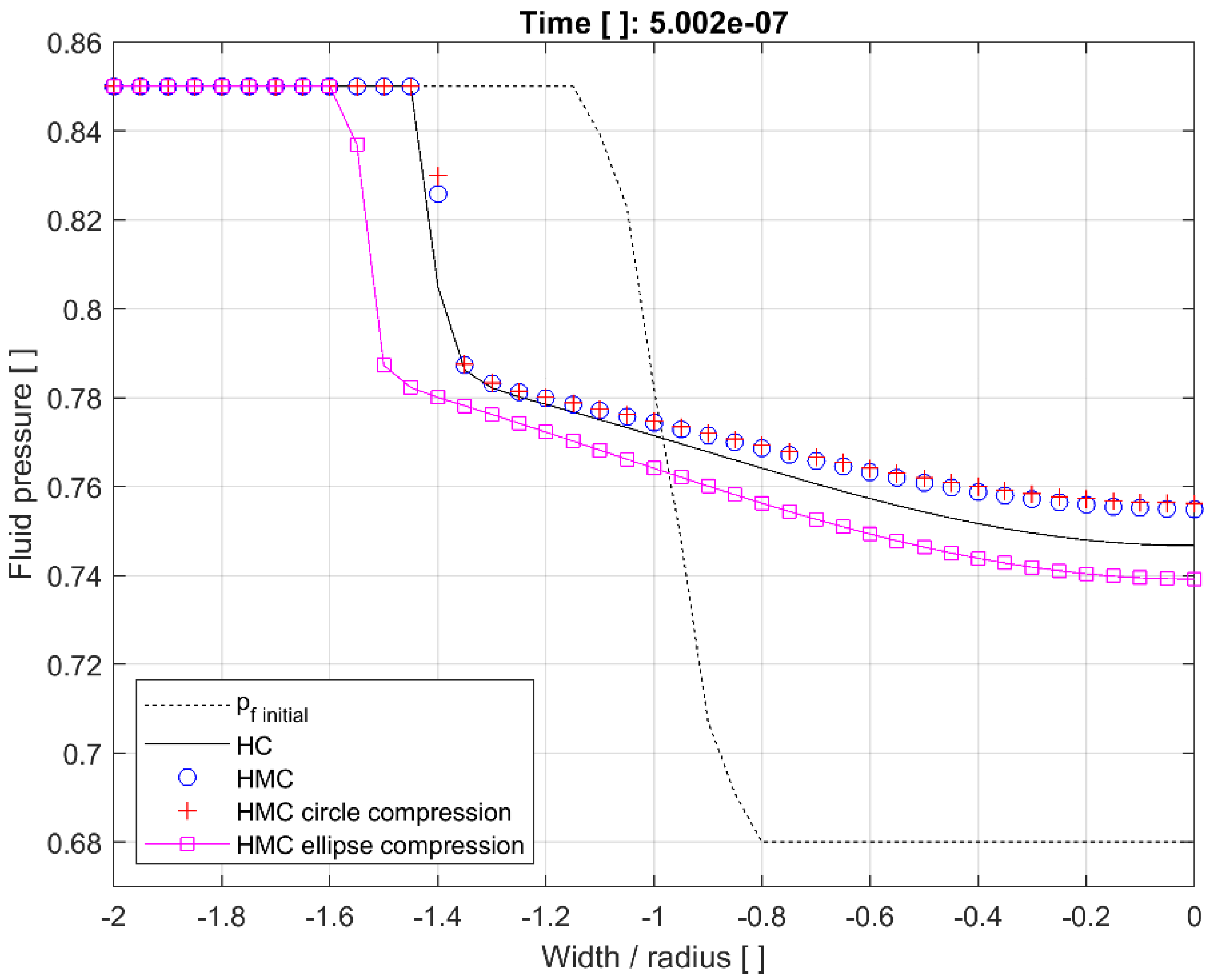
Hydro-mechanical-chemical model

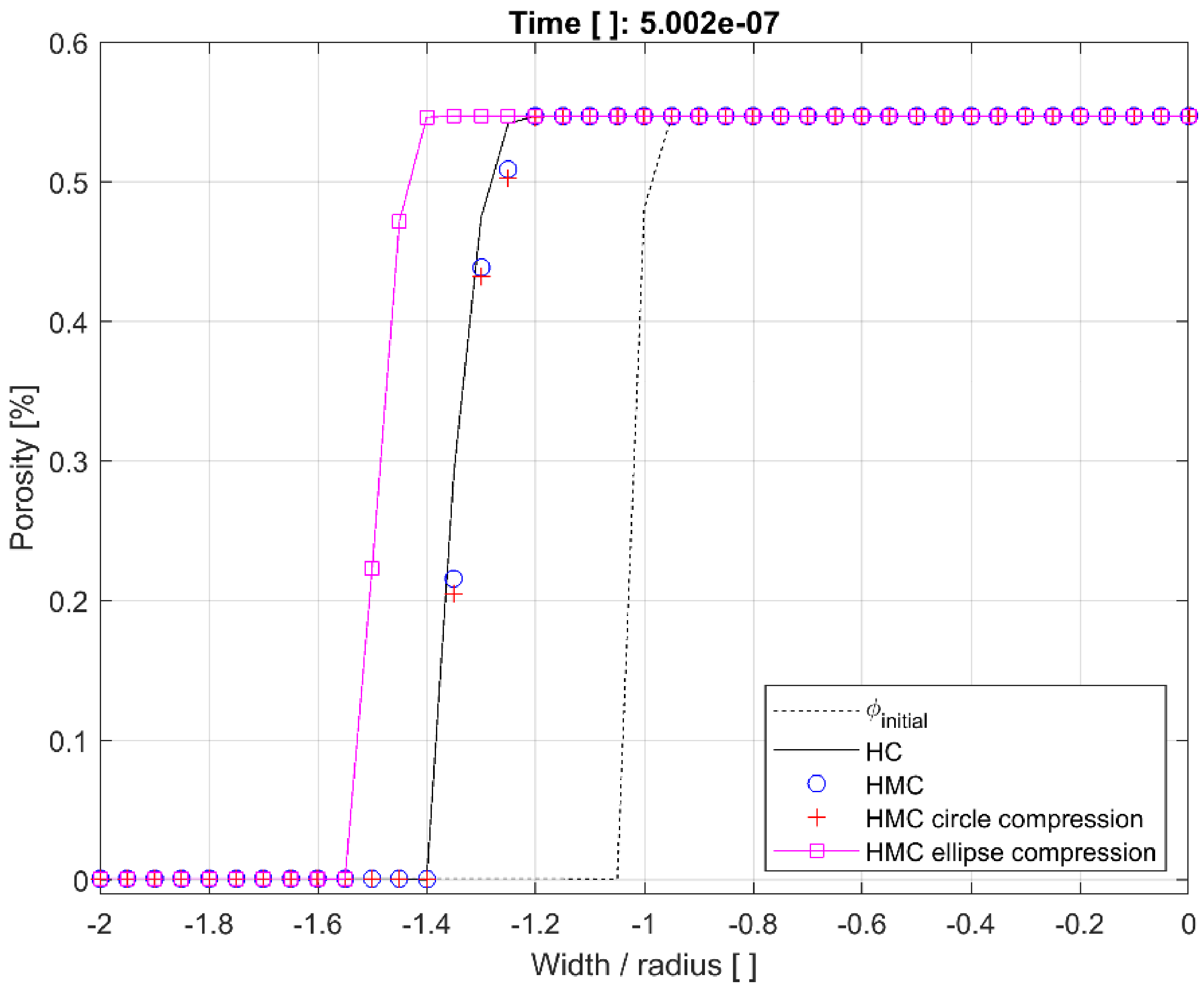
Colorplots of dimensionless fluid pressure



A hydro-chemical (HC) model, a hydro-mechanical-chemical (HMC) model with **NO** far field deformation, a HMC model **with** compression and a circular weak inlcusion and a HMC model **with** compression and an elliptical weak inlcusion (aspect ratio 3). Dashed white lines show initial area of pressure perturbation, which increases due to effective pressure diffusion. Models with compression show differences between fluid and solid velocities.

Hydro-mechanical-chemical model



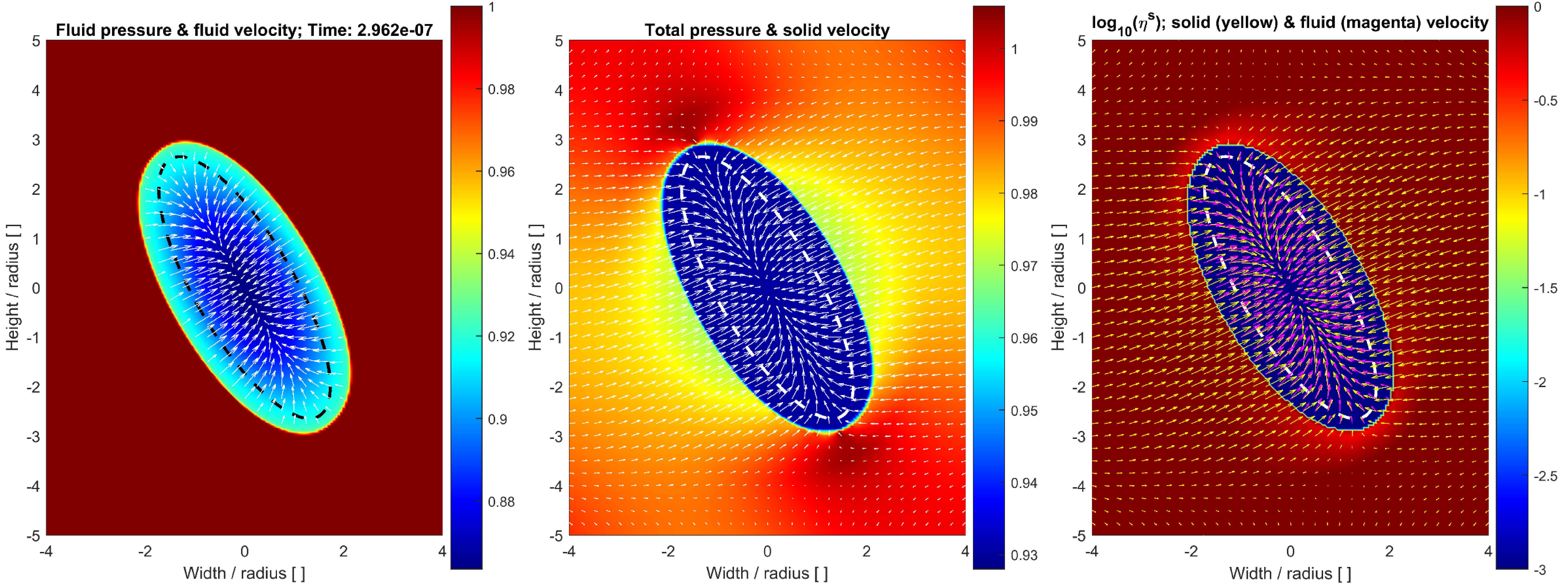


The fluid pressure and porosity profiles have a different shape after the same time. Hence, deformation of the viscous medium and compression have an impact on fluid pressure evolution and, hence, on the reaction.

All models are dimensionless. Initial fluid pressure is controlled by reaction pressure.

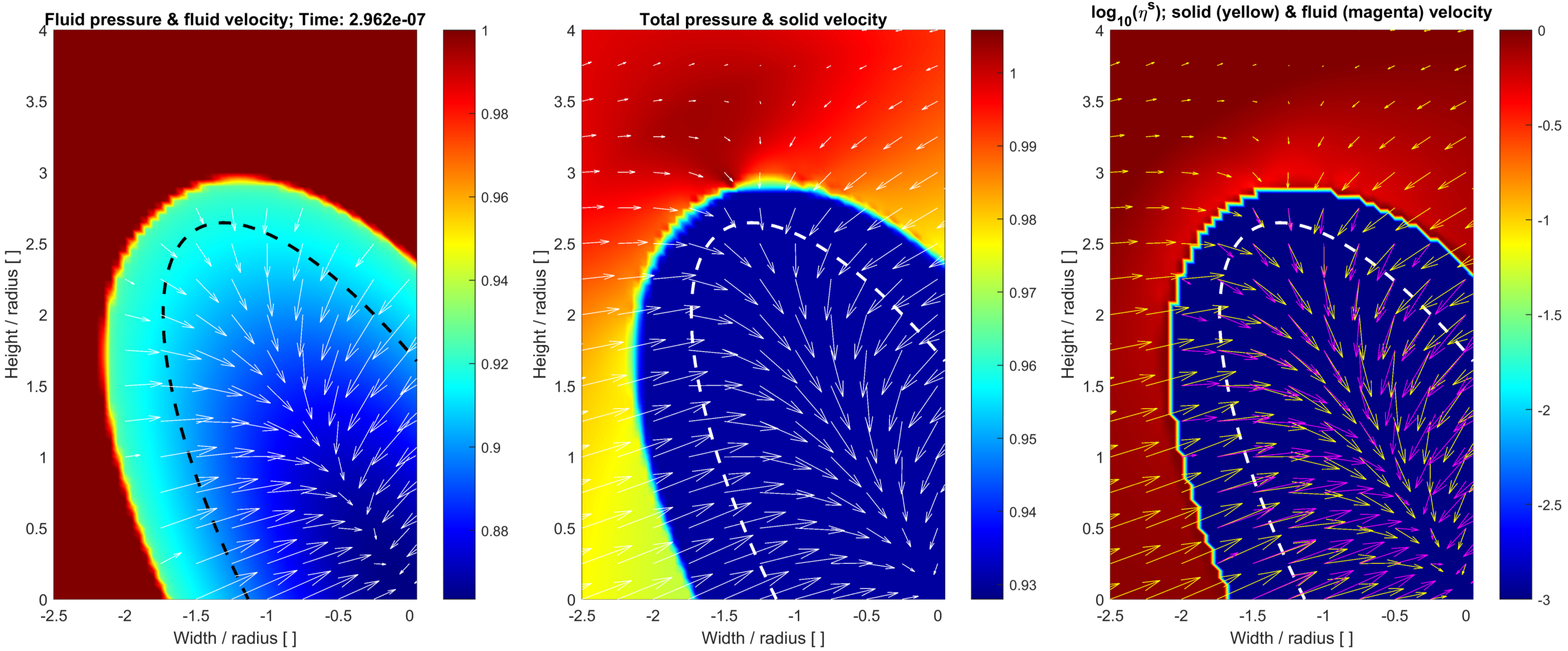
$$p_{ini} = 8.5 \text{ kbar}; \quad \frac{\lambda}{\eta^s} = 1; \quad \frac{k}{\eta_f}\frac{\eta^s}{r^2} = 10^8; \quad \frac{\dot{\varepsilon}\eta^s}{p_{ini}} = 0.0024$$

Hydro-mechanical-chemical model



Model with oblique, weak elliptical inclusion with horizontal pure shear shortening.
The colorplot of the effective shear viscosity (right panel) shows variable viscosity due to power-law flow law (n=3).
The dashed elliptical line shows the initial inclusion shape. The inclusion of periclase/water is increasing due to a moving dehydration front, which extracts water from the surrounding brucite.

Hydro-mechanical-chemical model



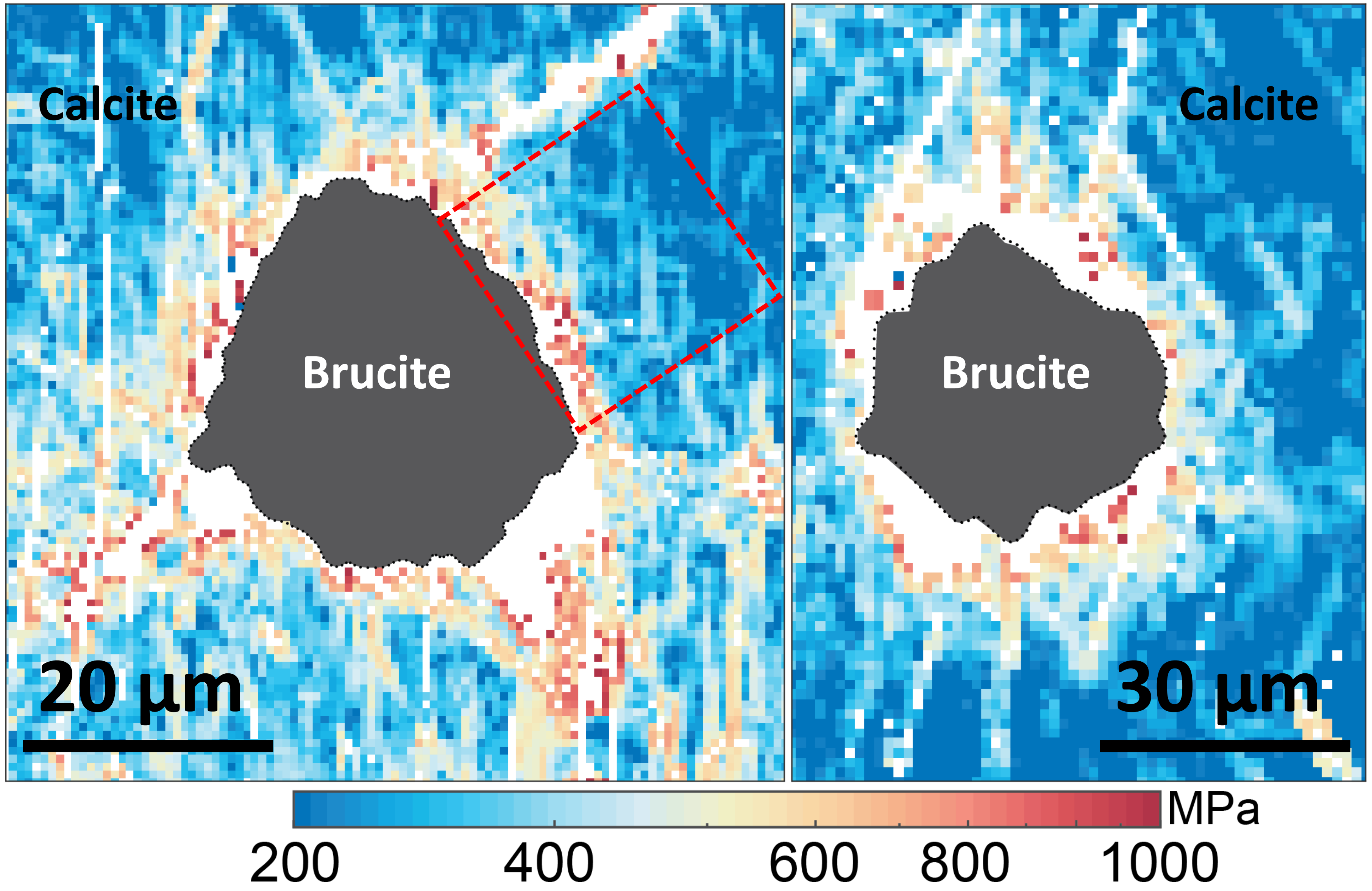
Enlargement of model from previous slide.
In deforming and mechanically heterogeneous systems, the total pressure and its gradients differ from the fluid pressure and its gradients. The solid and fluid velocities also differ.

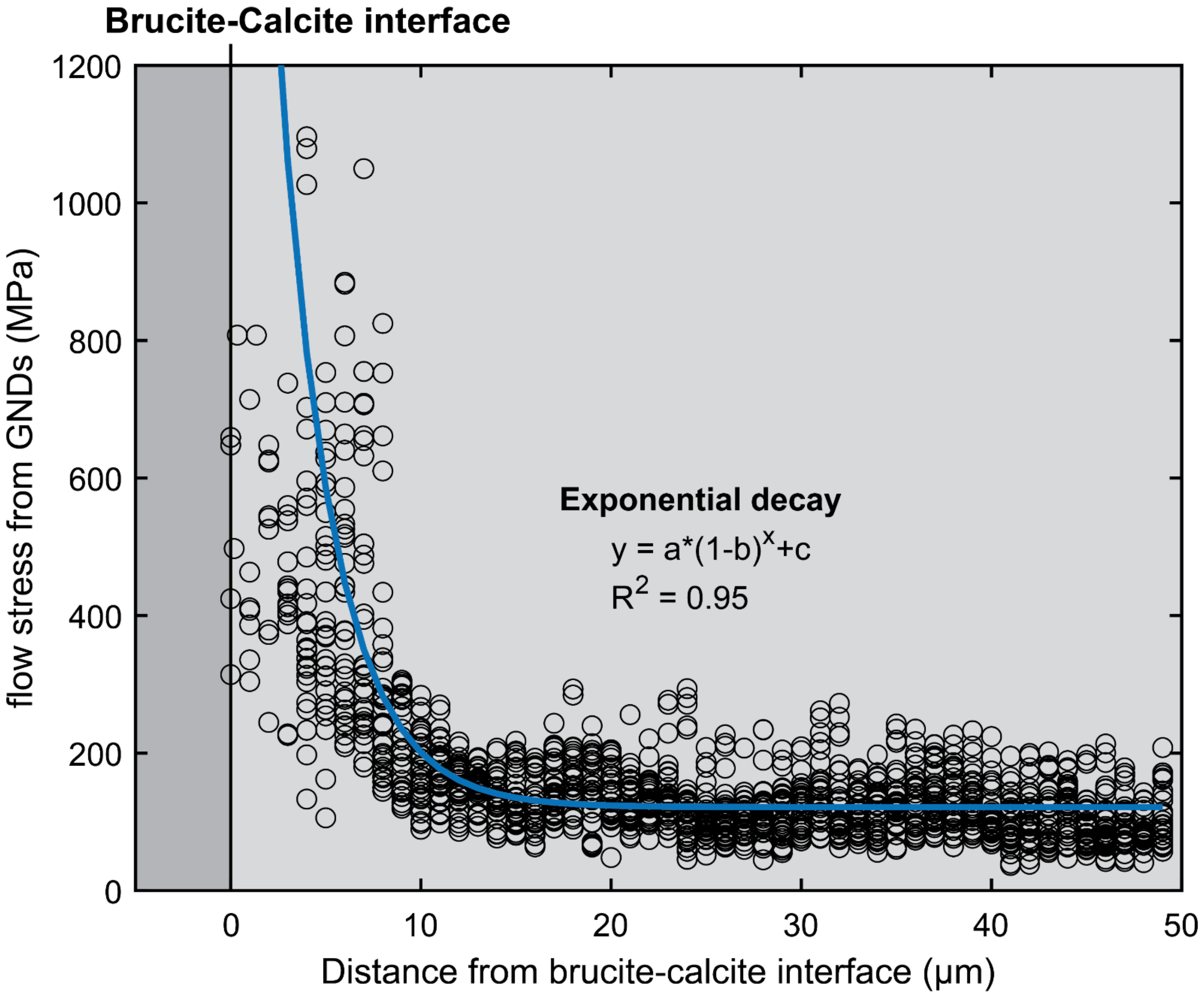
Acknowledgements: David Wallis, Floris Teuling, Thomas Müller

Next steps

Modelling an open system and the hydration of periclase, at pressures where brucite is also stable, and the resulting brucite formation to test whether volumetric expansion can generate significant reaction-induced stress in surrounding carbonate rocks, as suggested by flow stress estimates from dislocation densities estimated by high-angular resolution electron backscatter diffraction (HR-EBSD).

Stress distribution in calcite surrounding brucite using dislocation density-flow stress relationship (de Bresser, 1996)





Exponential stress decay away from brucite-calcite interface (calculated in area highlighted by dashed red box on the left)

De Bresser, J. H. P. (1996). *Journal of Geophysical Research: Solid Earth*, *101*(B10), 22189-22201.

Summary and conclusion

- We derived a mathematical model, which can describe 2D viscous compressible deformation coupled to hydro-chemical (de)hydration reactions.
- The pseudo-transient finite difference code can reproduce fundamental results for mechanically weak inclusions and fluid pressure diffusion across reaction boundaries. The code is suitable to numerically model hydro-mechanical-chemical processes during (de)hydration reactions.
- In deforming and mechanically heterogeneous systems, total pressure and fluid pressure are different, and fluid and solid velocities are different. Hence, mechanical deformation impacts (de)hydration reactions.