Pore-scale modeling of oil-shale pyrolysis with CFD-DEM method

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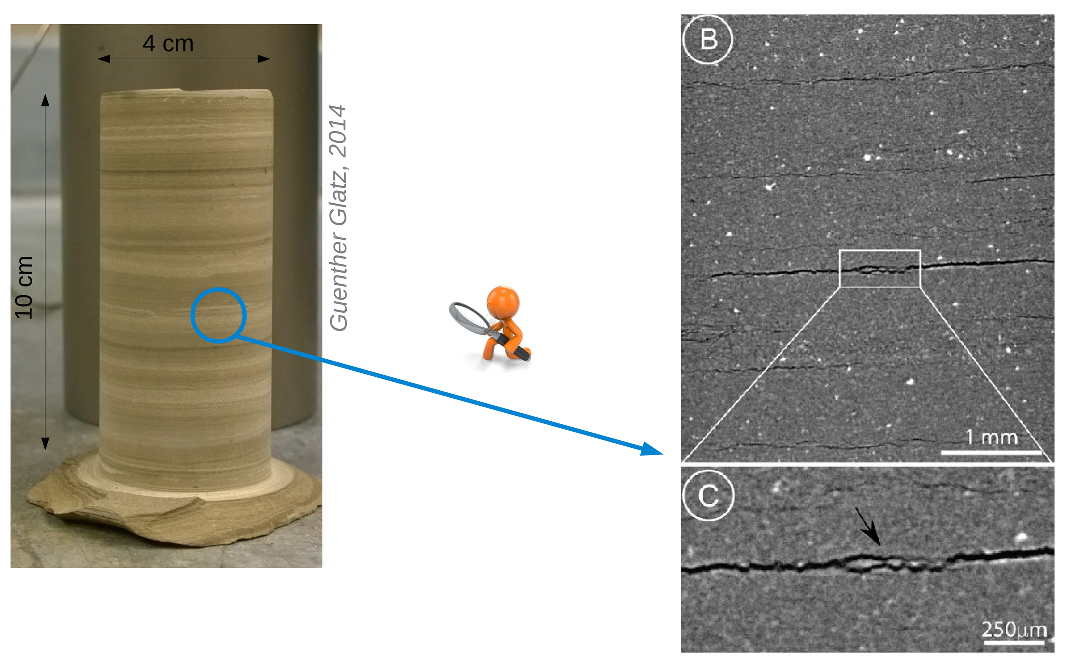
Introduction

Deposits of oil shale occur around the world and the estimates range from 4.8 to 5 trillion barrels of oil in place. Oil shale is a compact (very low permeability, very low porosity), laminated rock containing an organic matter called kerogen. The in-situ upgrading process uses heat to decompose the solid kerogen through a series of chemical reactions (the pyrolysis) into liquid and gas hydrocarbons. During the heat-up stage some micro-cracks will propagate wherein the mixture will flow.



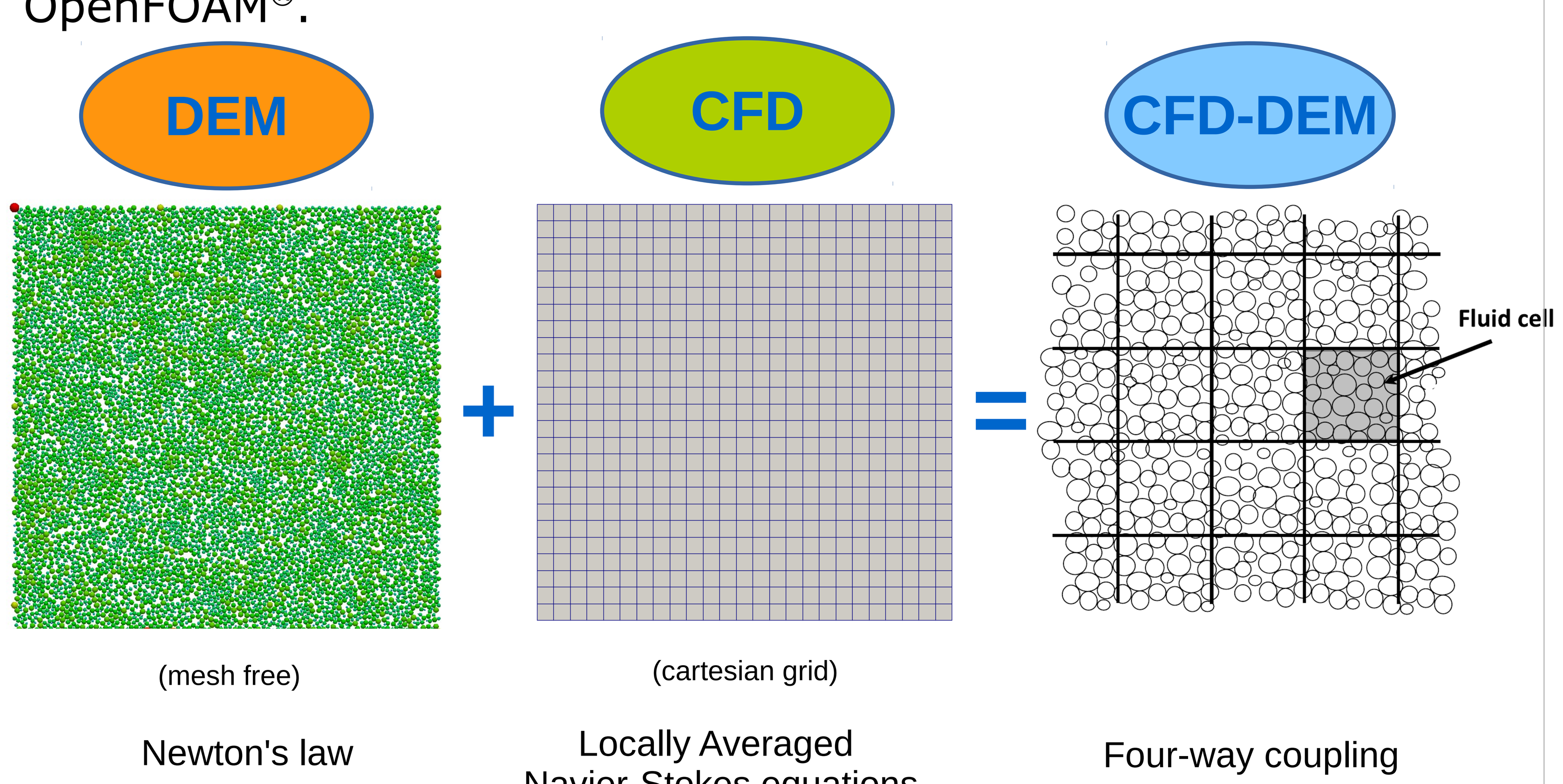
There are different origins to this creation of porosity:

- At high temperature, the kerogen starts to transform into volatile matter (pyrolysis),
- Fracturing due to the temperature induced brittle behavior of the solid,
- Fracturing due to the excessive pore-pressure.

We want to represent explicitly the cracks propagation and the mixture flowing through the generated micro-fractures.

CFD-DEM principle

To better understand the underlying physics of the in-situ oil shale pyrolysis, we propose to simulate the phenomenon at pore-scale using a CFD-DEM approach and the finite volume platform OpenFOAM®.

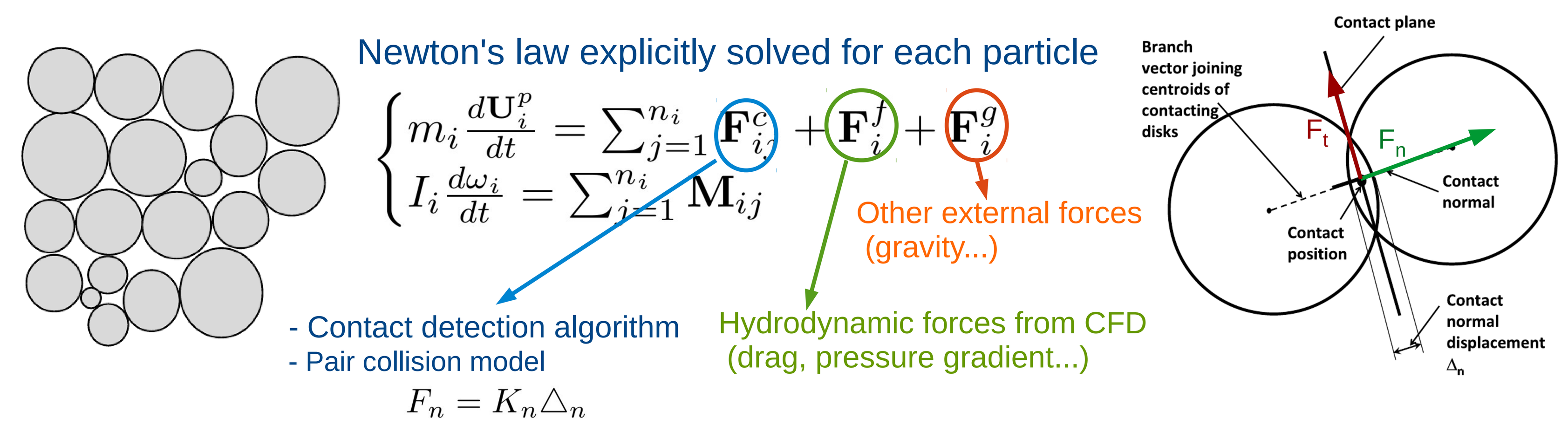


Requirements

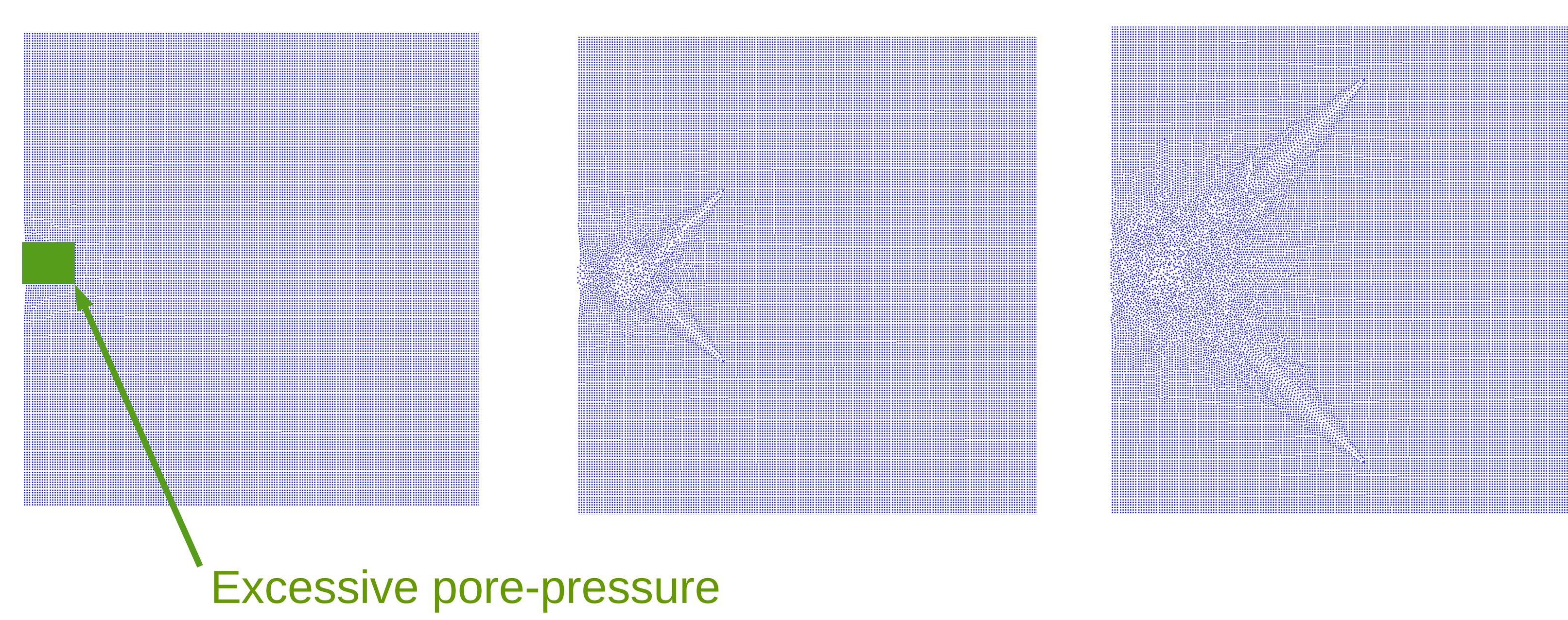
- Good initial packing of the particulate discrete elements
- Cell volume >> particle volume

The Discrete Element Method

In this method, the solid phase is represented by a cloud of solid particles in contact with each other. These particulate discrete elements evolve solving Newton's law accounting for inter-particles forces and the fluid interaction forces acting on each particle like the fluid pressure gradient.



Simulation example



- 80 000 identical particulate elements
- Regular packing, constrained at the domain boundaries
- No cohesion force

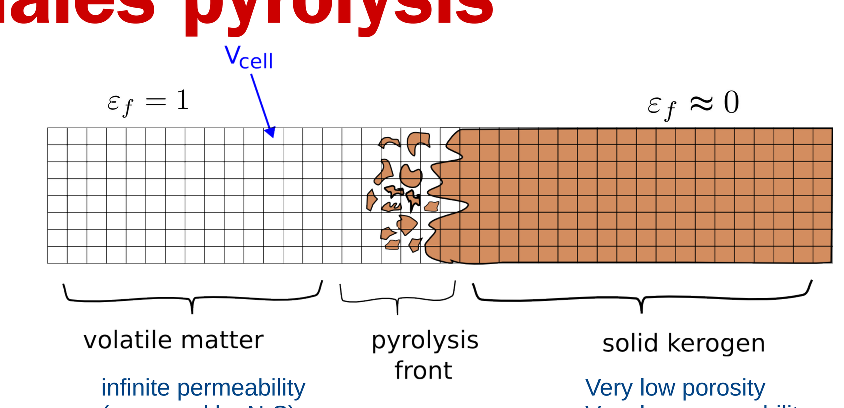
A CFD model for oil shales pyrolysis

$$\frac{\partial \varepsilon_k \rho_k}{\partial t} = -\dot{m},$$

$$\frac{\partial \varepsilon_f \rho_f}{\partial t} + \nabla.(\varepsilon_f \rho_f \mathbf{u}_f) = \dot{m},$$

$$\frac{\partial \varepsilon_f \rho_f \mathbf{u}_f}{\partial t} + \nabla.(\varepsilon_f \rho_f \mathbf{u}_f \mathbf{u}_f) = -\varepsilon_f \nabla p_f + \varepsilon_f \mu_f \nabla^2 \mathbf{u}_f - \mu_f k^{-1} \varepsilon_f^2 \mathbf{u}_f$$

$$\rho C_p \frac{\partial T}{\partial t} + \varepsilon_f \rho_f C_{p_f} \mathbf{u}_f.\nabla T = \nabla.(\lambda \nabla T) - \Delta H_{pyr} \frac{\partial \rho_k \varepsilon_k}{\partial t}$$

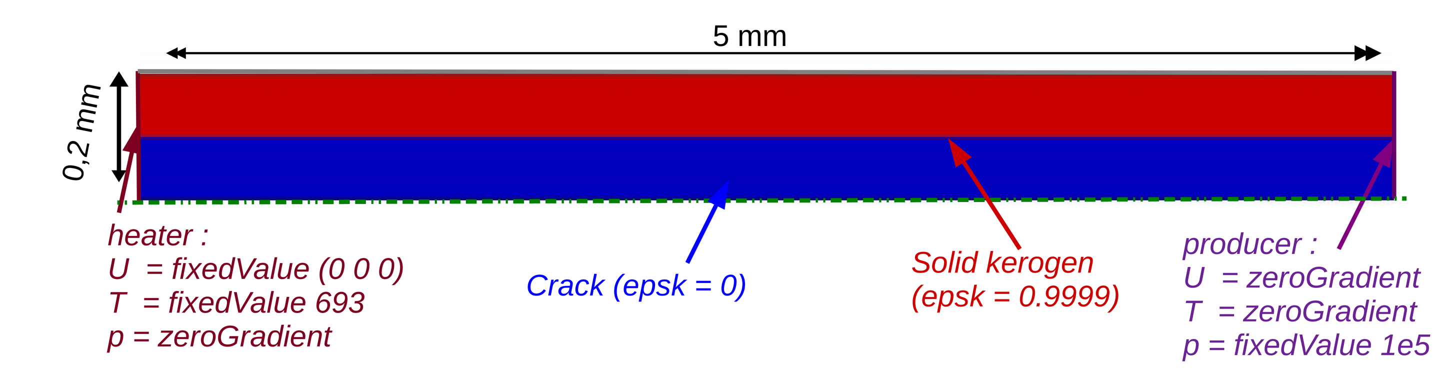


$$\dot{m} = A \exp\left(-\frac{E_a}{RT}\right)\varepsilon_k \rho_k \qquad \rho_f = \frac{M_f p_f}{RT} \qquad k^{-1} = k_0^{-1}\frac{(1-\varepsilon_f)^3}{\varepsilon_f^2}$$

This model allows to use the same formulation on a fixed grid in both the fractured area and the solid kerogen.

Some results: kerogen with an existing crack

The CFD model can be used independently of the DEM to simulate the oil shale decomposition when the mapping of the solid is known. Here we simulate the kerogen transformation in presence of an existing crack.

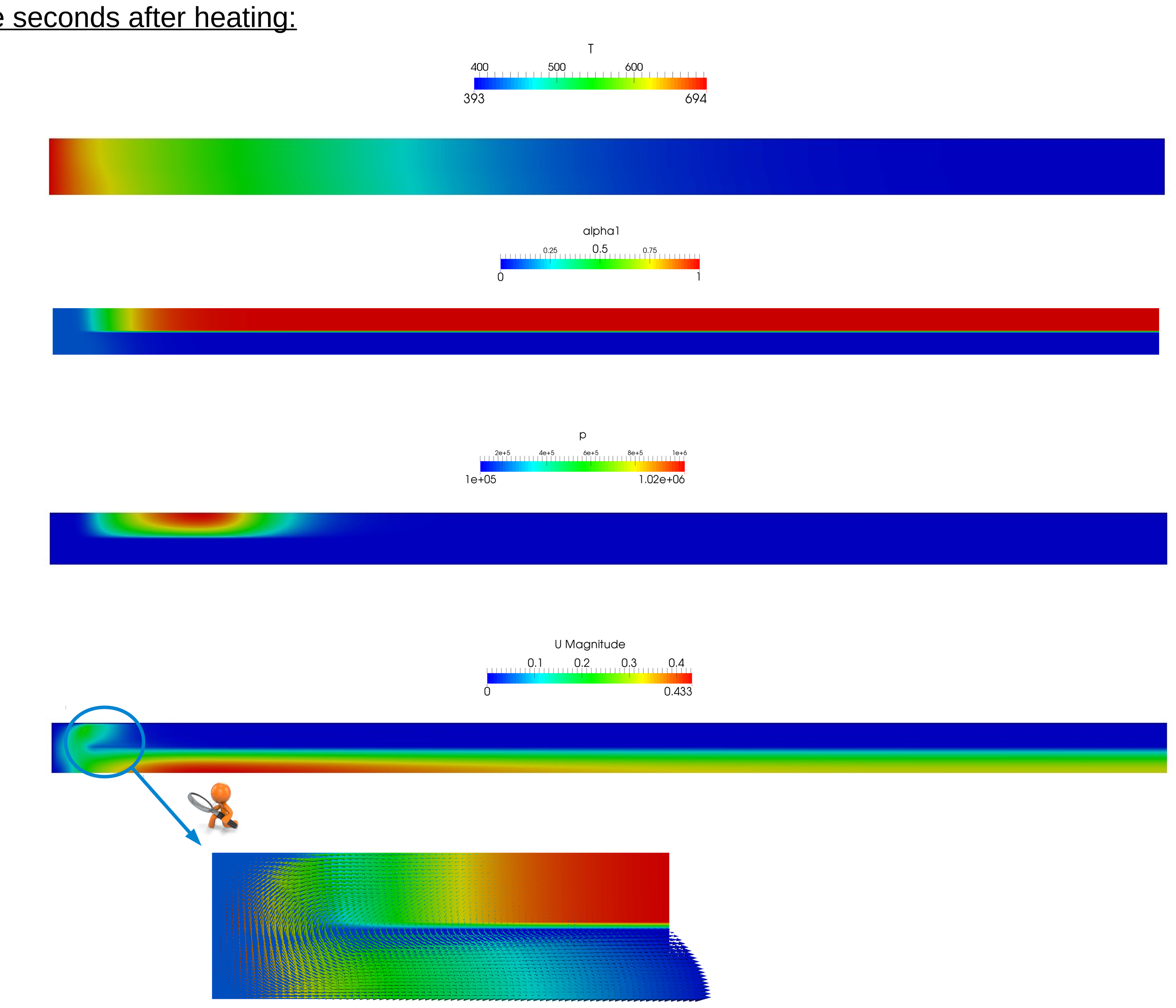


Mesh: 200 x 20 hexa

Initially, *U = 0 m/s ; T = 393 K ; p = 1e5 Pa ; epsk = 0.99999*

ρ_k	C_{p_k}	C_{p_f}	μ_f	λ_f	λ_k	M_f	E_a	A	ΔH_{pyr}	k_0
(kg/m^3)	(J/kg/K)	(J/kg/K)	(Pa.s)	(W/m/K)	(W/m/K)	(kg/kmol)	(J/kmol)	(s^{-1})	(J/kg)	(m^2)
1500	2700	1800	10^{-5}	0.07	1	20	160x10^6	3x10^{13}	375x10^3	10^{-16}

Some seconds after heating:



Conclusion and Future Work

- The CFD-DEM method seems promising to simulate fracturing due to excessive pressure.
- The CFD model developed for oil-shale pyrolysis can be used independently when the mapping of the void-space is known.
- Further work is needed to properly calibrate the DEM simulations.
- Future work will focus on the improvement of the CFD model (two-phase flow, more accurate kinetic model...)