NUMERICAL MODELLING OF CO_2-STORAGE

Ekkehard Holzbecher

German University of Technology in Oman, PO Box 1816,
130 Muscat, Sultanate of Oman

COMSOL CONFERENCE
2016 MUNICH

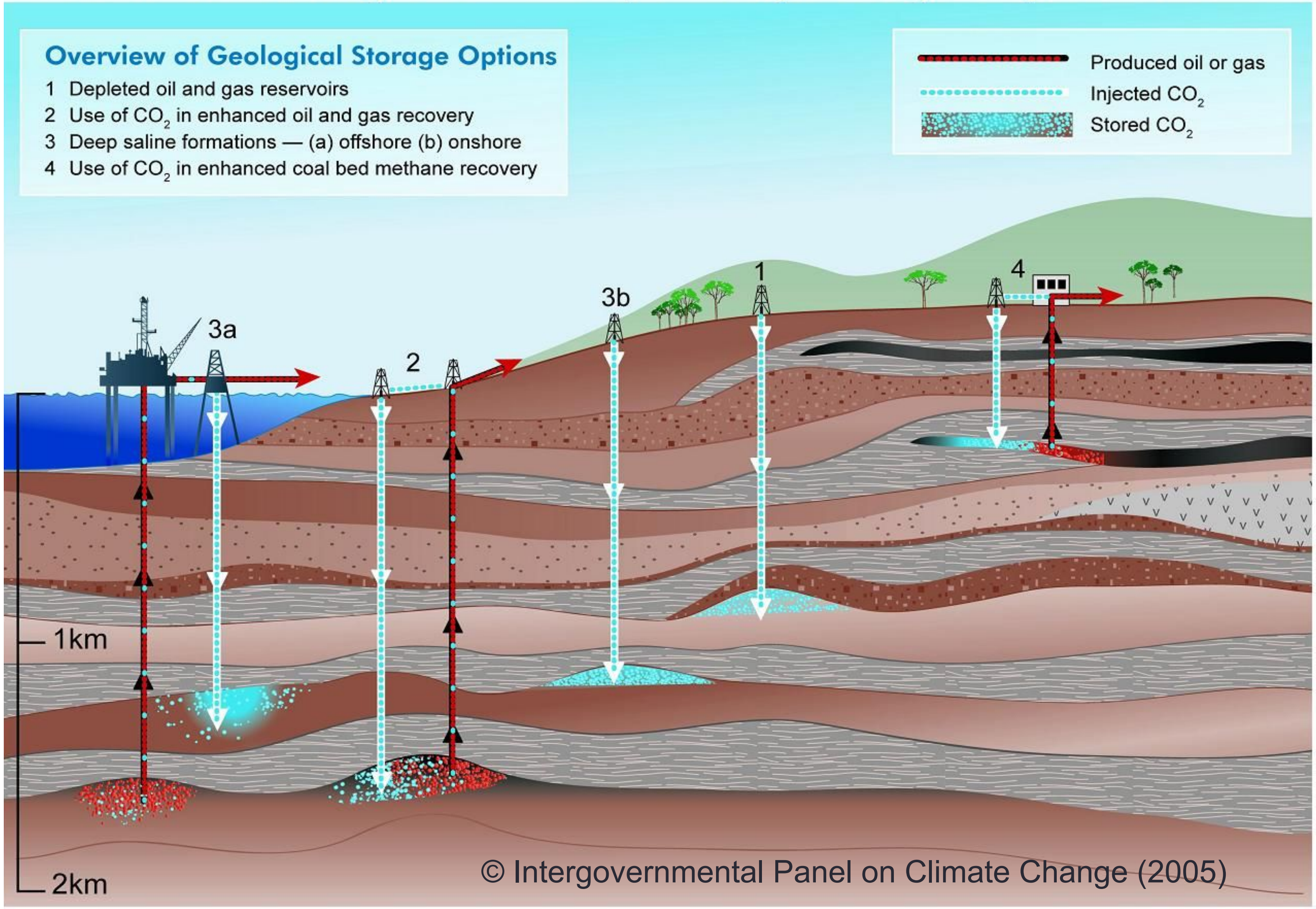
RWTH AACHEN
GUtech
الجامعة الألمانية للتكنولوجيا في عمان
German University of Technology in Oman

CO_2 Storage

Storage of CO_2 in the sub-surface is seen as a technology that can contribute to the generally accepted goal of a decarbonized society (climate treaty Paris 2015).

Concerning the practical application of CO_2 storage many questions are still unanswered. In the most favoured scenario CO_2 in supercritical state is pressed into a deep geological formation. Within the permeable layer CO_2 will come to overlie brine and will start to dissolve into the deeper part by diffusion and convection.

Geological Storage Options



Numerical Modelling

For the development of the storage technology real field experiments are hardly feasible. Therefore current studies utilize the capabilities of numerical modelling, to explore the basic behaviour of the underground system. Highly dynamic convective motions are induced by CO_2 entering at the top interface of a geological formation. The details of the flow patterns depend heavily on disturbances of physical parameters and also on numerical features, like mesh refinement.

Differential Equations (2D)

Flow (1) for streamfunction Ψ

Transport (2) for salinity c

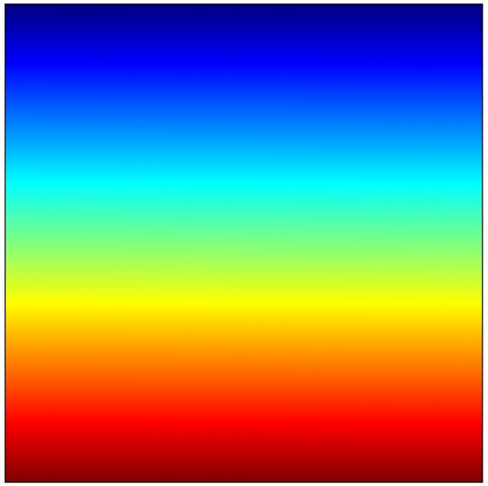
$$\frac{\partial}{\partial x}\left(\frac{\partial \Psi}{\partial x}\right)+\frac{\partial}{\partial z}\left(\frac{\partial \Psi}{\partial z}\right)=-Ra\frac{\partial c}{\partial x} \quad \text{with} \quad Ra=\frac{gk\Delta\rho H}{\mu D} \qquad (1)$$

$$\frac{\partial c}{\partial t}=\nabla\cdot(\nabla c-\mathbf{v}c) \quad \text{with} \quad v_x=-\frac{\partial \Psi}{\partial z} \quad \text{and} \quad v_z=\frac{\partial \Psi}{\partial x} \qquad (2)$$

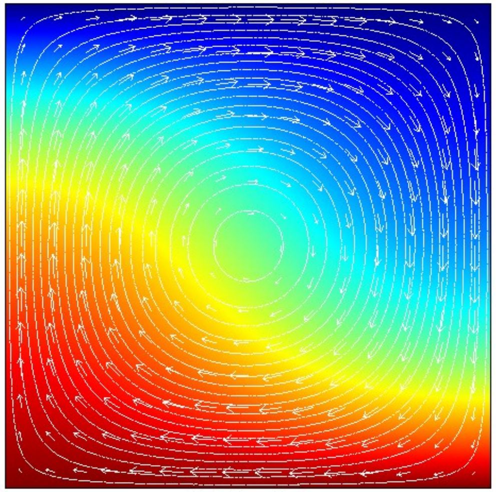
Rayleigh number Ra

Porous Media Convection

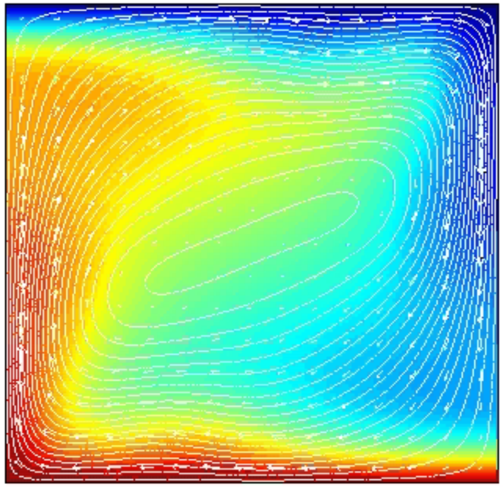
Conduction
(Ra=30)



Steady Convection
(Ra=50)

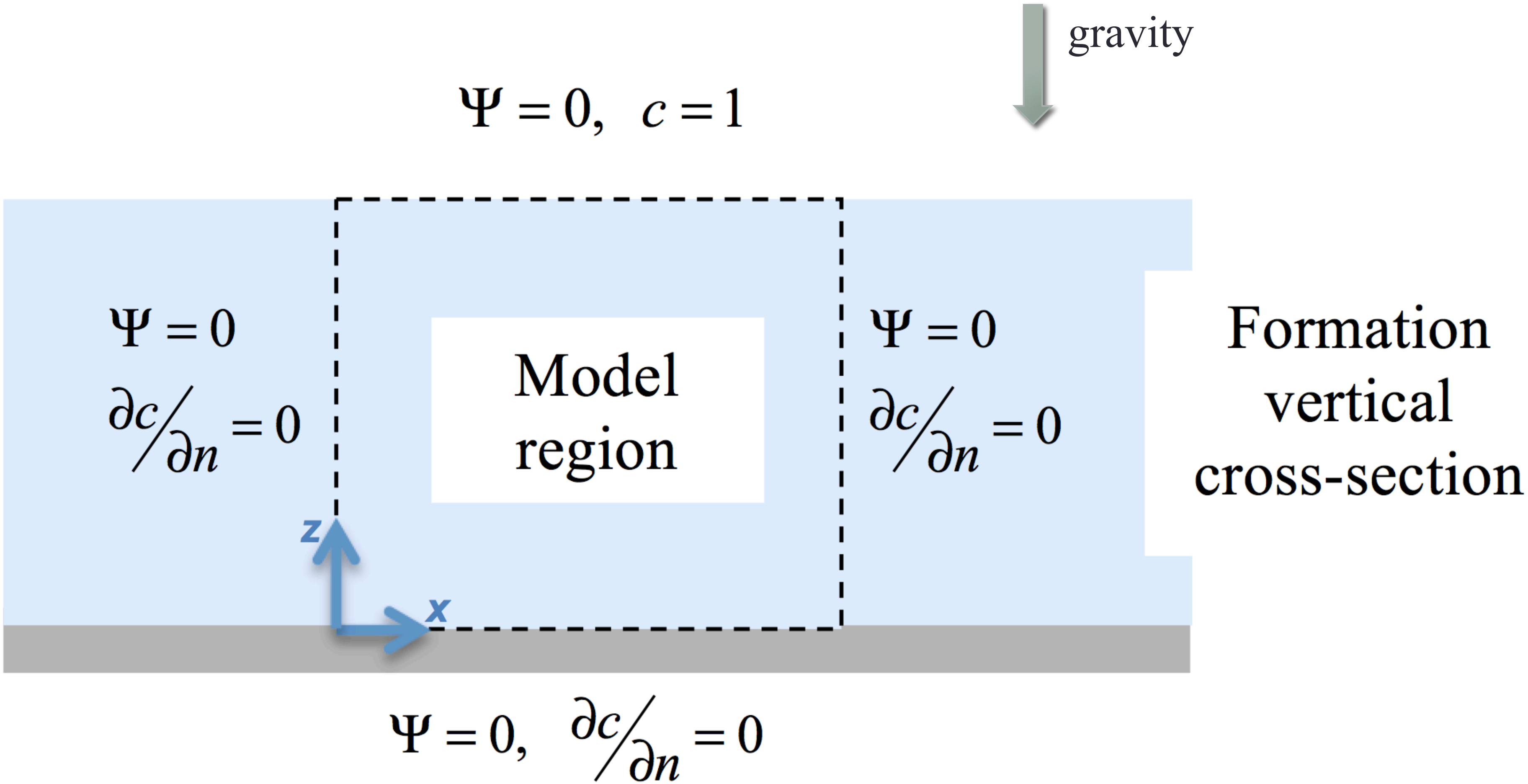


Oscillatory Convection
(Ra=400)



Ra = Porous medium Rayleigh number [1]

Model Region (2D) & Boundary Conditions



Parameters

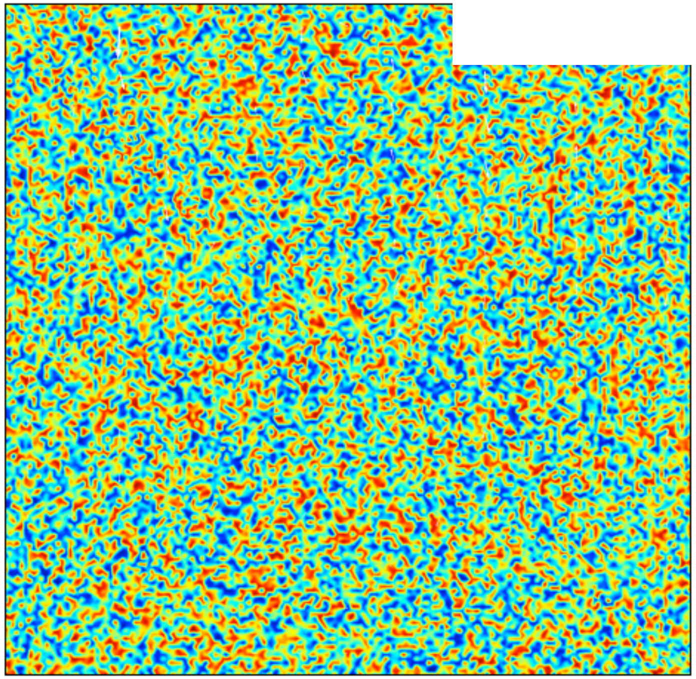
Parameter	**Value [Unit]**
Saturated CO_2 mass fraction	0.0493
Viscosity μ	$0.5947 \cdot 10^{-3}$ Pa·s
Brine density	994.56 kg/m^3
Density difference $\Delta\rho$	10.45 kg/m^3
Molecular diffusivity D	$2 \cdot 10^{-9}$ m^2/s
Reference permeability k_{ref}	$5 \cdot 10^{-13}$ m^2

Reference case parameters (partially taken from: Pau *et al*. 2010)

Ra = 5000

Meshes

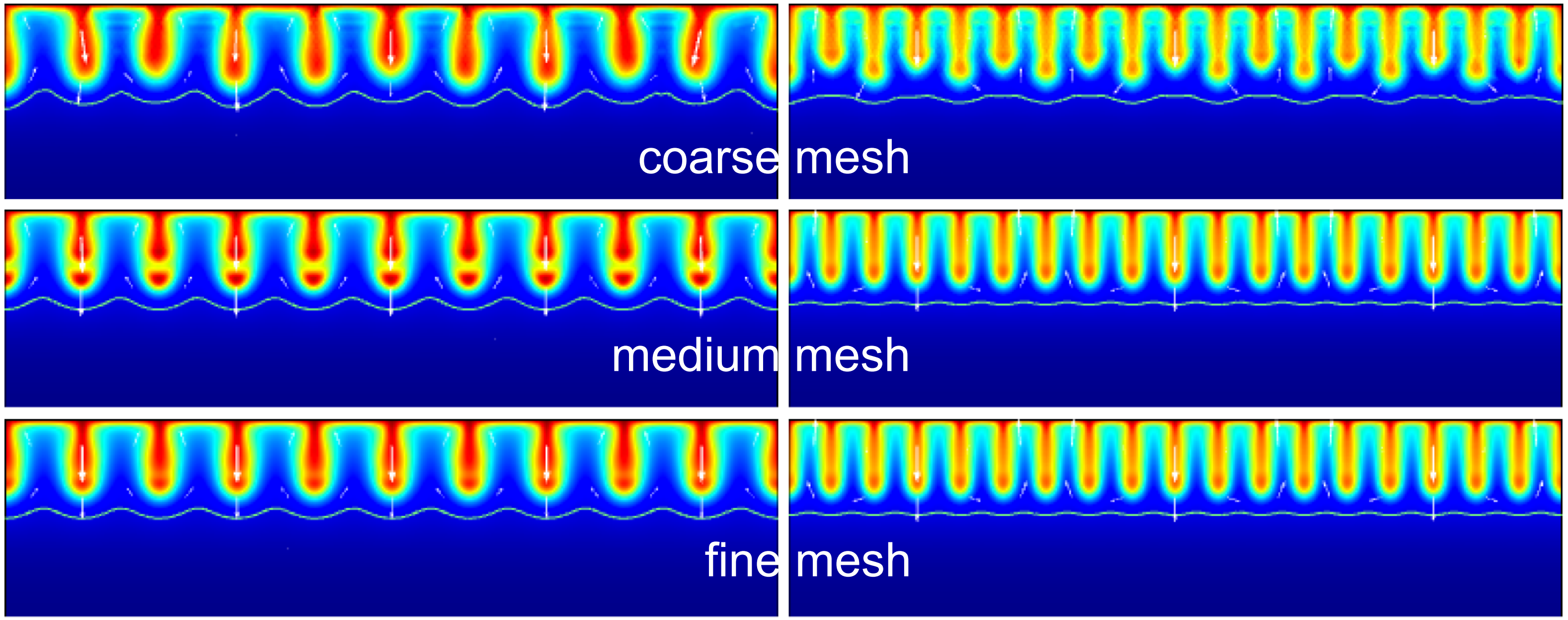
Mesh	No. of elements	Degrees of freedom (DOF)
Coarse	1856	17030
Medium	6282	57140
Fine	24912	225410



Example permeability random field distribution produced for the coarse mesh

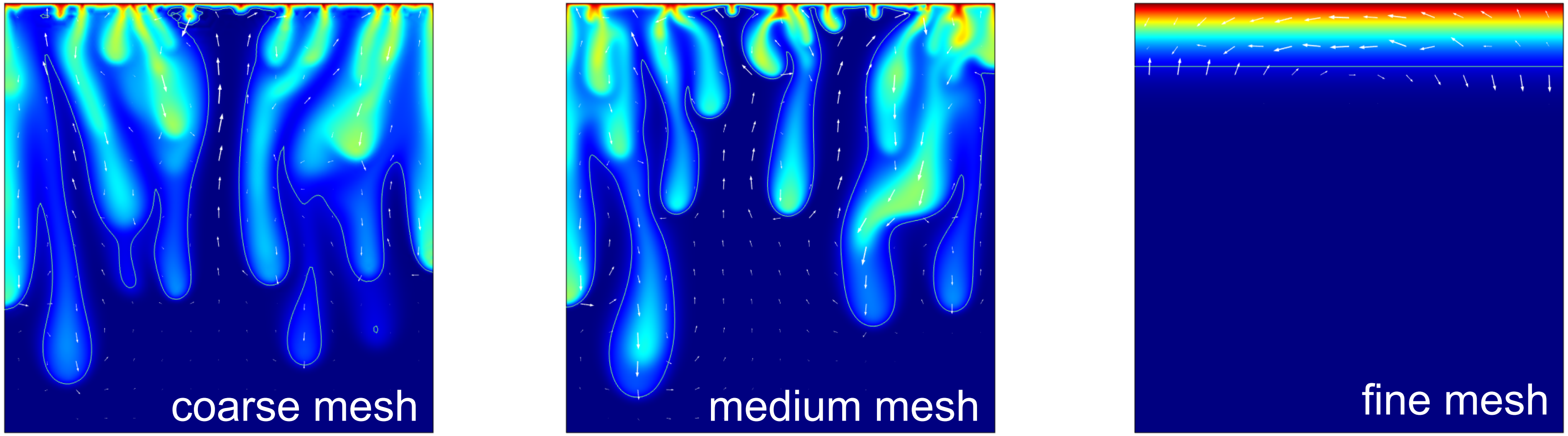
Onset of Convection

Near upper boundary,
red: high CO_2 content, blue: low CO_2 content

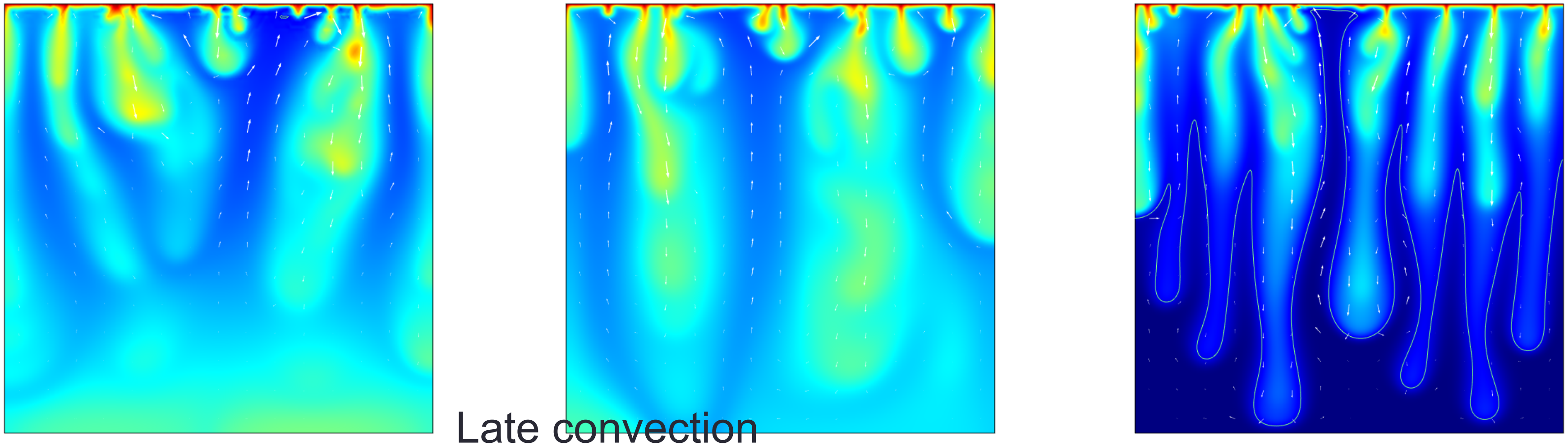


Created with oscillatory initial disturbance at the boundary
left: 10 periods, right: 18 periods

Convection Patterns

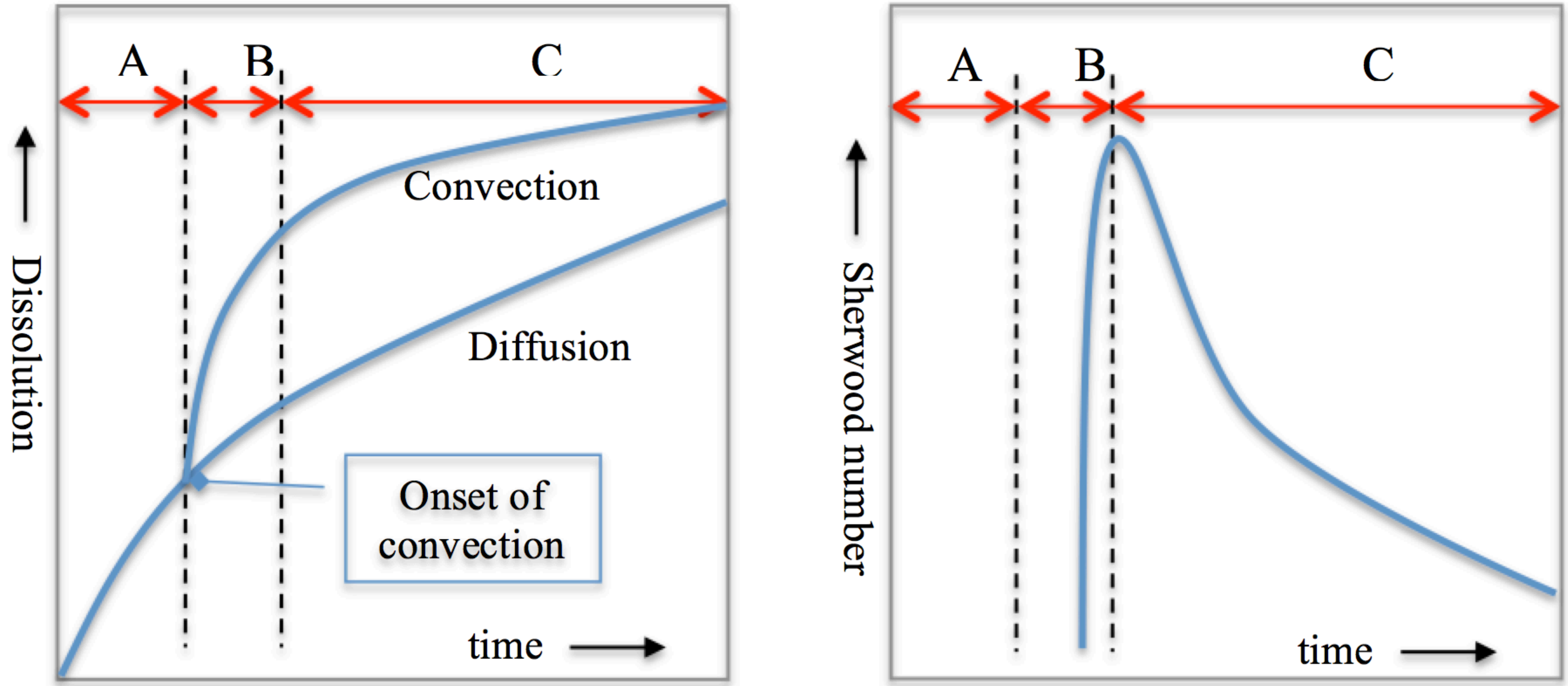


Early convection



Late convection

Mass Transfer

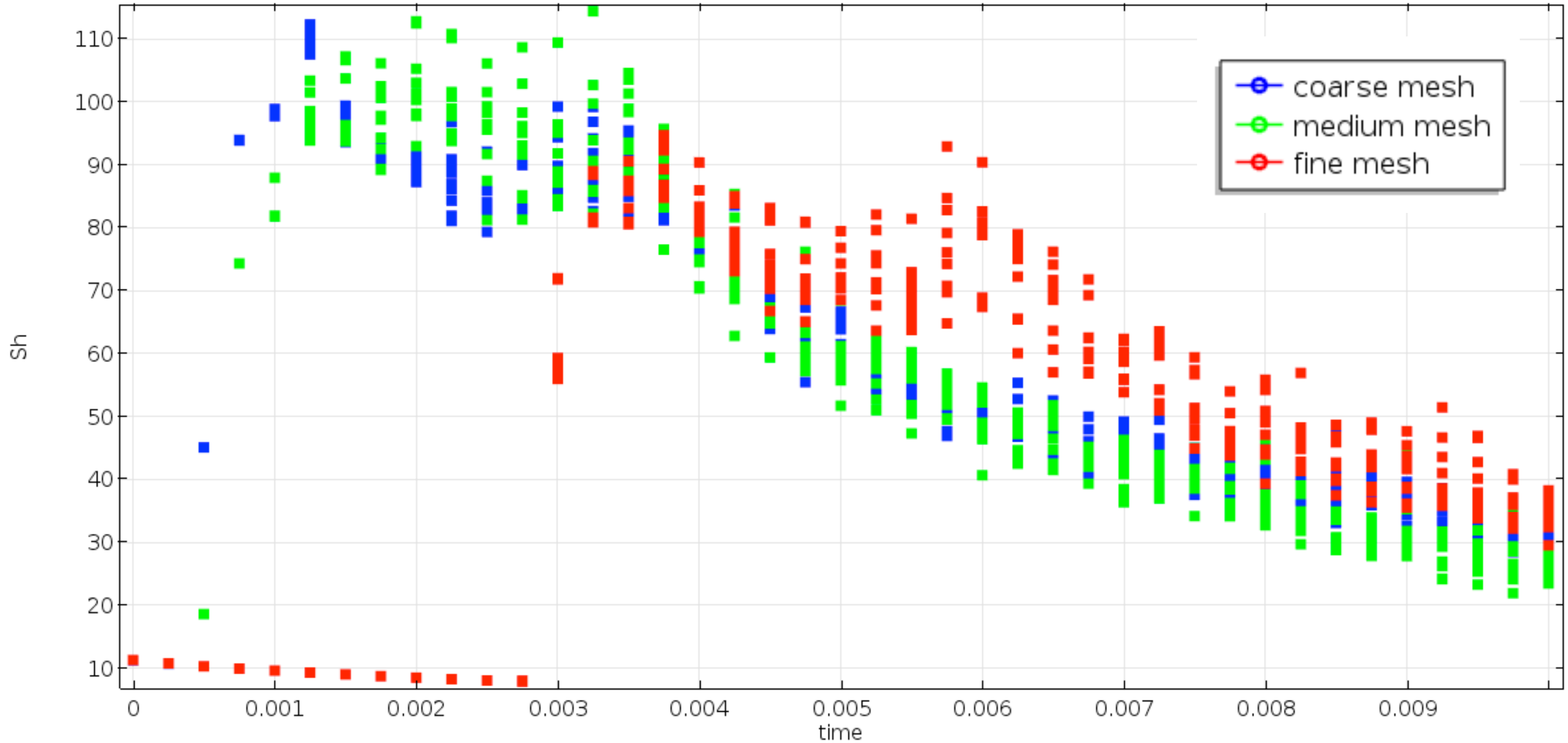


(A) diffusion, (B) early convection, (C) late convection

Sherwood number *Sh*

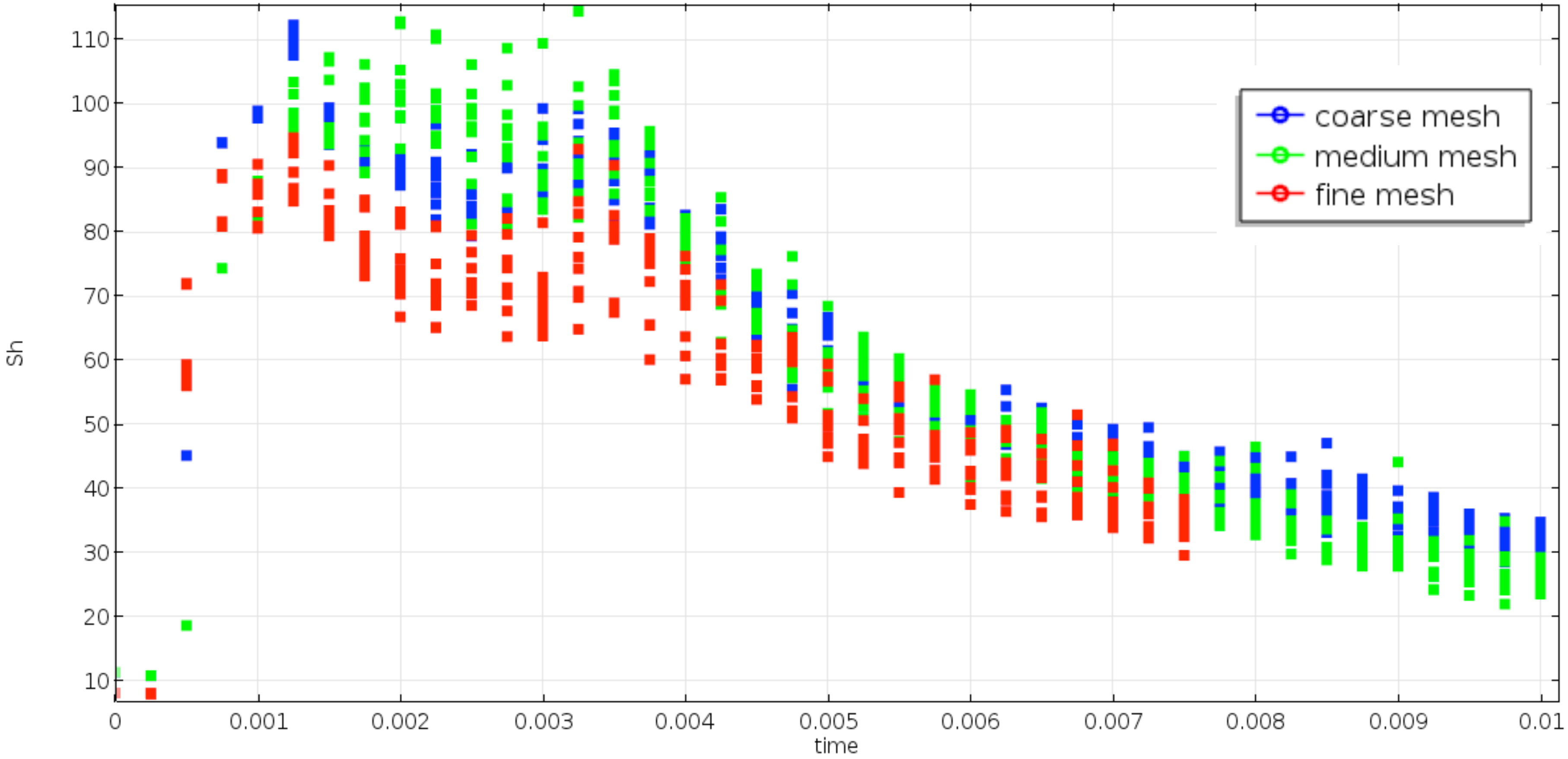
$$Sh = \int_0^1 \frac{\partial c}{\partial z} dx$$

Mass Transfer Results (1)



from 30 different random field realisations for permeability

Mass Transfer Results (2)



from 30 different random field realisations, fine mesh results shifted

Conclusions (1)

- The system is highly dynamic, i.e. the output of the simulations depends highly on slight disturbances of
  - Initial conditions
  - Boundary conditions
  - Heterogeneities
- Thus the development of a single simulation cannot be used for predictive purposes
- A series of scenarios, with different physical and numerical parameters has to be simulated for intercomparison

Conclusions (2)

- Time of onset of convective motions depends on mesh refinement
- Early convection phase does not show a single mass transfer peak
- The duration of the early convection phase is independent of mesh and random field
- In late convection with decreasing mass transfer, also the fluctuations of mass transfer decrease

References

- Farajzadeh, R., Salimi, H., Zitha, P., Bruining, H., Numerical simulation of density-driven natural convection in porous media with application for CO_2 injection projects. *Intern. Journal of Heat and Mass Transfer* 2007. 50: 5054–5064
- Hassanzadeh, H., Pooladi-Darvish, M., Keith, D- W., Scaling behavior of convective mixing with application to geological storage of CO_2, *AICHE Journal* 2007. 53(5): 1121-1131
- Holzbecher, E., *Modelling Density-Driven Flow in Porous Media*, Springer Publ., Heidelberg, 1998
- Holzbecher, E., The Henry-saltwater intrusion benchmark – alternatives in multiphysics formulations and solution strategies, *Int. Journal of Multiphysics* Vol. 10, No. 1, 21-41
- Holzbecher, E., Modeling pathways and stages of CO_2 storage, *Int. Journal of Multiphysics*, accepted

Further work (possible)

The modelling approach using COMSOL Multiphysics can be extended to consider further effects of

- increased disturbances or heterogeneities
- complex geometries
- consideration of anisotropies of
  - permeabilities
  - diffusivities
- consideration of dispersion
- 3D convective patterns
- temperature dependencies
- thermal coupling
- geomechanical coupling