COMSOL CONFERENCE
BANGALORE, 2012

Miscible Viscous Fingering: Application in Chromatographic Columns and Aquifers

Satyajit Pramanik, G. L. Kulukuru, and Manoranjan Mishra

Indian Institute of Technology Ropar,
Rupnagar – 140001, Punjab, India

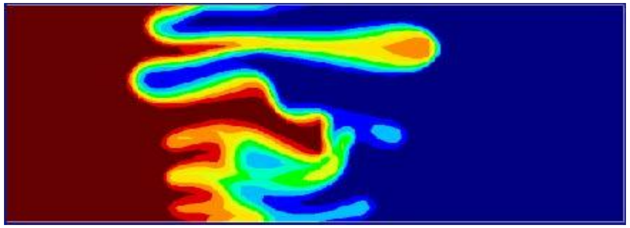
Viscous fingering instability

- The viscous fingering instability is a hydrodynamic instability that occurs when a less viscous fluid displaces a more viscous fluid in a porous medium.

- The interface between the two fluids is unstable and develops "fingers" of the more mobile solution that invade the less mobile one.

Viscous fingering instability

Rectilinear displacement



Radial displacement

Fingering occurs in both

- immiscible solutions in which case surface tension must be taken into account
- miscible solutions for which dispersion plays a key role

Here we focus on miscible solutions in rectilinear displacements

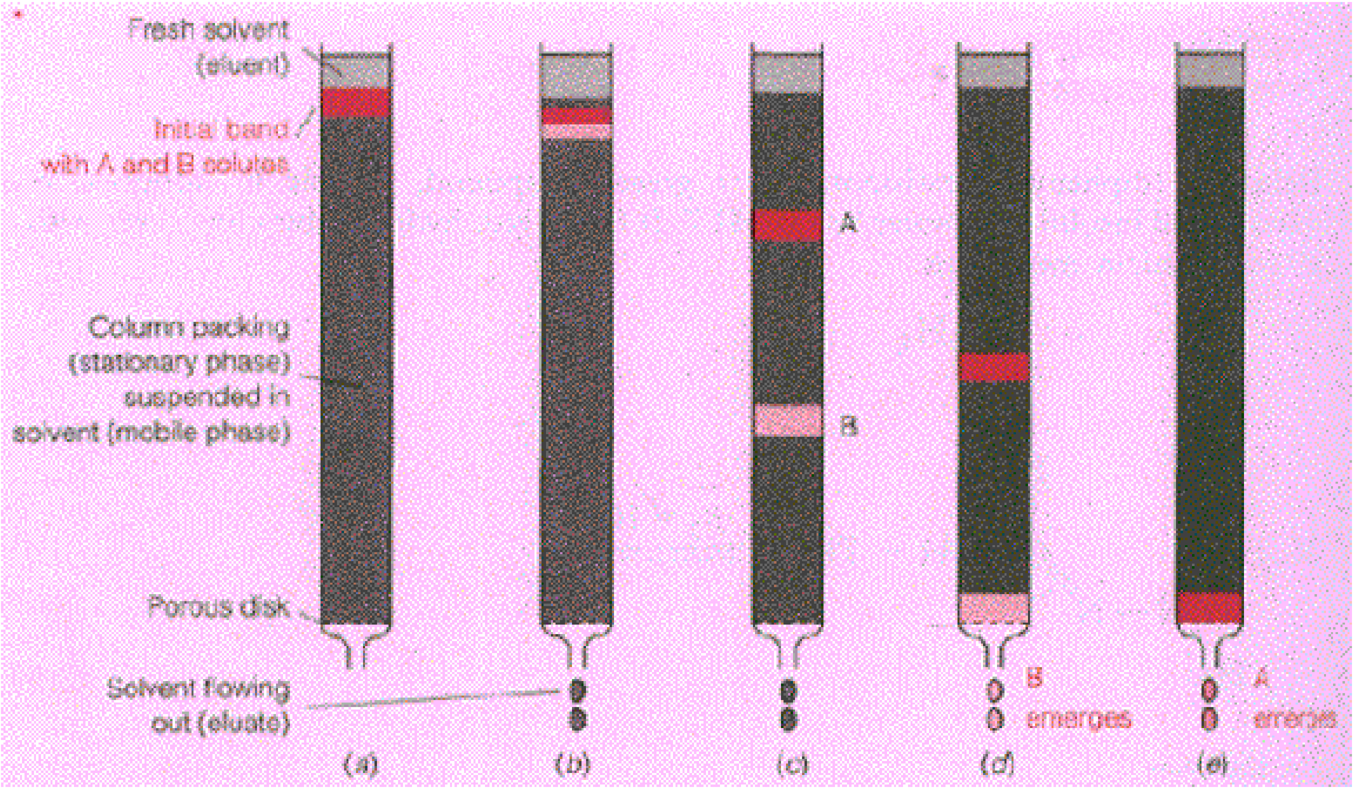
Nevertheless, two main applications where viscous fingering is important are not appropriate in the semi-infinite domain:

1. Chromatographic separation
2. Dispersion of pollutants in aquifers

Each of them involve displacement of a <u>fluid sample of finite extent</u> by another carrying fluid.

Chromatography

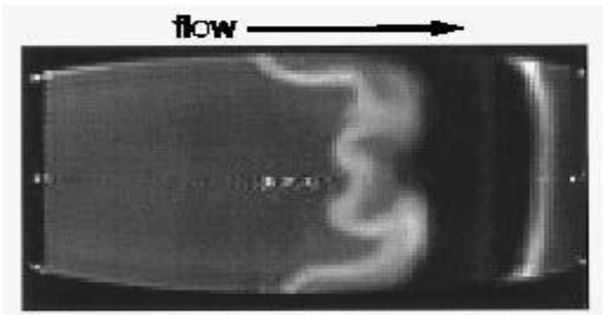
- A mechanism, used to separate or to analyze the chemical components of a given mixture by passing it through a porous medium.



- This separates the analyte or solute to be measured from other molecules in the mixture and allows it to be isolated.

Evidence in chromatography

Magnetic resonance imaging

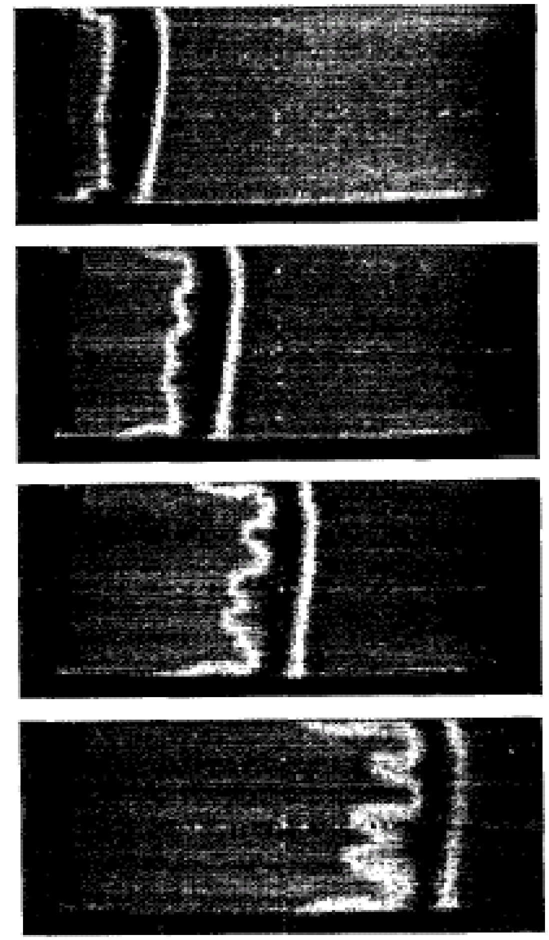


Fernandez et al., Biotechn. Progress, (1996)

A 5ml sample of 40% glycerol is displaced by water through a resin.

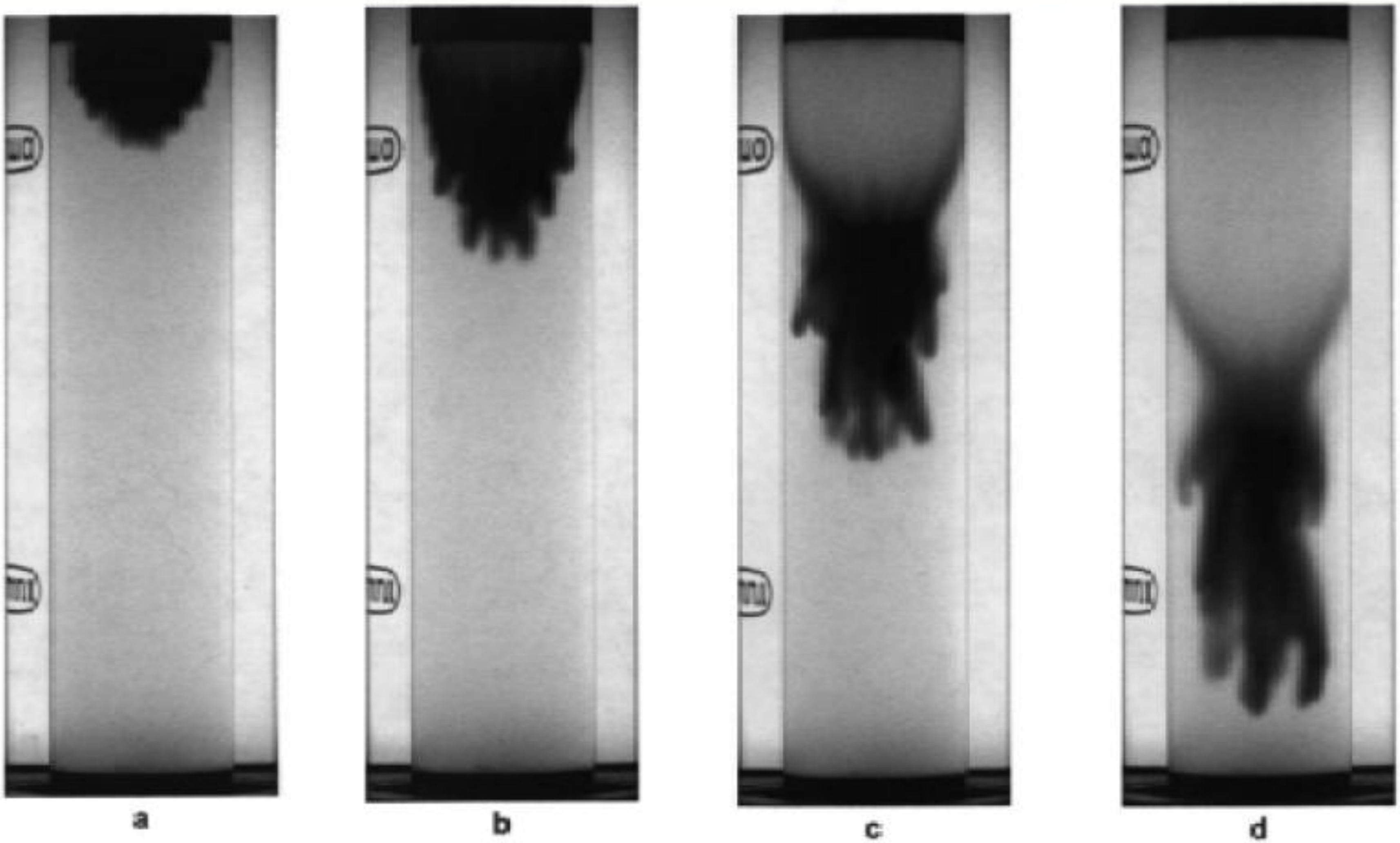
The inlet is at the left side.

The flow rate is 5 ml/min.



E.J. Fernandez *et al.*

Phys. Fluids, 7 (1995) 468

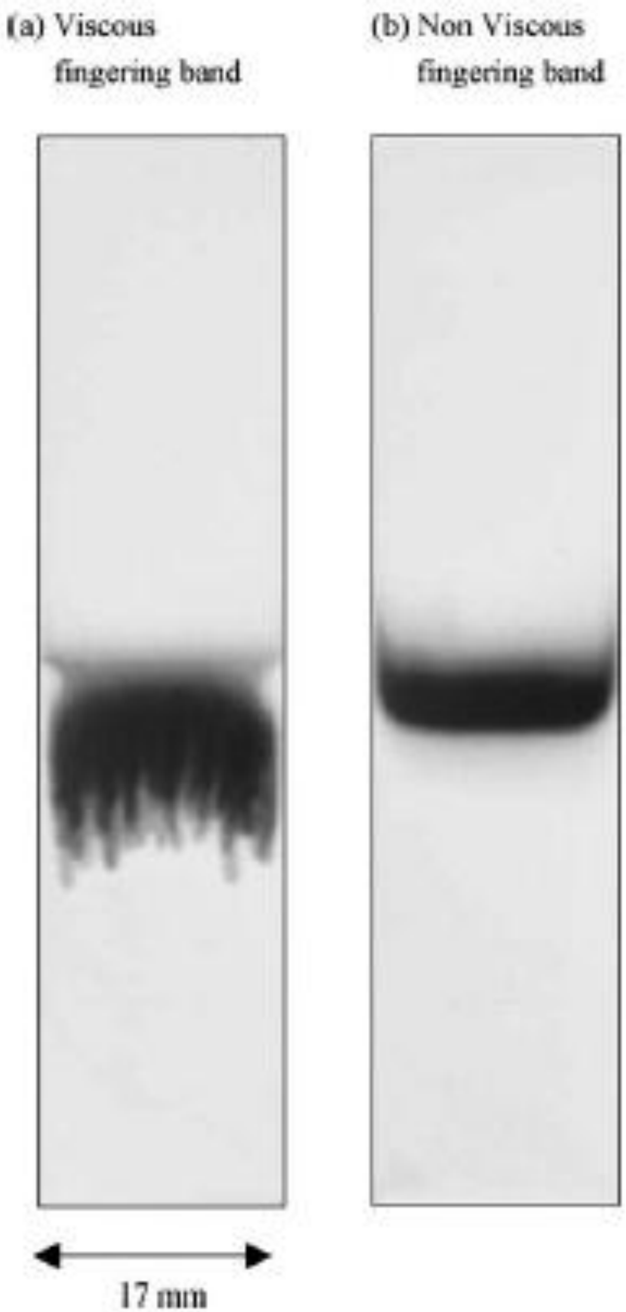


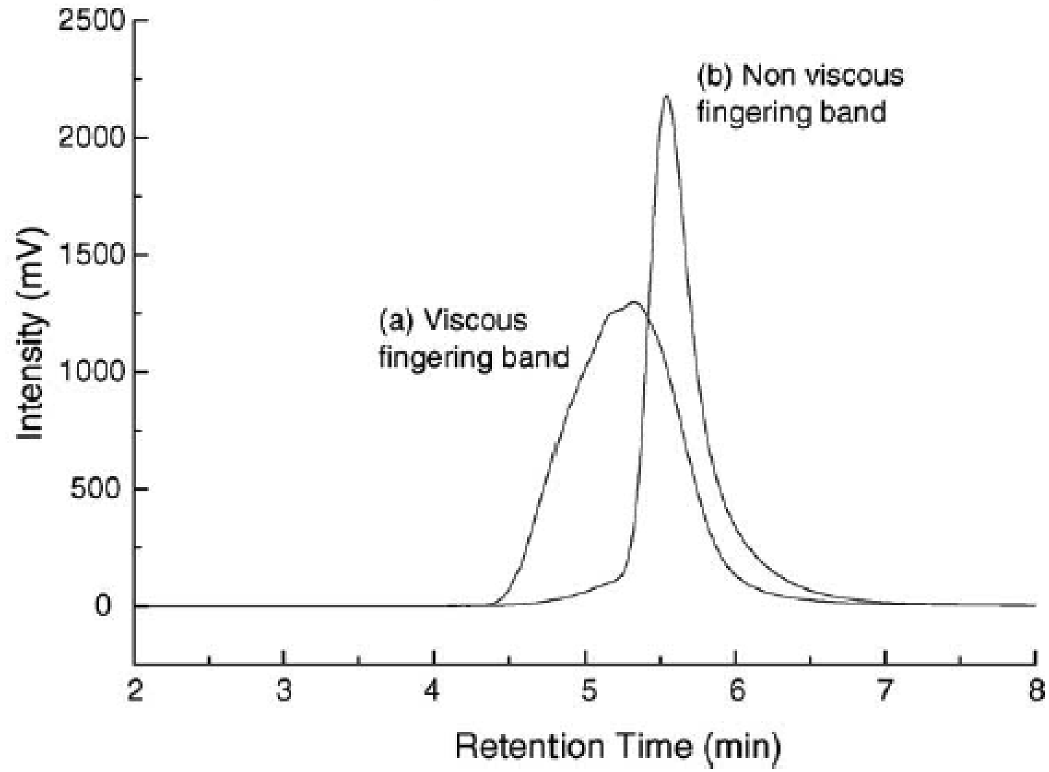
R.A. Shalliker et al. / J. Chromatog. A 865 (1999) 73–82

Fig. 6. Photographs of a 500 μl injection of a saturated iodine in pentane solution through the narrow (4.6 mm diameter) frit. Flow rate=1.5 ml/min. (a) t=30 s, (b) t=60 s, (c) t=120 s, and (d) t=210 s.

Visualization by matching of index of refraction
Shalliker et al. (1999).

Mayfield et al. (2005)

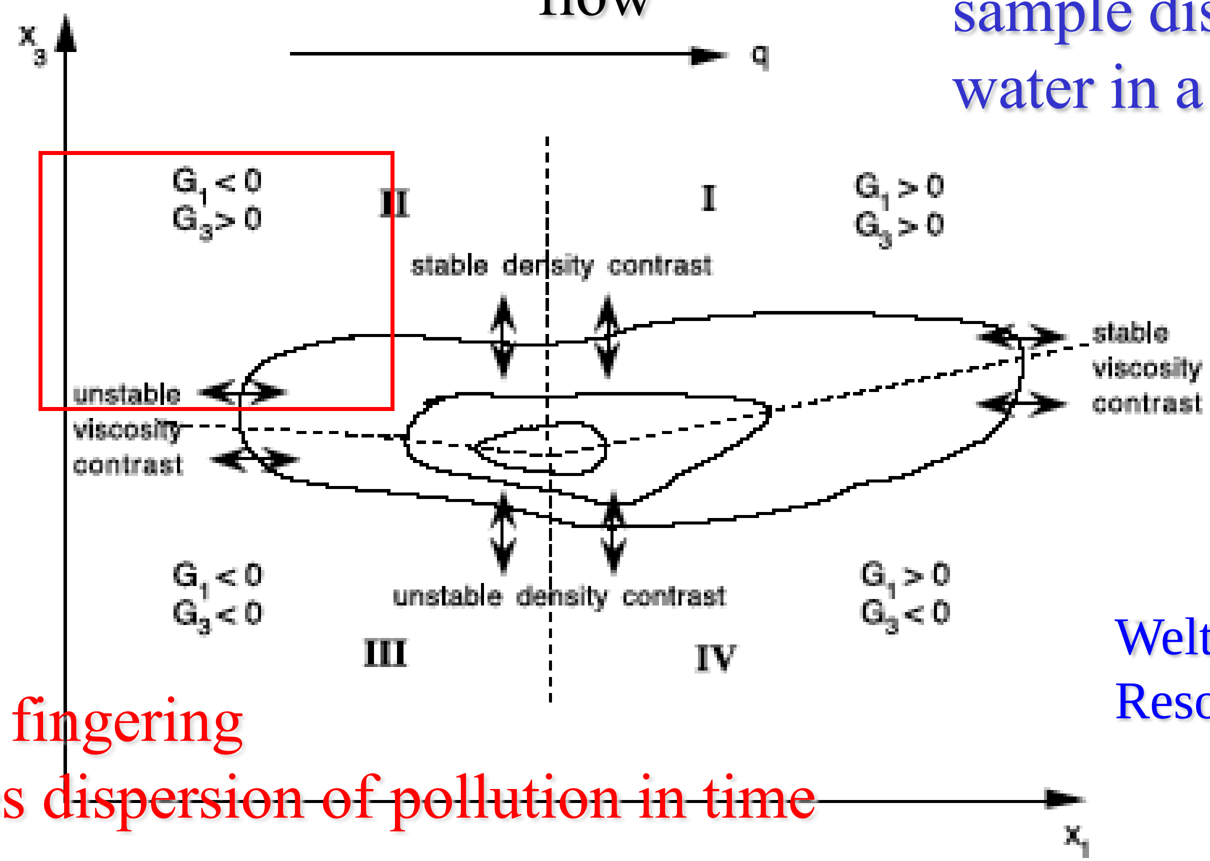




In chromatography, viscous fingering distorts the sample and increases peak broadening:
<u>dramatic for the separation technique</u>!!!

Dispersion of pollutants in aquifers

Heavy and viscous sample displaced by water in a porous medium

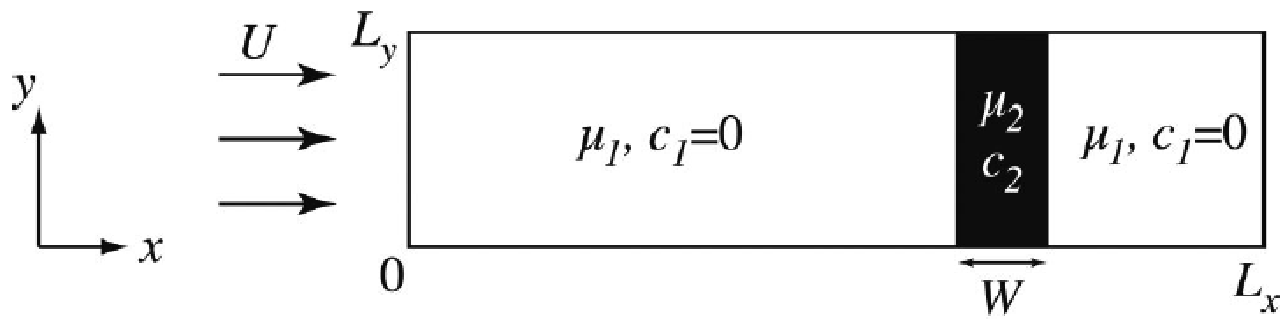


Viscous fingering enhances dispersion of pollution in time

Welty et al., Water Resources Res. (2003)

Figure 4. Schematic of hypothetical solute body with signs of concentration gradients indicated in each quadrant.

Theoretical model (two component)



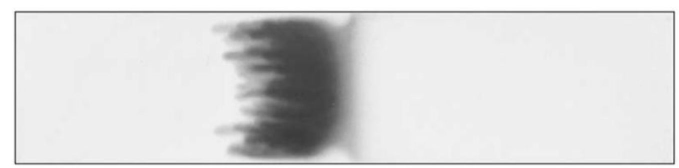
Model Equations

$$\underline{\nabla} \cdot \underline{u} = 0,$$

$$\underline{\nabla} p = -\frac{\mu(c)}{K} \underline{u}, \qquad \text{Darcy's law}$$

$$\frac{\partial c}{\partial t} + \underline{u} \cdot \underline{\nabla} c = D_x \frac{\partial^2 c}{\partial x^2} + D_y \frac{\partial^2 c}{\partial y^2},$$

$$m = m_1 e^{Rc}$$



$\underline{u}$: 2D velocity field

K: permeability

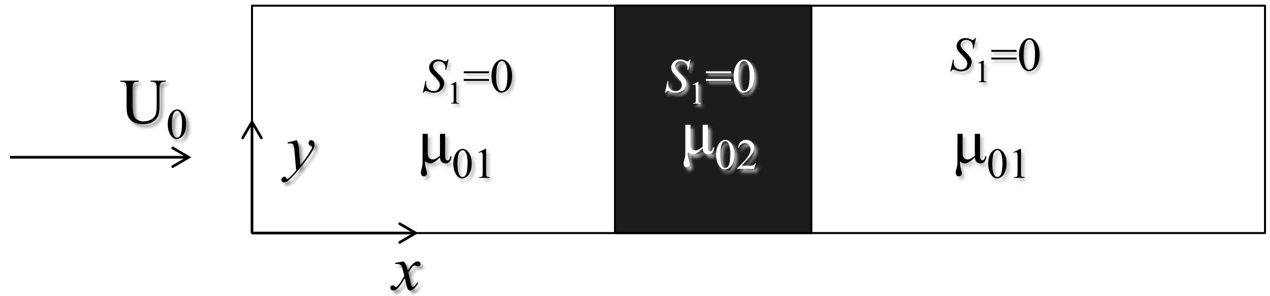
p: pressure

c: solute ruling the viscosity of the miscible fluids

D_x, D_y: axial and transverse dispersion coefficients

COMSOL Multiphysics model

Two-Phase Darcy's Law



$$\frac{\partial \epsilon_p \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0, \quad \mathbf{u} = -\frac{\mathbf{\kappa}}{\mu} \cdot \nabla p$$

$$\rho = s_1 \rho_1 + s_2 \rho_2, \quad \frac{1}{\mu} = s_1 \frac{\kappa_{r1}}{\mu_1} + s_2 \frac{\kappa_{r2}}{\mu_2}, \quad s_1 + s_2 = 1$$

$$\frac{\partial \epsilon_p c_1}{\partial t} + \nabla \cdot c_1 \mathbf{u} = \nabla \cdot D_c \nabla c_1, \quad c_1 = s_1 \rho_1$$

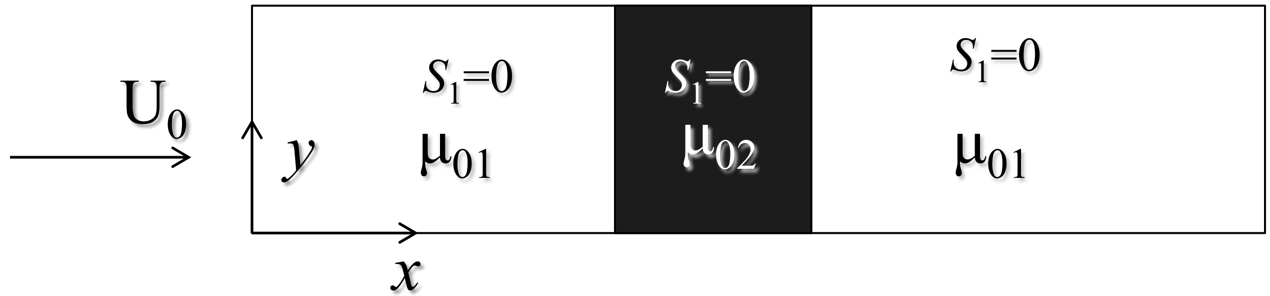
$$m_1 = m_2 = m_{01} e^{R s_1}$$

$\rho = \rho_1 = \rho_2$ = constant

ϵ_p, $\mathbf{\kappa}$ = constant

$\kappa_{r1} = \kappa_{r2} = 1$

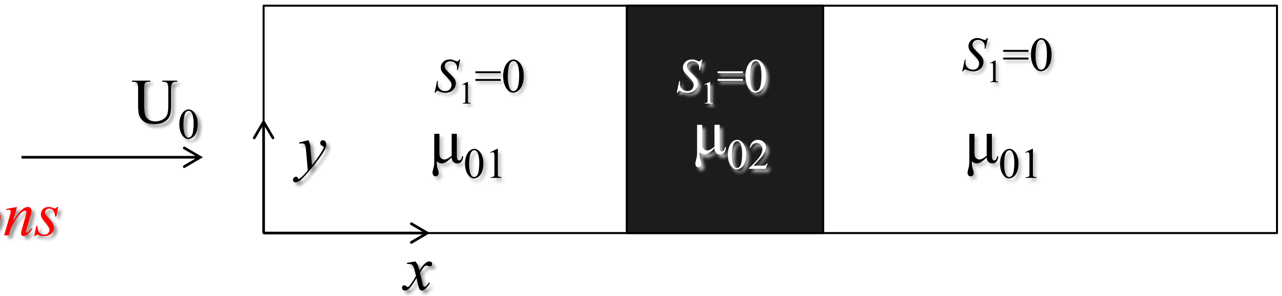
COMSOL Multiphysics model



Initial conditions

$$s_1(t=0)=\begin{cases} 0, & x < L_x/8 \\ 0.5(1+\xi f(x,y)), & x = L_x/8 \\ 1, & L_x/8 < x < L_x/8 + W \\ 0.5(1+\xi f(x,y)), & x = L_x/8 + W \\ 0, & x > L_x/8 + W \end{cases}$$

COMSOL Multiphysics model



Boundary conditions

$$-n \times r u = 0$$ *No Flux*

$$-n \cdot D_c \nabla c_1 = 0$$ *Outflow*

$$-n \times r u = (s_1 r_1 + s_2 r_2) U_0,$$ *inflow*

Normal inflow velocity U_0

COMSOL Multiphysics model

Parameters	Symbols	Value & Unit
Length of the domain	L_x	0.08 mm 0.128 mm
Width of the domain	L_y	0.02 mm 0.032 mm
Amplitude of the disturbance	ζ	0.01
Log-mobility ratio	R	-2, 2, 3
Injection speed	U_0	1 mm/s 0.5 mm/s
Viscosity of the displacing fluid	μ_1	10^{-3} Pa-s
Aspect ratio	A	4
Length of the finite sample	$W = L_x/8$	0.01 mm 0.016 mm

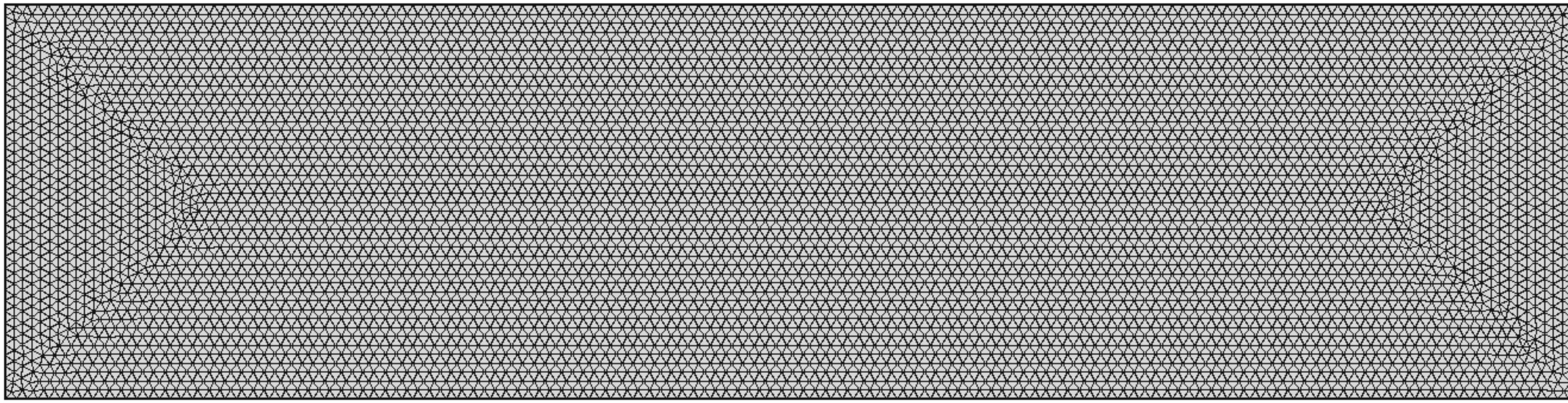


Fig. Finer grids

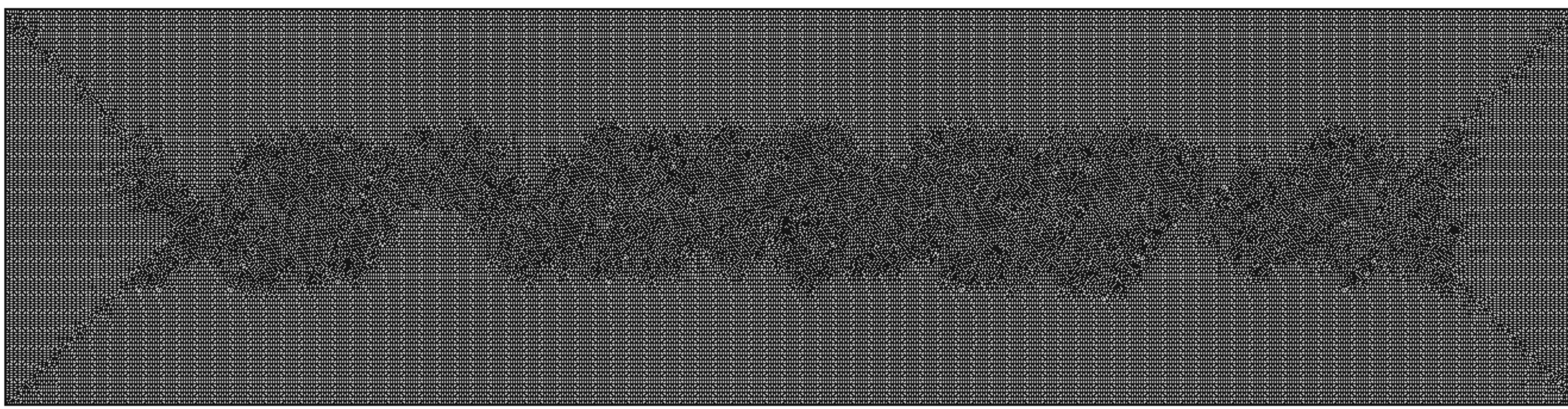


Fig. Extra Fine grids

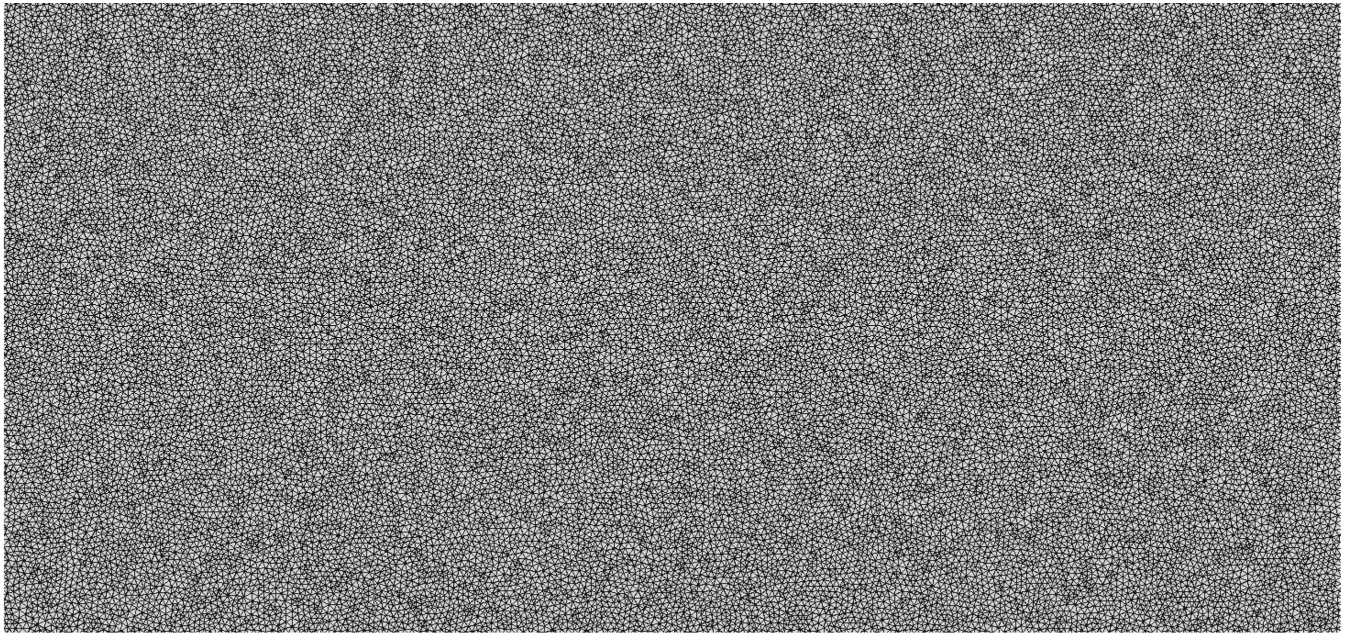
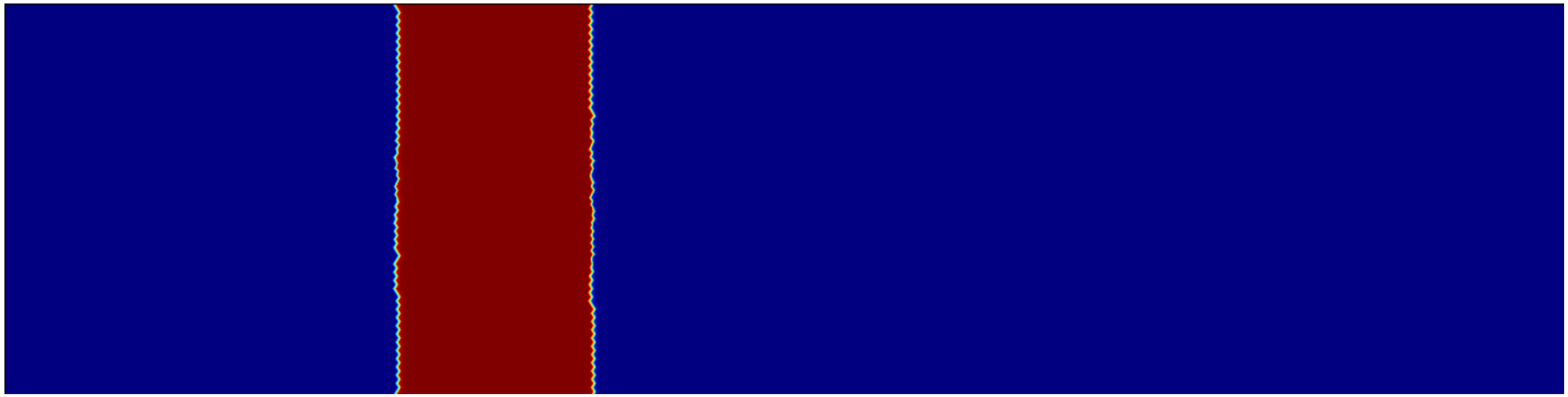


Fig. Extremely Fine grids (magnified)

No. of elements	**Degrees of freedom**	**Computation time (s)**
12684	32249	250
63930	160982	1475
383814	961778	6111

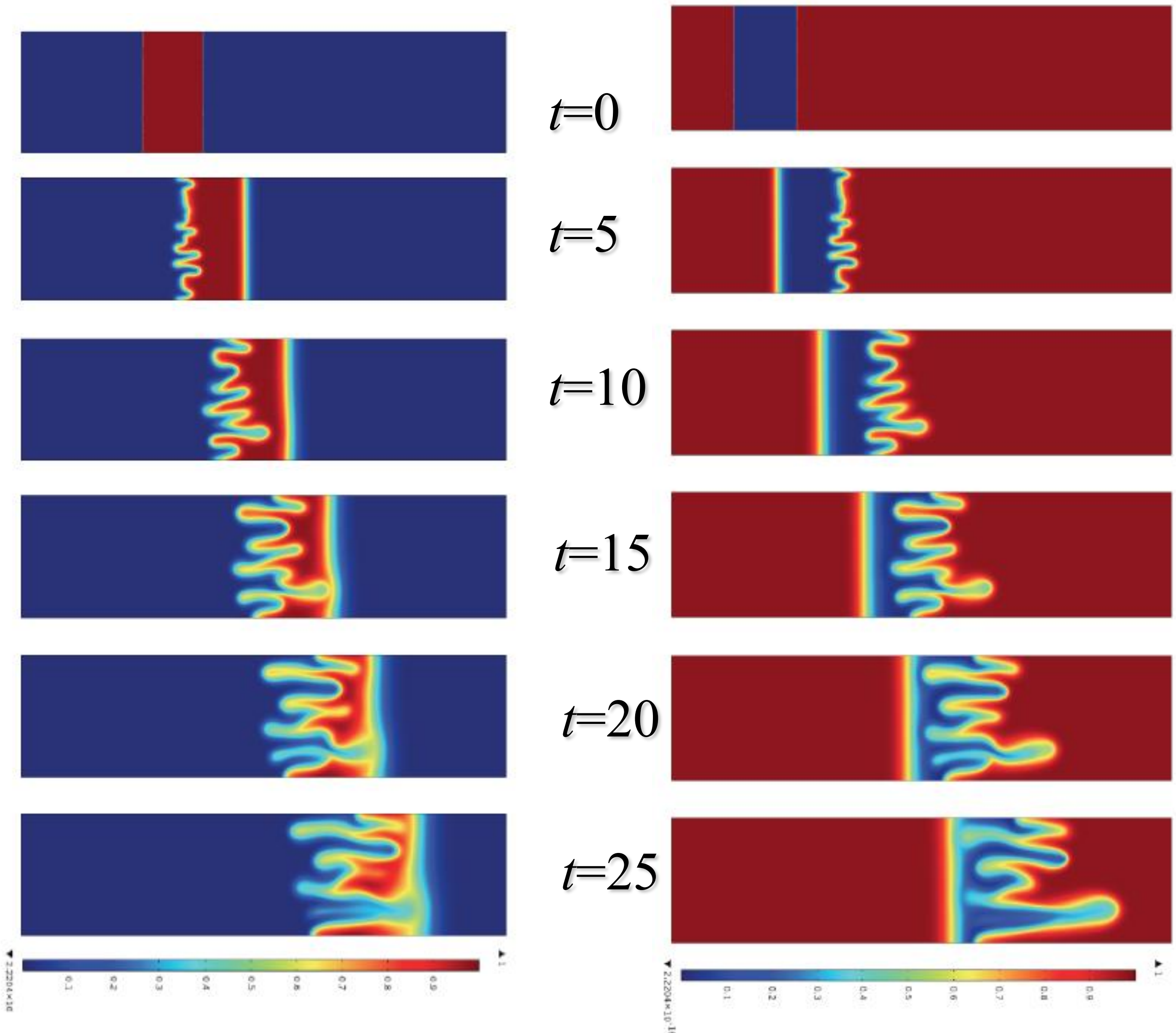
Results



R = 2, A = 4, U_0 = 1 mm/s

R = -2, A = 4, U_0 = 1 mm/s

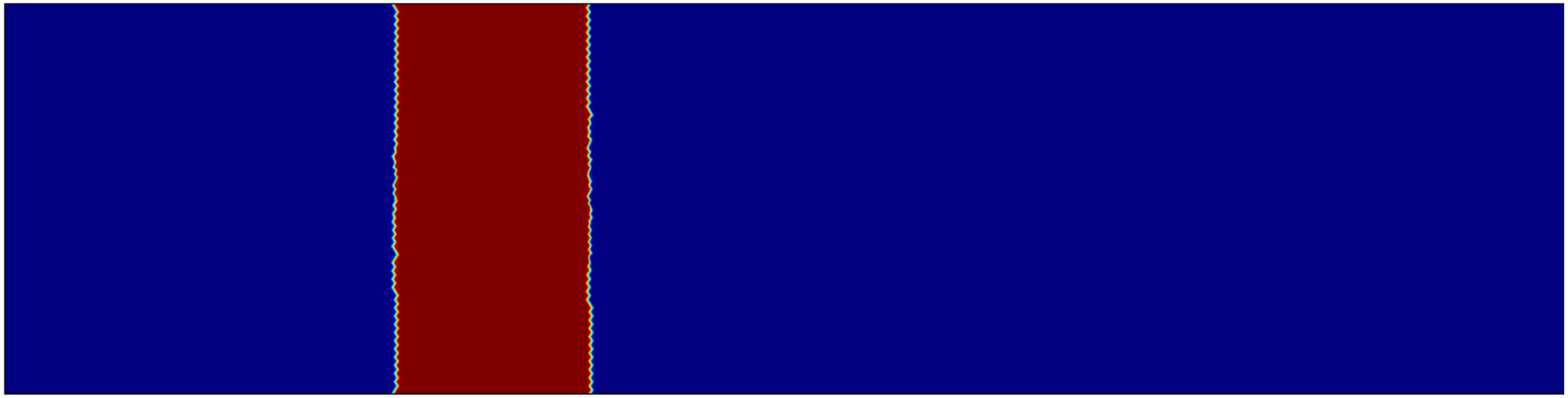
Results



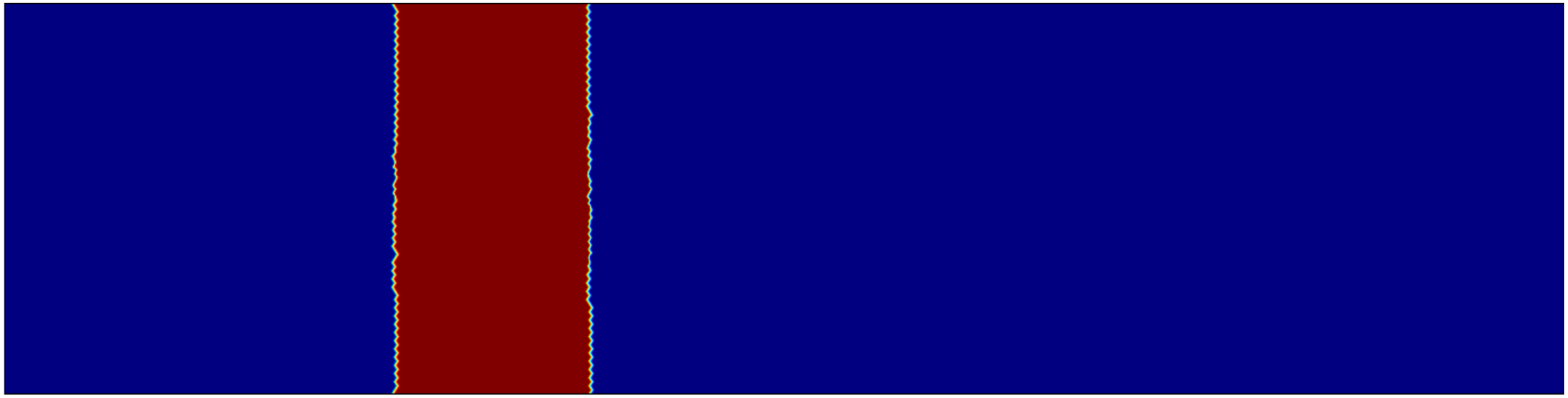
Mishra et al.
Phy. Rev. E 78, 066306, 2008

Using Fourier Spectral Method

Results

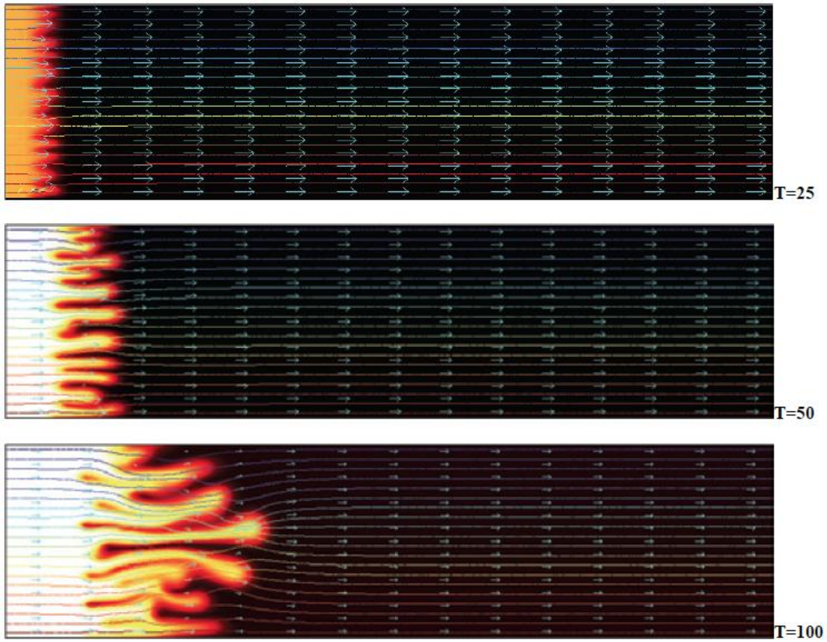


R = 2, A = 4, U_0 = 0.5 mm/s



R = 3, A = 4, U_0 = 0.5 mm/s

Modeling of Viscous Fingering using COMSOL Multiphysics



Ekkehard Holzbecher “Modeling of Viscous Fingering”, Proceedings of the COMSOL Conference 2009 Milan

In version 3.5a:
By coupling:
Poisson and convection-diffusion

The initial state for the concentration distribution is implemented as a MATLAB@ function

$$c(t=0) = \begin{cases} \xi f(x,y)\exp(-x^2/\sigma^2) & \text{for } x < L/128 \\ 0 & \text{else} \end{cases}$$

f describes a random disturbance of the initial concentration pattern and $\zeta = 0.01$

Conclusions

- Miscible viscous fingering of finite sample can be modeled using COMSOL Multiphysics.
- The classical VF phenomenon like, merging and tip splitting are observed through this COMSOL Multiphysics simulation model.
- The results and dynamics are reproducible.
- Quantification of the influence of fingering of the broadening of peaks as a function of the various parameters of the problem can be obtained