Advanced Numerical Methods for Modelling Two-Phase Flow in Heterogeneous Porous Media

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PhD Thesis Defense

Outline

1. Two-phase flow in porous media
2. Semi-analytical solutions in 1D
3. Dynamic effect in capillary pressure–saturation relationship
4. Mixed-Hybrid Finite Element – Discontinuous Galerkin method
5. Conclusion

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Motivation

- Two-phase flow in porous media
  - Immiscible
  - Incompressible
- Capillarity
  - Capillary barrier in heterogeneous porous media
  - Dynamic effect

Figure: Laboratory experiment provided by CESEP, Colorado School of Mines

Single phase flow

Darcy law

$$\mathbf{u} = -\frac{1}{\mu}\mathbf{K}\left(\nabla p - \rho \mathbf{g}\right) = -\frac{1}{\mu}\mathbf{K}\nabla\psi$$

Continuity theorem

$$\Phi\frac{\partial \varrho}{\partial t} + \nabla \cdot (\varrho\, \mathbf{u}) = \varrho F$$

Figure: H. Darcy [1803-1858]

Two-phase flow

Darcy law

$$\mathbf{u}_\alpha = -\frac{k_{r\alpha}}{\mu_\alpha}\mathbf{K}\left(\nabla p_\alpha - \rho_\alpha \mathbf{g}\right) = -\lambda_\alpha \mathbf{K}\nabla\psi_\alpha$$

Continuity theorem
(incompressible and immiscible)

$$\Phi\frac{\partial S_\alpha}{\partial t} + \nabla\cdot\mathbf{u}_\alpha = F_\alpha$$

Figure: H. Darcy [1803-1858]

$$\alpha \in \{w, n\}$$

Two-phase flow

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Capillary pressure

$$p_c = p_n - p_w$$

Saturation

$$S_w + S_n = 1$$

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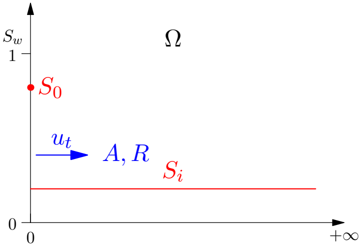
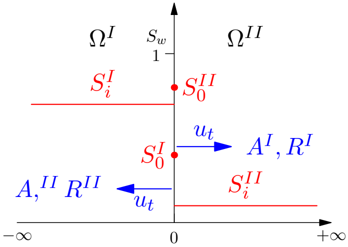
Problem Formulation

1D two-phase flow equation

$$\Phi \frac{\partial S_w}{\partial t} + \frac{AR}{\sqrt{t}} \, \frac{\partial f_w(S_w)}{\partial x} - \frac{\partial}{\partial x}\left(D(S_w)\, \frac{\partial S_w}{\partial x} \right) = 0$$



(a) Homogeneous setup
McWhorter and Sunada (1992)



(b) Heterogeneous setup
Fučík *et al.* (2008)

Exact Solution

1D two-phase flow equation

$$\Phi\frac{\partial S_w}{\partial t}+\frac{AR}{\sqrt{t}}\ \frac{\partial f_w(S_w)}{\partial x}-\frac{\partial}{\partial x}\left(D(S_w)\ \frac{\partial S_w}{\partial x}\right)=0$$

- Exact solution $S_w = S_w(t,x)$ is implicitly obtained from

$$x = F'(S_w)\frac{2A(1-Rf_w(S_i))}{\Phi}\sqrt{t}$$

- Function $F = F(S_w)$ satisfies the integral equation

$$F(S_w) = 1 - \frac{\int\limits_{S}^{S_0} \frac{(v-S_w)\ D(v)}{F(v)-\varphi(v)}\ \mathrm{d}v}{\int\limits_{S_i}^{S_0} \frac{(v-S_i)\ D(v)}{F(v)-\varphi(v)}\ \mathrm{d}v}$$

Modified Integral Equation

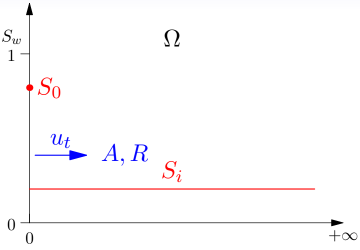
- Substitution $G \equiv \frac{D}{F-\varphi}$ allows to obtain modified integral equations :
variant A :

$$G_{k+1}(S_w) = D(S_w) + G_k(S_w) \left(\varphi(S_w) + \frac{\int_{S}^{S_0} (v - S_e)\, G_k(v)\, \mathrm{d}v}{\int_{S_i}^{S_0} (v - S_i)\, G_k(v)\, \mathrm{d}v} \right)$$

variant B :

$$G_{k+1}(S_w) = \left(D(S_w) + G_k(S_w)\, \varphi(S_w)\right) \left(1 - \frac{\int_{S_e}^{S_0} (v - S)\, G_k(v)\, \mathrm{d}v}{\int_{S_i}^{S_0} (v - S_i)\, G_k(v)\, \mathrm{d}v} \right)^{-1}$$

Exact Solution for Layered Porous Media



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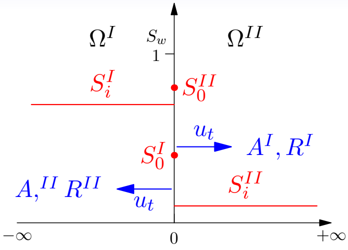
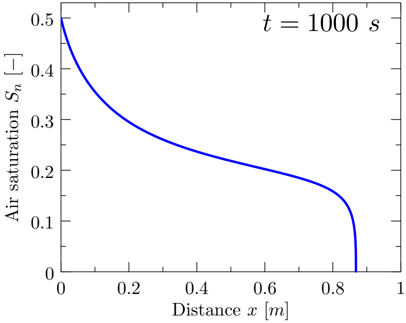


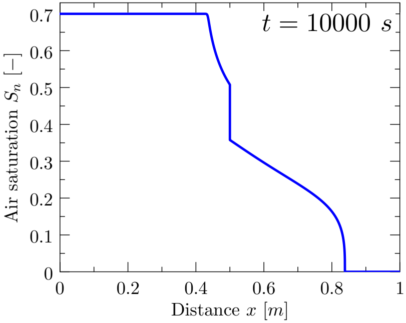
(b) Heterogeneous setup
Fučík *et al.* (2008)

- Combination of two exact solutions for the homogeneous problems
- Interfacial conditions:
  - $A^I R^I = A^{II} R^{II}$
  - $R^I - R^I R^{II} + R^{II} = 0$
  - $p_c^I(S_0^I) = p_c^{II}(S_0^{II})$

Example Solutions



Homogeneous medium



Heterogeneous medium

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Dynamic Effect in Capillarity

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- $p_c =< p_n > - < p_w >$ holds only in thermodynamic equilibrium
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$$p_c(S_w) = p_c^{eq}(S_w) - \tau(S_w)\frac{\partial S_w}{\partial t}$$

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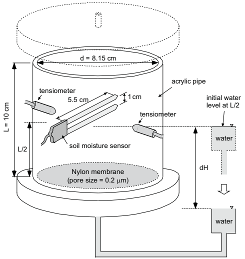
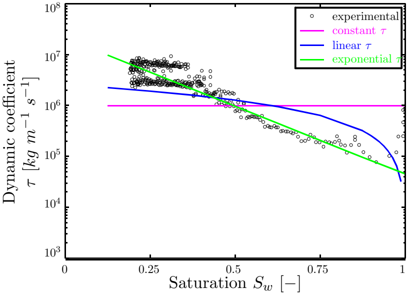
$$p_c(S_w) = p_c^{eq}(S_w) - \tau(S_w)\frac{\partial S_w}{\partial t}$$

Dynamic effect coefficient $\tau = \tau(S_w)$ (exp. data from CESEP)





Two-phase flow incl. dynamic effect

Darcy law

$$\mathbf{u}_\alpha = -\frac{k_{r\alpha}}{\mu_\alpha}\mathbf{K}\left(\nabla p_\alpha - \rho_\alpha \mathbf{g}\right) = -\lambda_\alpha \mathbf{K}\nabla\psi_\alpha$$

Figure: H. Darcy [1803-1858]

Continuity theorem
(incompressible and immiscible)

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Capillary pressure

$$p_c = p_n - p_w = p_c^{eq} - \tau(S_w)\frac{\partial S_w}{\partial t}$$

$$\alpha \in \{w, n\}$$

Saturation

$$S_w + S_n = 1$$

Dynamic Effect in Capillarity

How does the inclusion of dynamic effect in capillarity influence results of numerical models?

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- Vertex–Centered Finite Volume Method (VCFVM) in 1D
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Results:

- Verification of VCFVM using semi-analytical solutions
- Simulation of the laboratory experiment

Simulation of Laboratory Experiment

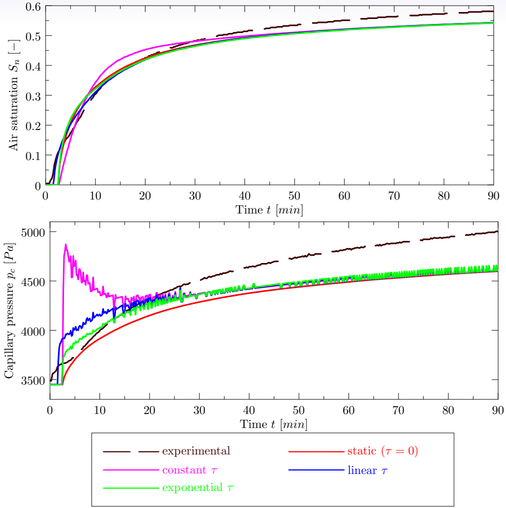

Figure: Simulation of the laboratory experiment in homogeneous medium.

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  - Dynamic effect in capillarity not found to be important in homogeneous medium

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- Vertex–Centered Finite Volume Method (VCFVM) in 1D
- Fully implicit in time
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Results:

- Verification of VCFVM using semi-analytical solutions
- Simulation of the laboratory experiment
  - Dynamic effect in capillarity not found to be important in homogeneous medium
- Barrier effect sensitivity analysis (heterogeneous medium)
  - Dynamic effect in capillarity influenced the speed of propagation of non-wetting phase through material interfaces

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MHFE-DG Problem Formulation

Model equations (without dynamic effect, $\psi_c = \psi_c(S_w)$)

$$\Phi \frac{\partial S_\alpha}{\partial t} + \nabla \cdot \mathbf{u}_\alpha = F_\alpha \quad (1)$$

$$\mathbf{u}_\alpha = -\lambda_\alpha \mathbf{K} \nabla \psi_\alpha \quad (2)$$

$$\psi_c = \psi_n - \psi_w \quad (3)$$

$$S_w + S_n = 1 \quad (4)$$

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Total velocity $\mathbf{u}_t$ splitting

$$\mathbf{u}_t = \mathbf{u}_w + \mathbf{u}_n = -\lambda_w \mathbf{K} \nabla \psi_w - \lambda_n \mathbf{K} \nabla \psi_n = \underbrace{-\lambda_t \mathbf{K} \nabla \psi_w}_{\mathbf{u}_a} + f_n (\underbrace{-\lambda_t \mathbf{K} \nabla \psi_c}_{\mathbf{u}_c})$$

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Eq. (1):

$$\Phi \frac{\partial S_\alpha}{\partial t} + \nabla \cdot (f_w \mathbf{u}_a) = F_\alpha$$

Key Steps of MHFE-DG Discretization

- Approximation of $\mathbf{u}_c$ and $\mathbf{u}_a$ in the Raviart–Thomas space $\mathbf{RT}_0(K)$ space (MHFE)

$$\mathbf{u}_\alpha = \sum_{E \in \mathcal{E}_K} u_{\alpha,K,E} \mathbf{w}_{K,E}(\mathbf{x}), \quad \alpha \in \{c, a\}$$

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- Expression of $\mathbf{u}_c$ and $\mathbf{u}_a$ as a function of side-average potentials $\psi_{c,E}$ and $\psi_{w,E}$

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- Satisfying the extended capillary pressure condition at material interfaces

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- Expression of $\mathbf{u}_c$ and $\mathbf{u}_a$ as a function of side-average potentials $\psi_{c,E}$ and $\psi_{w,E}$
- Satisfying the extended capillary pressure condition at material interfaces
- Approximation of S_w in the discontinuous Galerkin space $\mathcal{D}_1(K)$ (DG)

$$S_w(t, \mathbf{x}) = \sum_{E \in \mathcal{E}_K} S_{w,K,E}(t) \varphi_{K,E}(\mathbf{x})$$

Computational Algorithm (IMPES)

$S^i_{w,K,E}$

- Implicit system of equations for side-average potentials $\psi_{c,E}$ based on known saturation $S_{w,K,E}$ from previous time step i

Computational Algorithm (IMPES)

$$S^i_{w,K,E} \rightarrow \psi_{c,E}$$

- Implicit system of equations for side-average potentials $\psi_{c,E}$ based on known saturation $S_{w,K,E}$ from previous time step i
- Computation of velocities $u_{c,K,E}$

Computational Algorithm (IMPES)

$$S^i_{w,K,E} \to \psi_{c,E} \to u_{c,K,E}$$

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- Discretization of the saturation equation based on known velocities $u_{a,K,E}$ leads to a system of ODE for $S_{w,K,E} = S_{w,K,E}(t)$

Computational Algorithm (IMPES)

$$S^i_{w,K,E} \to \psi_{c,E} \to u_{c,K,E} \to \psi_{w,E} \to u_{a,K,E} \to \hat{S}^{i+1}_{w,K,E}$$

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- Explicit solution of the system of ODE using Forward Euler method

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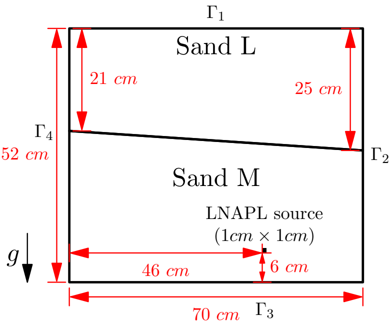
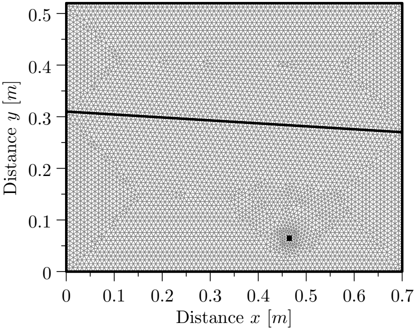
- Explicit solution of the system of ODE using Forward Euler method
- Slope limiting procedure to stabilize the numerical method

Results: LNAPL at Inclined Interface



Domain setup



Mesh: 32374 triangles

Results: LNAPL at Inclined Interface

Time t=27 min

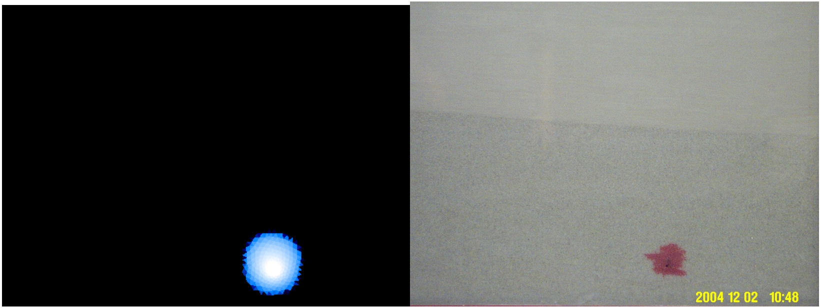


Figure: MHFE-DG simulation vs. laboratory experiment (CESEP).

Results: LNAPL at Inclined Interface

Time t=42 min

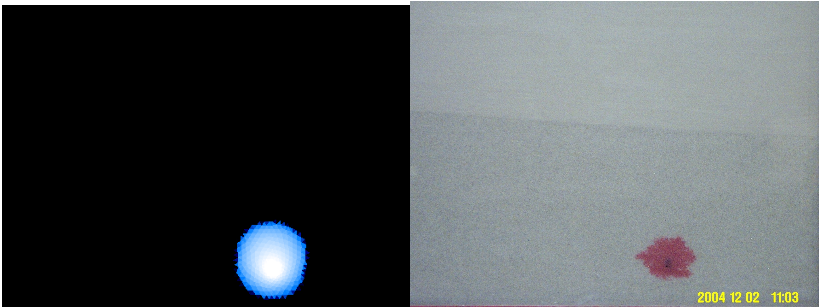


Figure: MHFE-DG simulation vs. laboratory experiment (CESEP).

Results: LNAPL at Inclined Interface

Time t=1 h

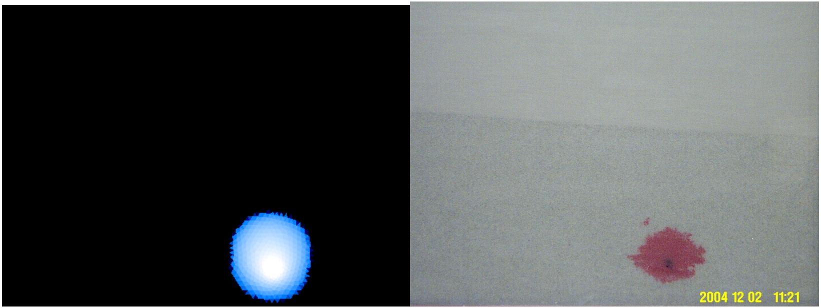
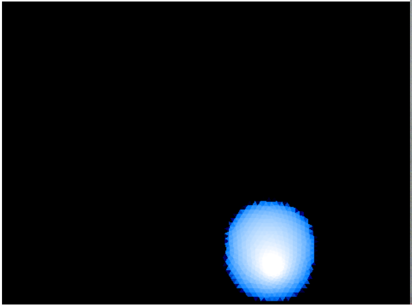


Figure: MHFE-DG simulation vs. laboratory experiment (CESEP).

Results: LNAPL at Inclined Interface

Time t=1 h 15 min



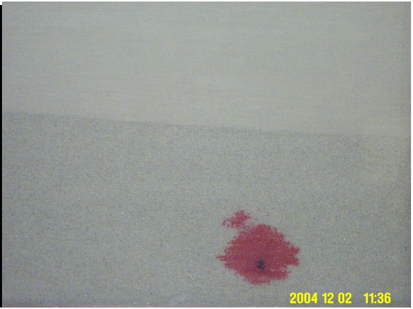


Figure: MHFE-DG simulation vs. laboratory experiment (CESEP).

Results: LNAPL at Inclined Interface

Time t=1 h 30 min

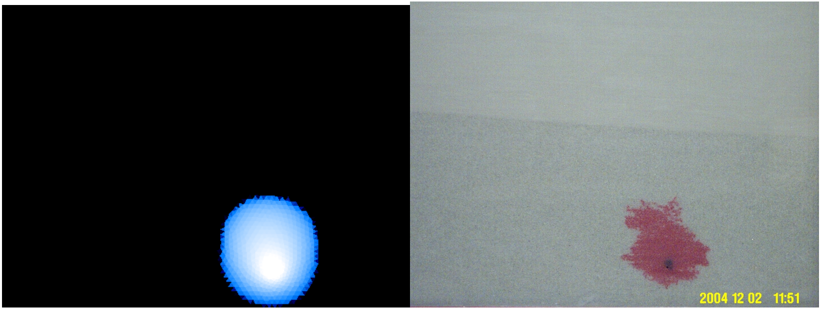


Figure: MHFE-DG simulation vs. laboratory experiment (CESEP).

Results: LNAPL at Inclined Interface

Time t=2 h 10 min

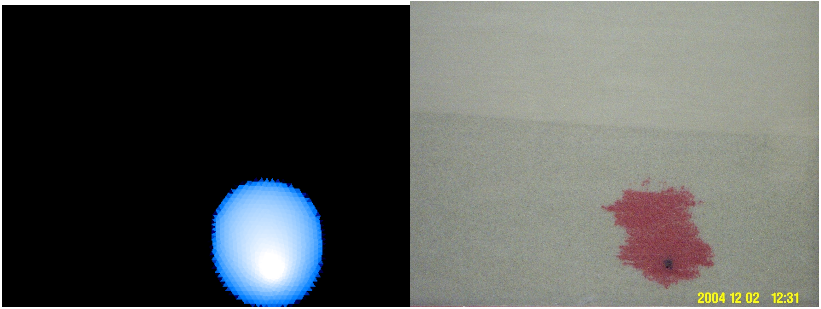


Figure: MHFE-DG simulation vs. laboratory experiment (CESEP).

Results: LNAPL at Inclined Interface

Time t=3 h 32 min

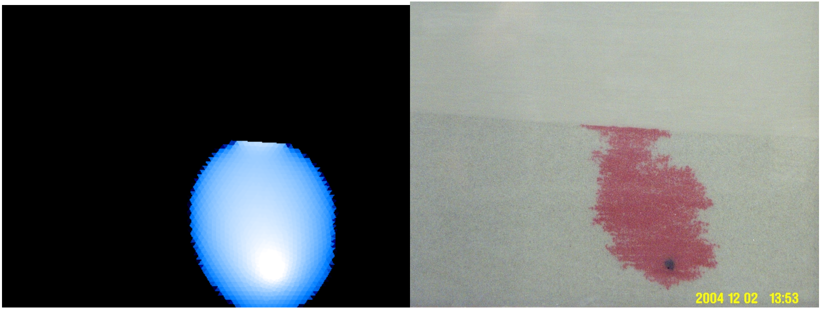


Figure: MHFE-DG simulation vs. laboratory experiment (CESEP).

Results: LNAPL at Inclined Interface

Time t=3 h 50 min

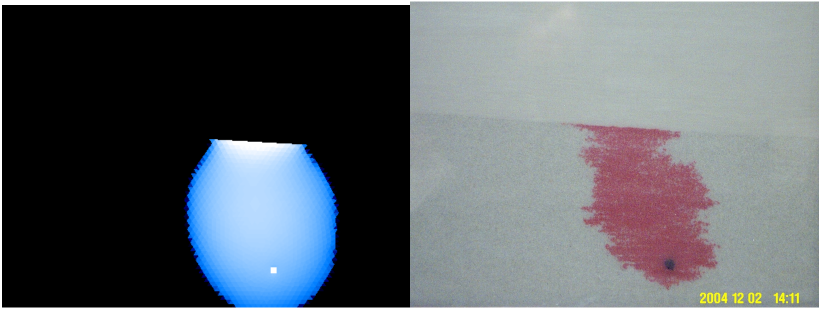


Figure: MHFE-DG simulation vs. laboratory experiment (CESEP).

Results: LNAPL at Inclined Interface

Time t=3 h 52 min

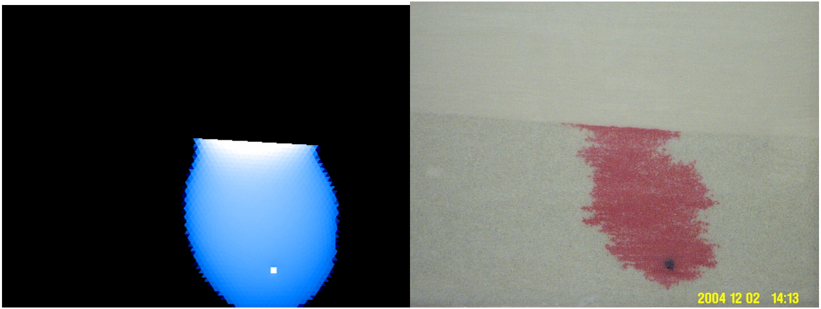
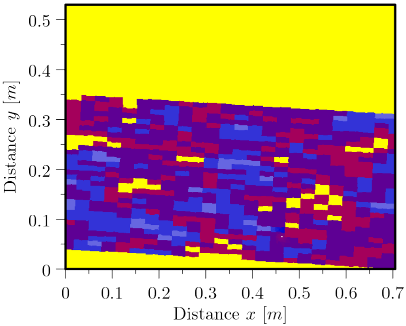
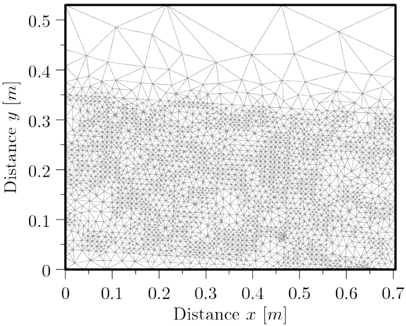


Figure: MHFE-DG simulation vs. laboratory experiment (CESEP).

Results: Random Heterogeneous Medium



Domain setup (CESEP)



Mesh : 5503 triangles

Results: Random Heterogeneous Medium

Time t=10 min

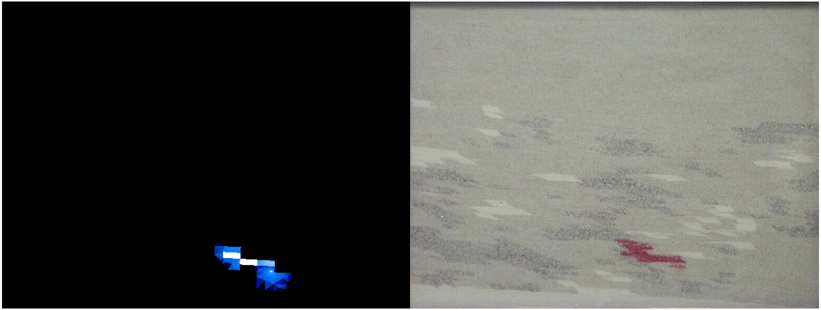


Figure: MHFE-DG simulation vs. laboratory experiment (CESEP).

Results: Random Heterogeneous Medium

Time t= 20 min

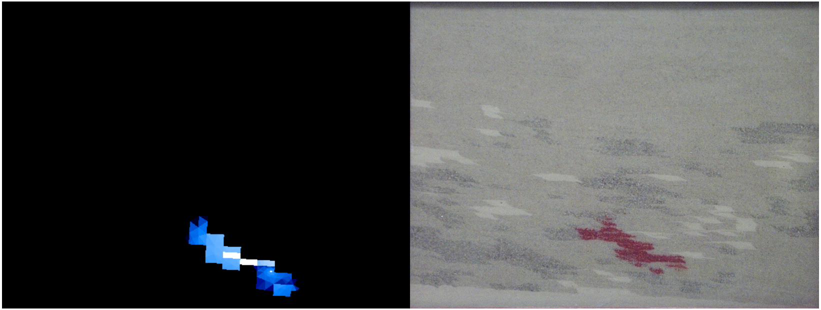


Figure: MHFE-DG simulation vs. laboratory experiment (CESEP).

Results: Random Heterogeneous Medium

Time t= 30 min

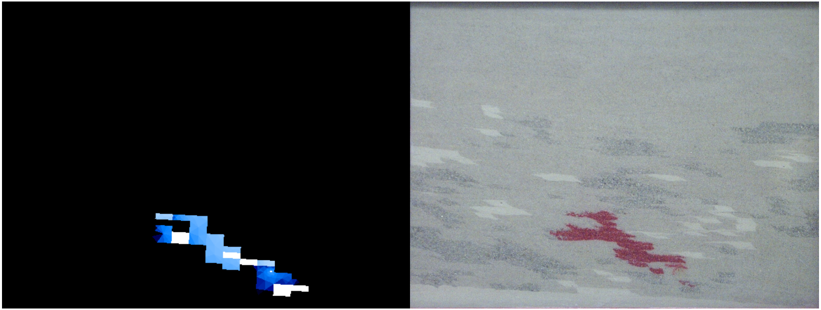


Figure: MHFE-DG simulation vs. laboratory experiment (CESEP).

Results: Random Heterogeneous Medium

Time t= 40 min

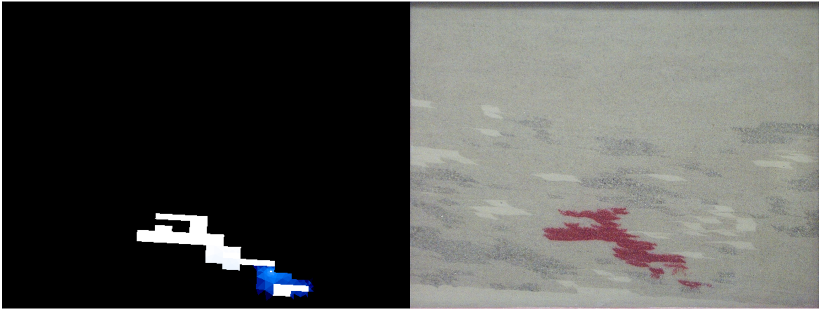


Figure: MHFE-DG simulation vs. laboratory experiment (CESEP).

Results: Random Heterogeneous Medium

Time t= 50 min

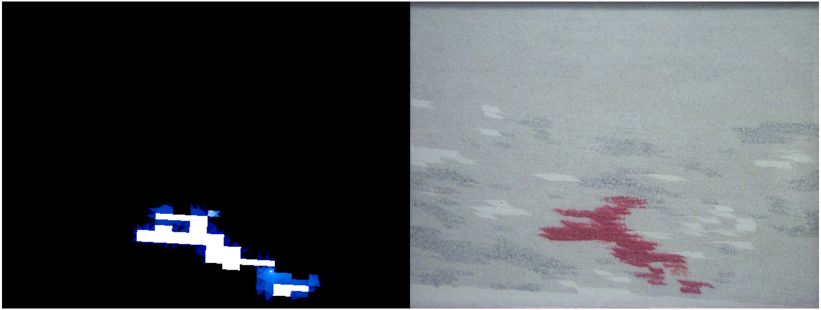


Figure: MHFE-DG simulation vs. laboratory experiment (CESEP).

Results: Random Heterogeneous Medium

Time t= 1 h

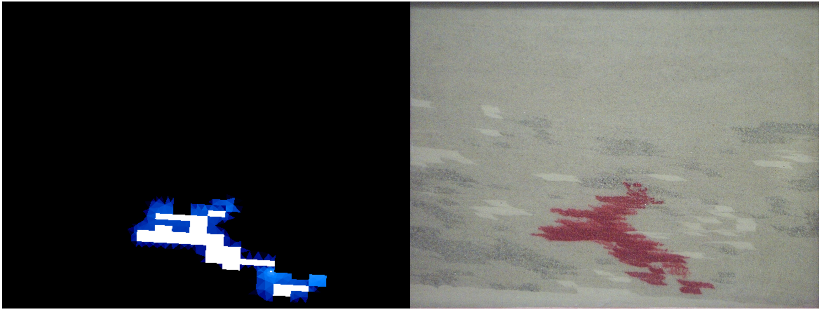


Figure: MHFE-DG simulation vs. laboratory experiment (CESEP).

Results: Random Heterogeneous Medium

Time t= 1.2 h

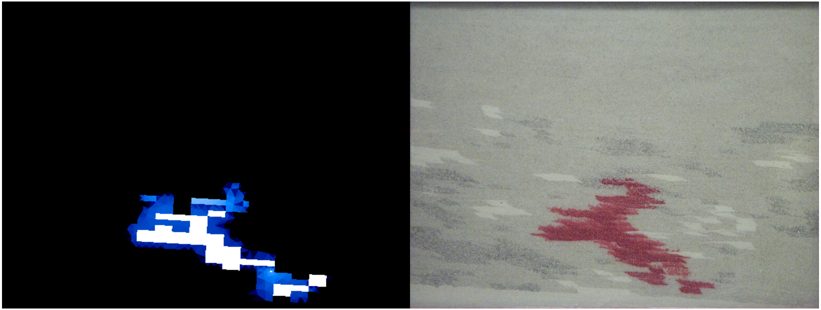


Figure: MHFE-DG simulation vs. laboratory experiment (CESEP).

Results: Random Heterogeneous Medium

Time t= 1.7 h

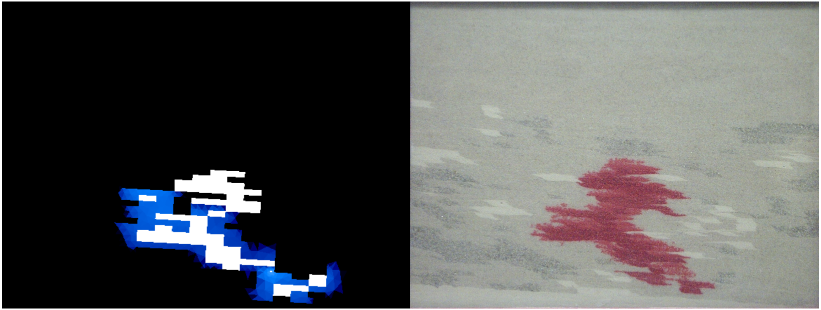


Figure: MHFE-DG simulation vs. laboratory experiment (CESEP).

Results: Random Heterogeneous Medium

Time t= 2.4 h

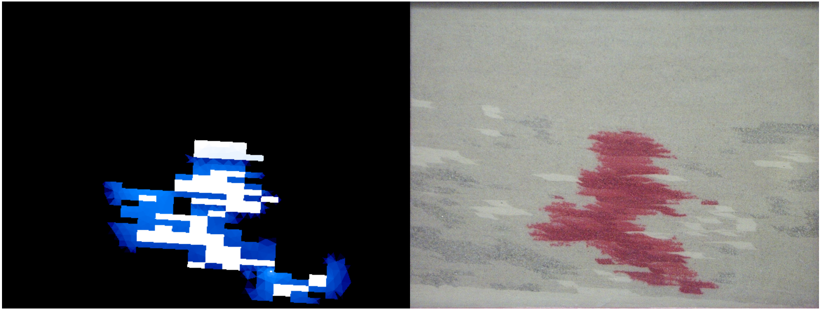


Figure: MHFE-DG simulation vs. laboratory experiment (CESEP).

Results: Random Heterogeneous Medium

Time t= 2.6 h

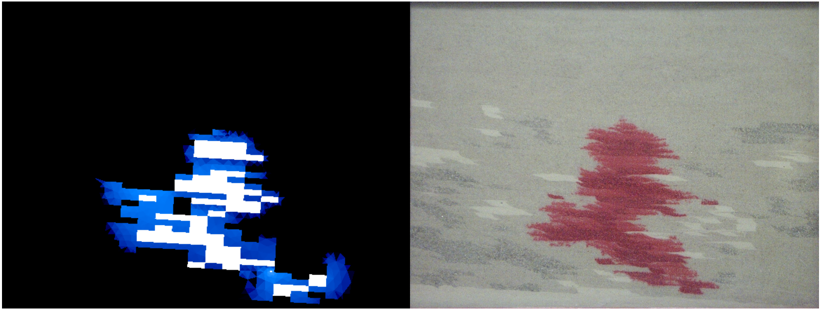


Figure: MHFE-DG simulation vs. laboratory experiment (CESEP).

Results: Random Heterogeneous Medium

Time t= 2.7 h

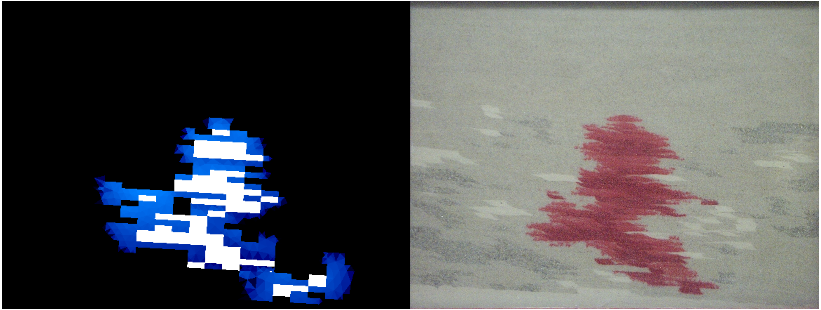


Figure: MHFE-DG simulation vs. laboratory experiment (CESEP).

Results: Random Heterogeneous Medium

Time t= 3.6 h

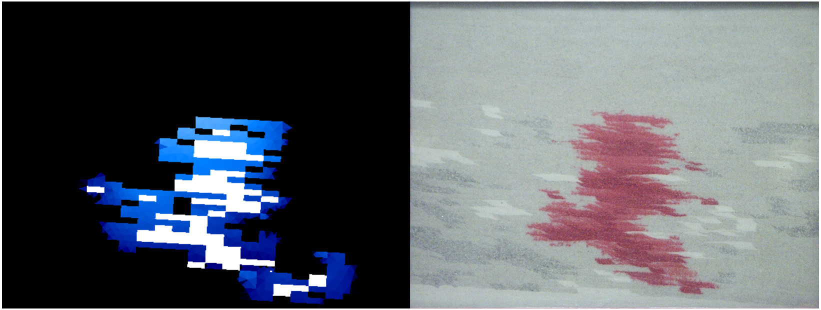


Figure: MHFE-DG simulation vs. laboratory experiment (CESEP).

Results: Random Heterogeneous Medium

Time t= 3.7 h

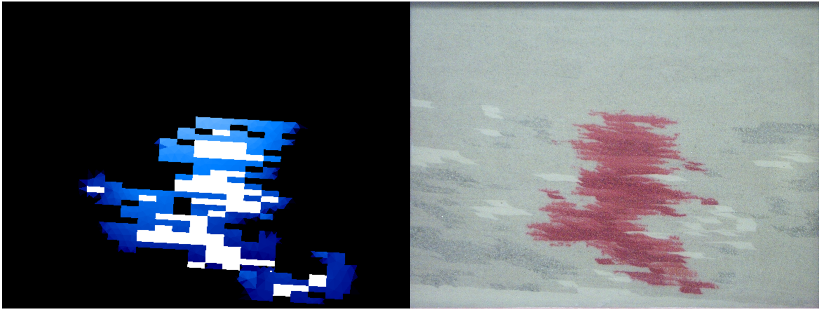


Figure: MHFE-DG simulation vs. laboratory experiment (CESEP).

Results: Random Heterogeneous Medium

Time t= 4.6 h

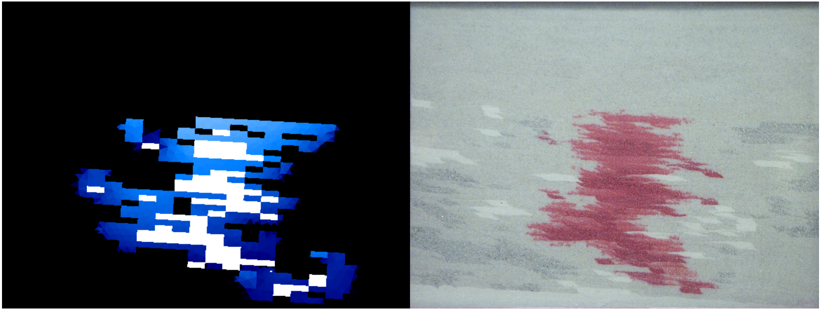


Figure: MHFE-DG simulation vs. laboratory experiment (CESEP).

Outline

1. Two-phase flow in porous media
2. Semi-analytical solutions in 1D
3. Dynamic effect in capillary pressure–saturation relationship
4. Mixed-Hybrid Finite Element – Discontinuous Galerkin method
5. Conclusion

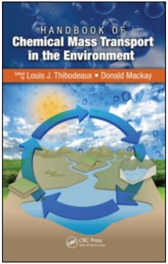
Conclusion: Key Results

1. McWhorter and Sunada semi-analytical solution
   - New, more robust iterative method for solving integral equation
   - Extension to heterogeneous porous media
2. Dynamic effect in capillary pressure–saturation relationship
   - Fully implicit VCFVM method in 1D
   - Numerical scheme verification using 1D benchmark problems
   - Simulation of laboratory experiment using laboratory measured data (CESEP)
   - Dynamic effect found to be important in heterogeneous porous materials
3. Mixed-hybrid finite element and discontinuous Galerkin method
   - Improvements to the MHFE-DG method by Hoteit and Firoozabadi [2008]
   - Inclusion of the extended capillary pressure condition
   - Numerical scheme verification using 1D and 2D benchmark problems
   - Good agreement with laboratory experiments (CESEP)
4. Future work
   - More realistic computational time: parallel implementation of the CG solver on nVidia graphics cards using CUDA (original research in progress within our group MMG)

Publications

- Book Chapter:

  T. H. Illangasekare, C. C. Frippiat, R. Fučík
  Dispersion and Mass Transfer Coefficients in Groundwater of Near-surface Geologic Formations
  in Handbook of Estimation Methods: Environmental Mass Transport Coefficients, Dispersion and Mass Transfer Coefficients
  Editors L. J. Thibodeaux and D. Mackay,
  CRC Press / Taylor and Francis Group, UK, 2010



- Impacted Periodicals: 5 (next page)
- Contributions in Proceedings: 10 + 1 submitted
- International conference presentations: 7 talks, 9 posters

Publications in Impacted Periodicals

R.Fučík, J. Mikyška, T. Sakaki, M. Beneš and T. H. Illangasekare
Significance of Dynamic Effect in Capillarity in Layered Soils
Vadose Zone Journal, vol. 9, pages 697–708, 2010

Beneš M., Fučík R., Mikyška J., and Illangasekare T.H.
Analytical and Numerical Solution for One-Dimensional Two-Phase Flow in Homogeneous Porous Medium
Journal of Porous Media, vol. 12, no. 12, pages 1139–1152, 2009

R.Fučík , I. Cheddadi, M. Prieto and M. Vohralík
Guaranteed and robust a posteriori error estimates for singularly perturbed reaction-diffusion problems
ESAIM: Mathematical Modelling and Numerical Analysis, no. 43, pages 867–888, 2009

R.Fučík, J. Mikyška, T. H. Illangasekare and M. Beneš
Semi-Analytical Solution for Two-Phase flow in Porous Media with a Discontinuity
Vadose Zone Journal, vol. 7 no. 3, pages 1001–1009, 2008

R.Fučík, J. Mikyška, T. H. Illangasekare and M. Beneš
An Improved Semi-Analytical Solution for Verification of Numerical Models of Two-Phase Flow in Porous Media
Vadose Zone Journal, no. 6, pages 93–104 2007