Heterogeneous Reacting Fluid Flow

in

Catalytically Active Porous Electrode Regions

Finite Element Analysis (FEA) using Comsol Multiphysics

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Acknowledgement

The FEA Model Presented here was greatly assisted by the work
of
Johan Sundqvist
and his colleagues and academic associates
at
COMSOL - a publisher of Finite Element Software

The porous region geometry I used comes from the pore-scale flow experiments

conducted by A. Keller, M. Auset, and S. Sirivithayapakorn

at the University of California.

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Overview – Volume Averaging

Typical analysis starts with the idea that one can average across macroscopic regions

1. Volume averaging

In a porous medium, see Figure 3.1, the transport processes, such as e.g. conservation of mass and momentum, can be solved on a microscale.

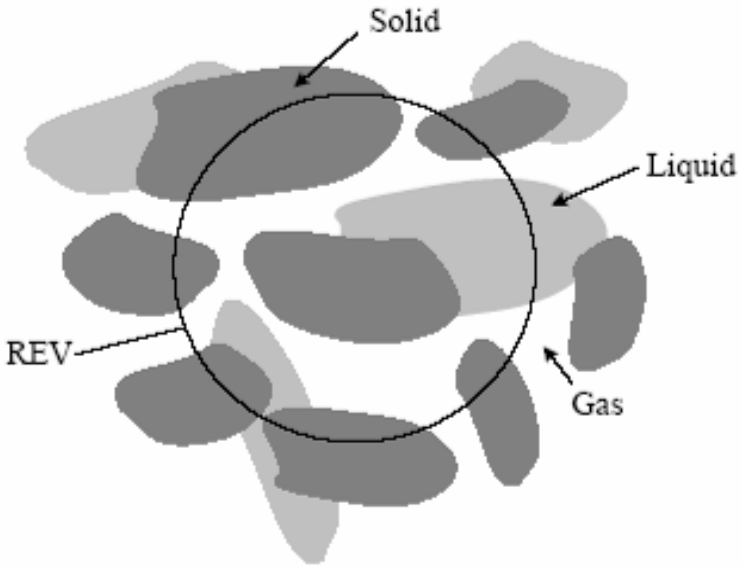

Figure 3.1. A schematic of a porous medium with a gas and liquid phase present and the representative elementary volume (REV).

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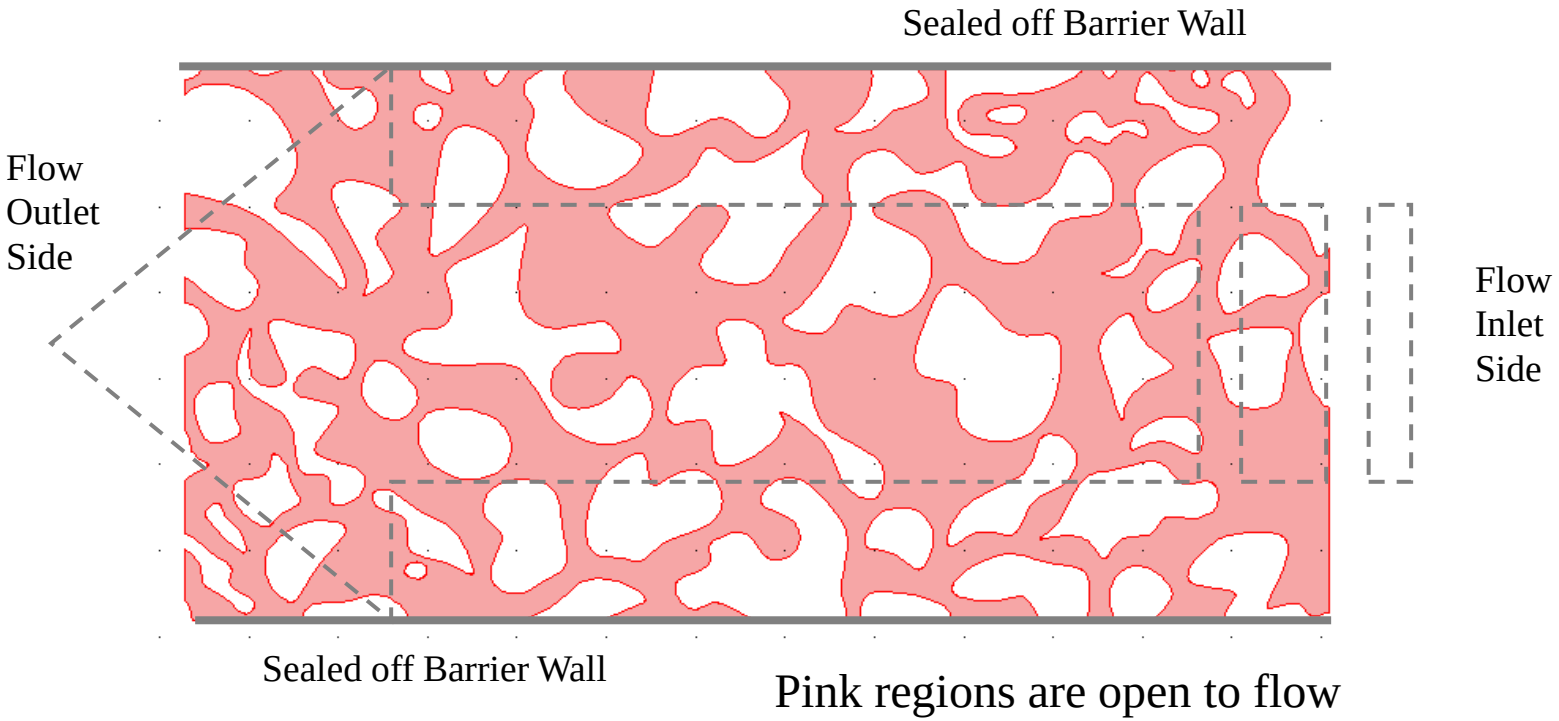
Overview – Microscale Finite Element Modeling (FEA)

In this presentation, we will not volume average. We keep the micro-structure and observe how fluid flow and chemical reactions take place. This "Micro-Picture" is very instructive. Here is our domain. It was digitized from an actual porous structure



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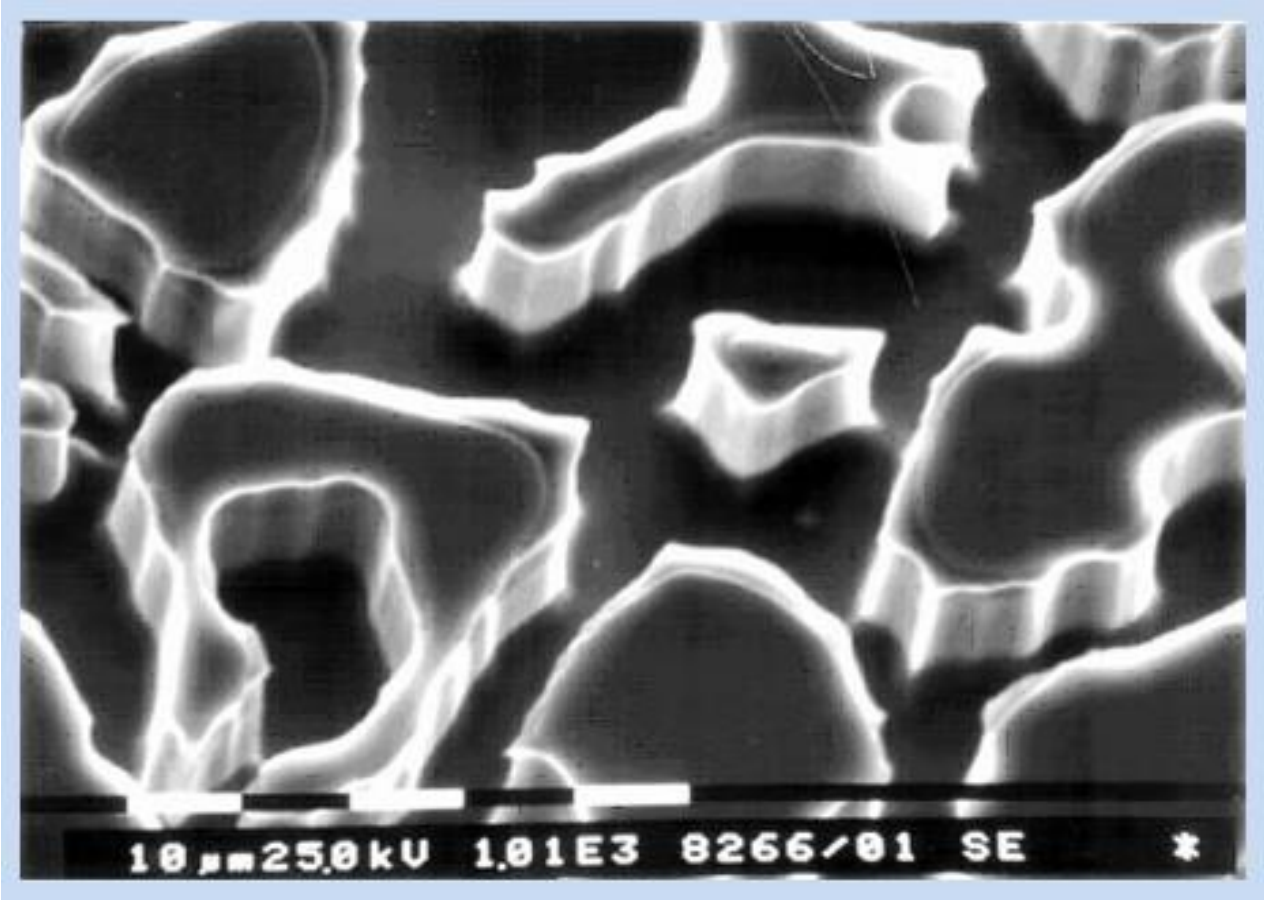
Overview

Here is an SEM of the structure from which the pore model was made



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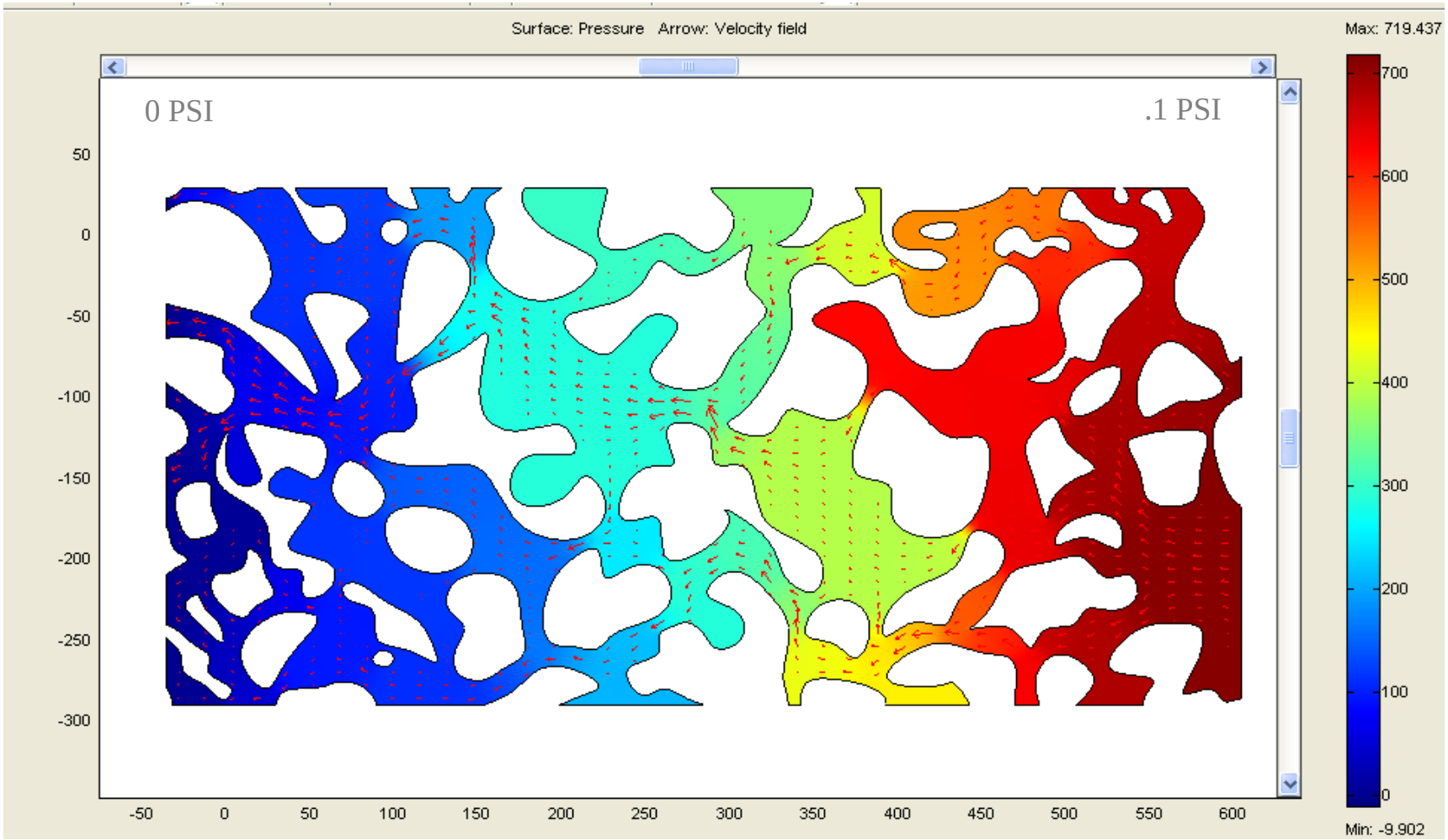
Pressure and Flow Velocity Through Porous Regions



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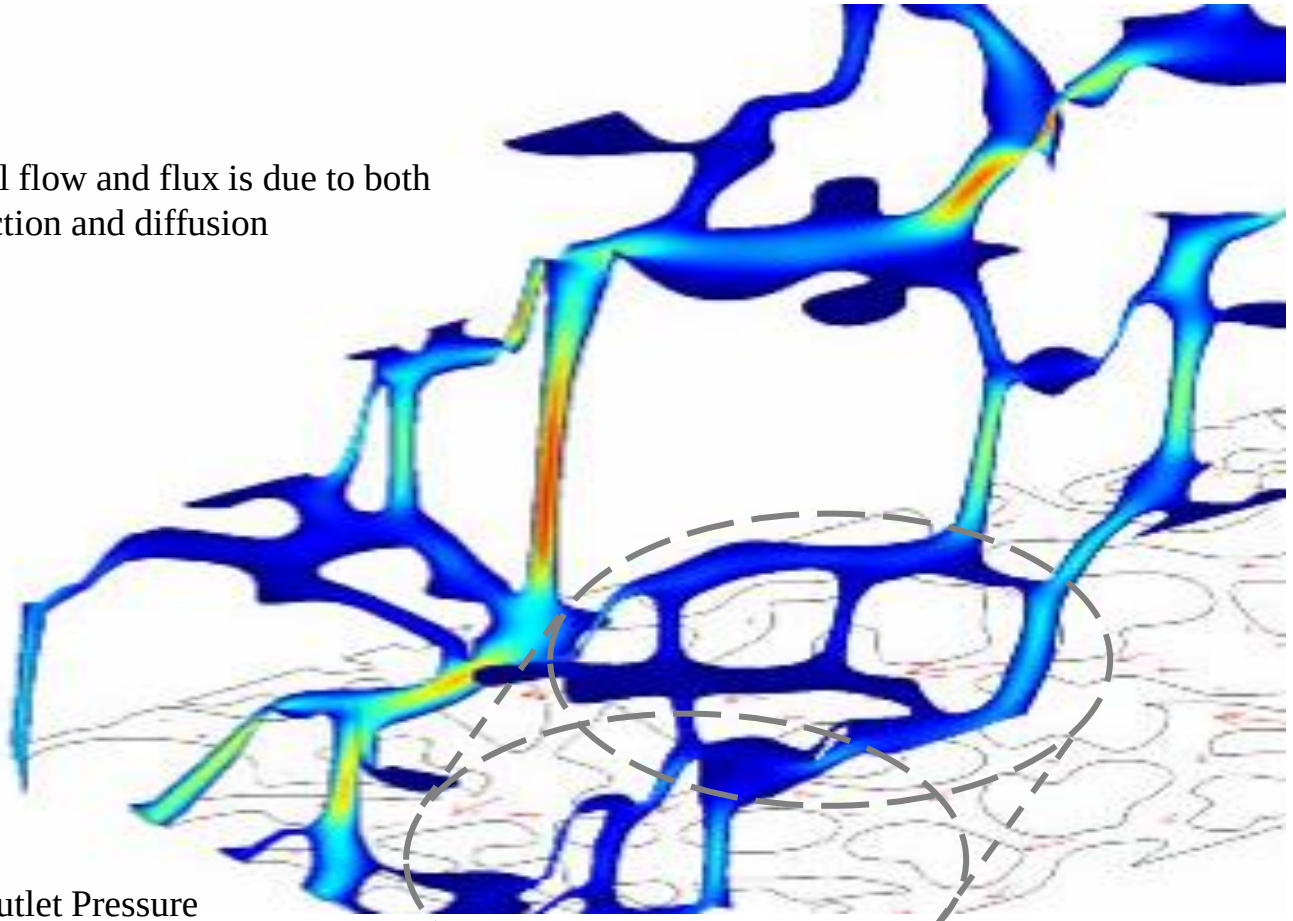
Pressure and Flow Velocity Through Porous Regions

Overall flow and flux is due to both convection and diffusion



.1 PSI Inlet Pressure

0 PSI Outlet Pressure

Partially Occluded Region

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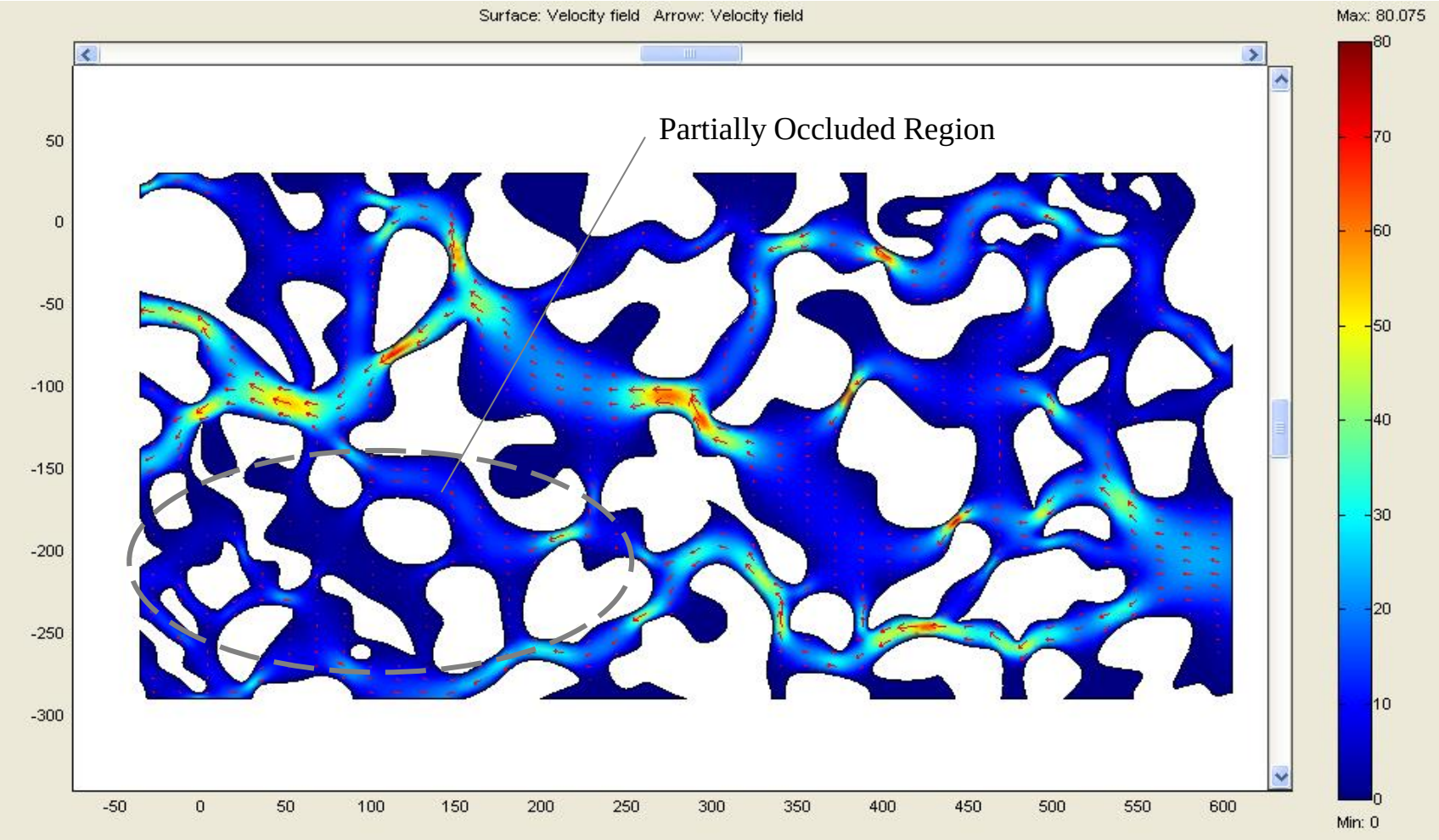
Flow Velocity Through Porous Regions



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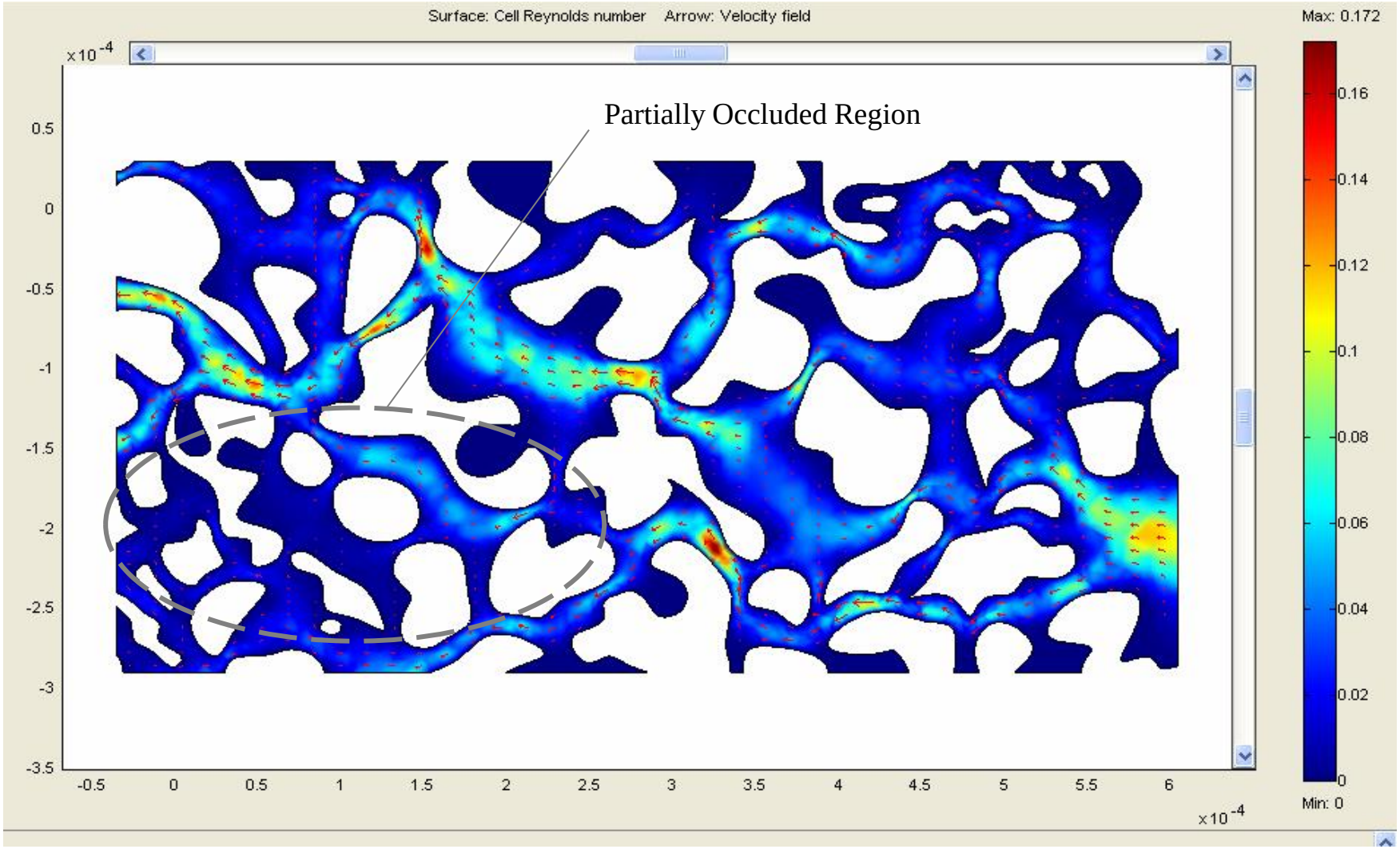
Plot of Reynolds Number Through Porous Regions



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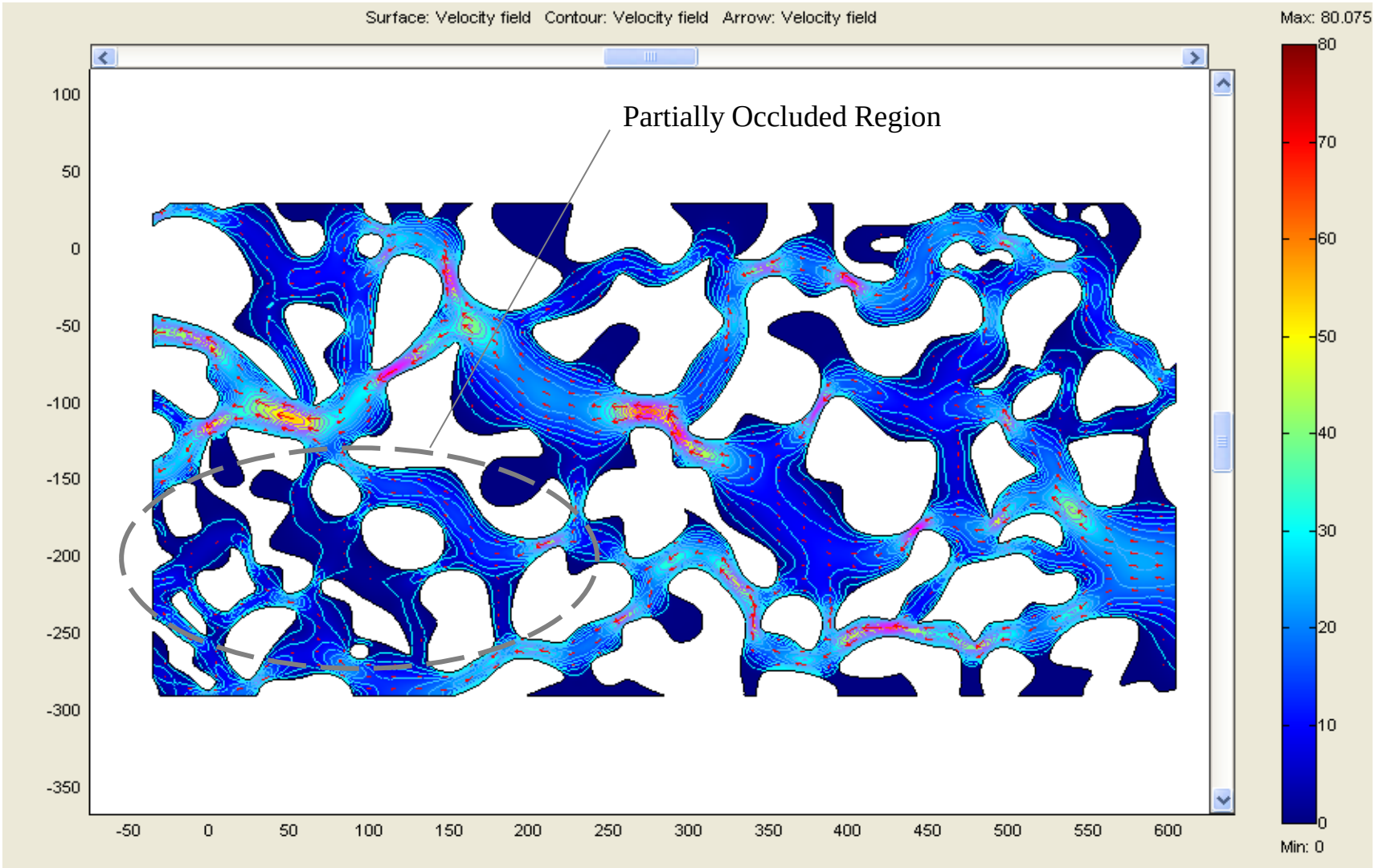
Velocity Contours Through Porous Regions



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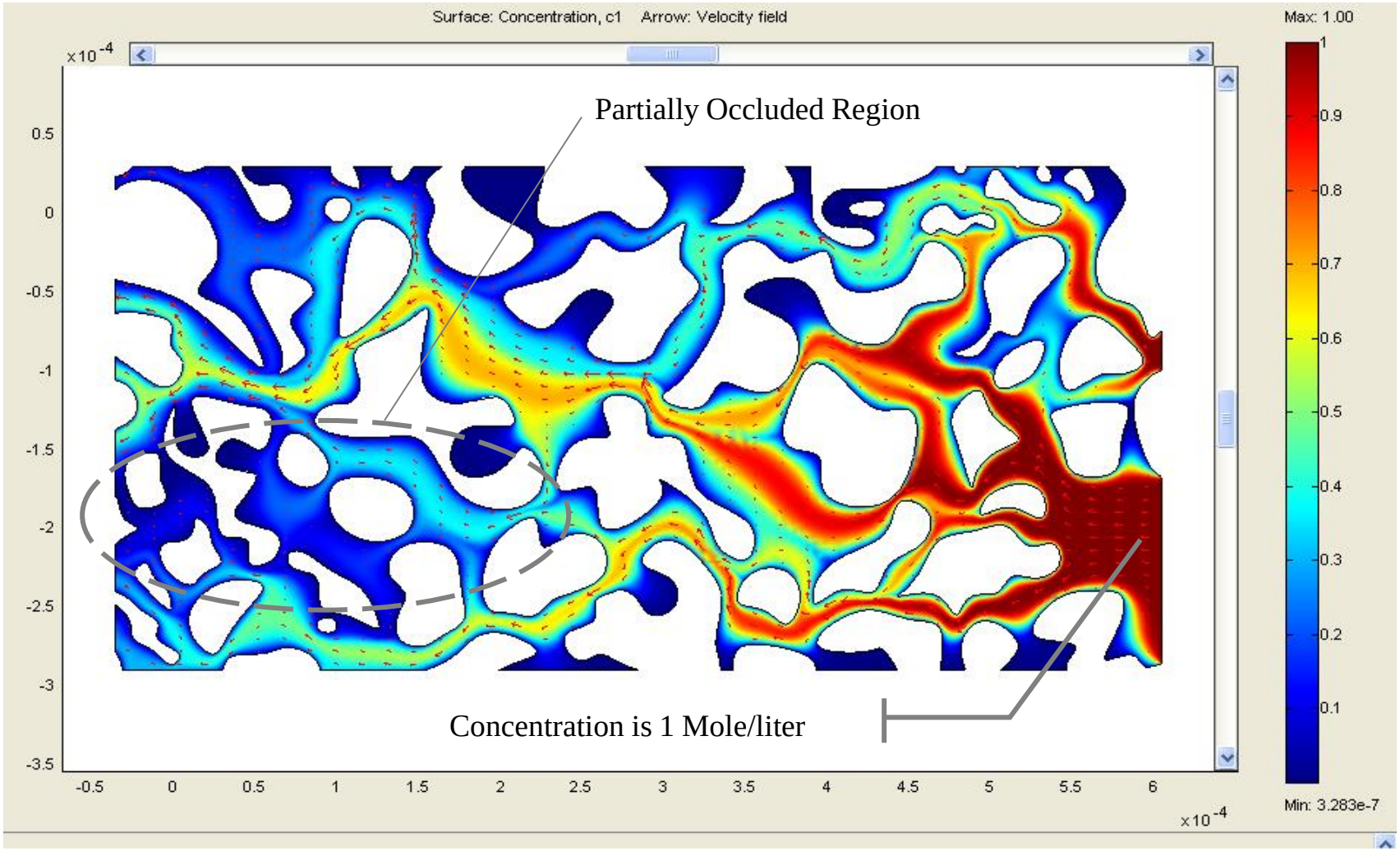
In-flowing Reactant Concentration Field



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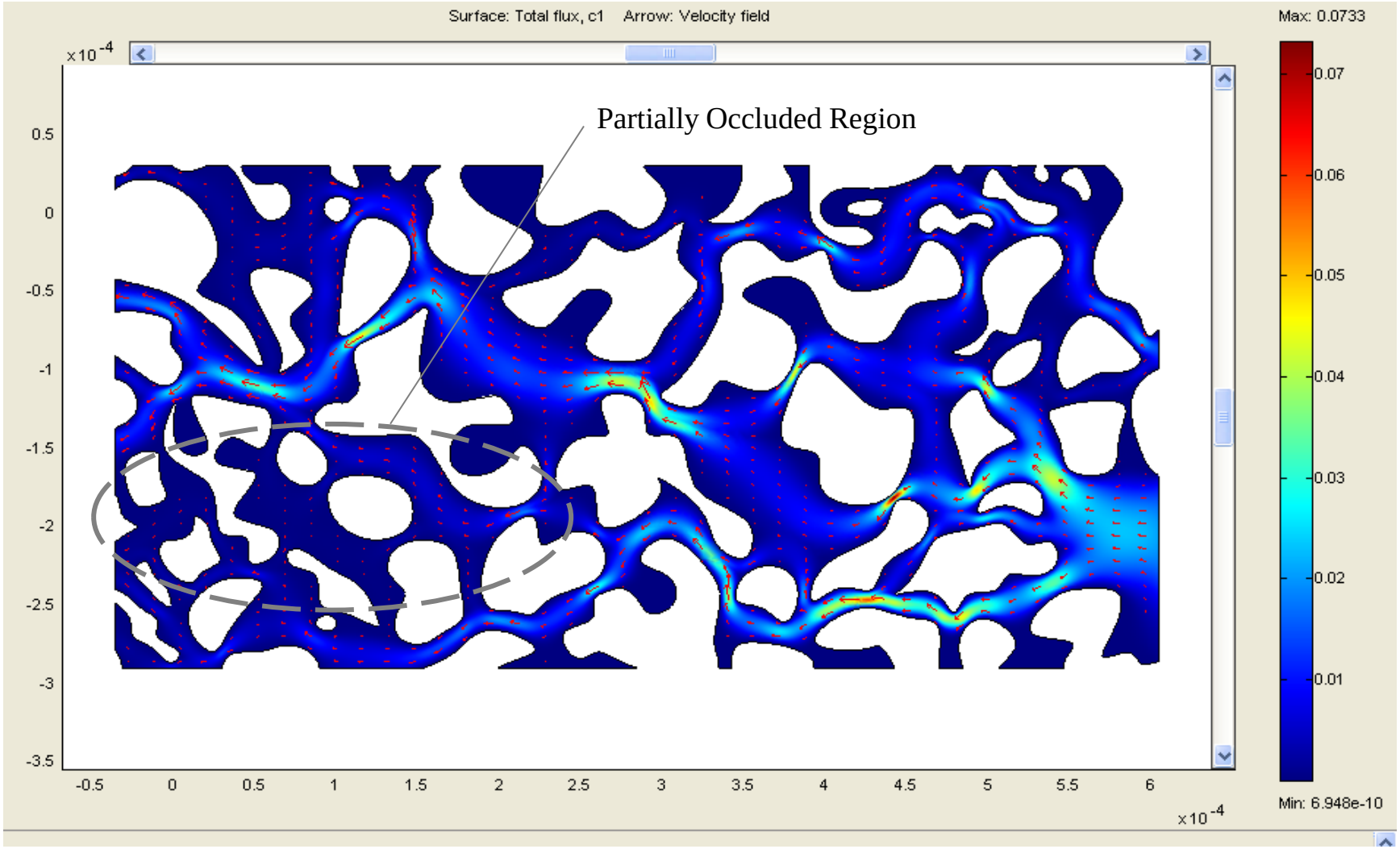
Inflowing Reactant Flux



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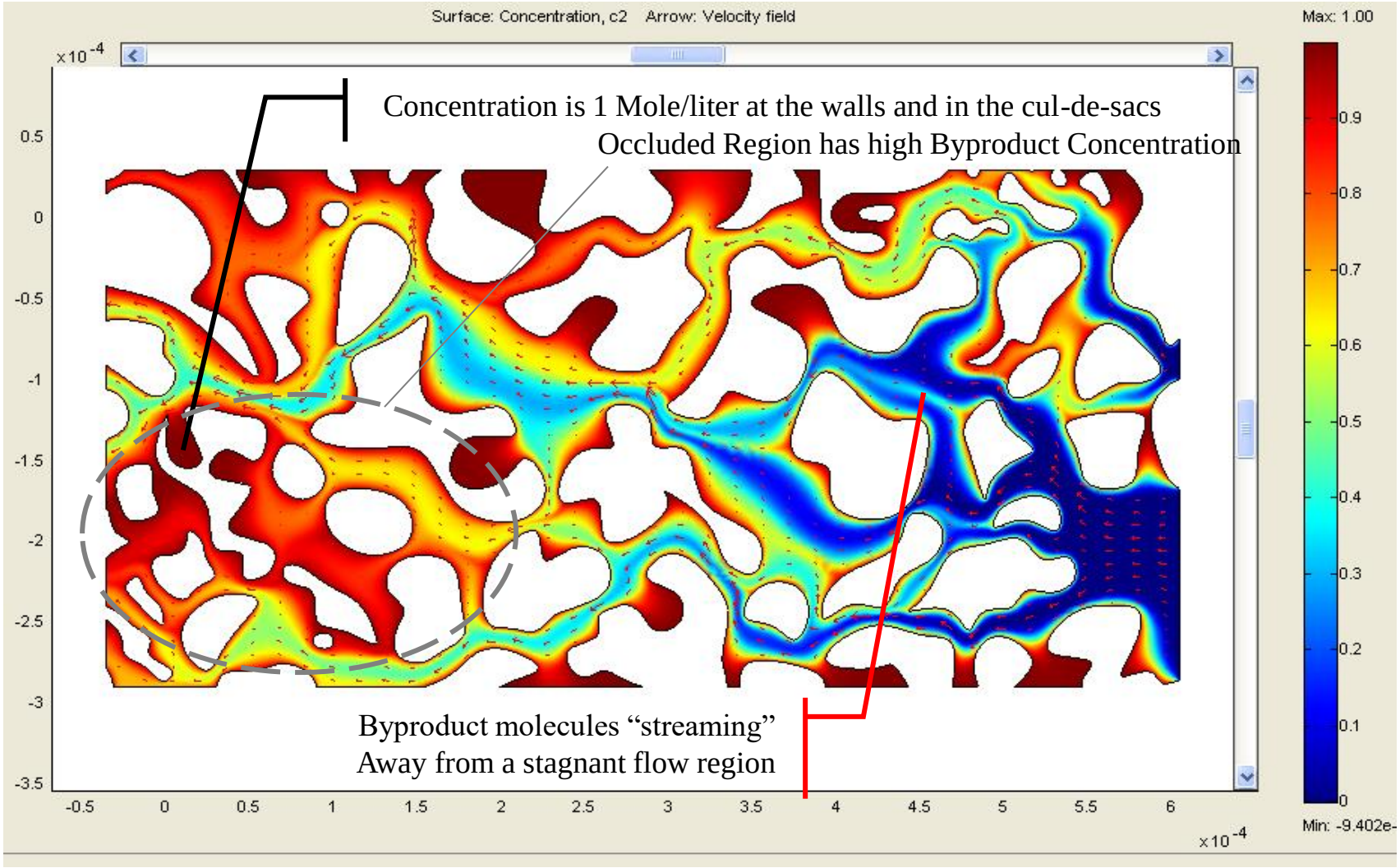
Outflowing Reactant Byproduct Concentration



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Conclusions

1. A relatively few number of accidental “Choke Points” can easily occlude a relatively large region that would otherwise be catalytically active.

2. Reaction byproduct gas bubbles will tend to form in the larger cul-de-sacs where capillary force bubble compression is low and gas concentration is high.

3. Once reaction byproduct gas bubbles form, they may remain in place indefinitely

4. Mass transfer by diffusion processes will be slowed down in porous regions by the same amount for all reactant and reaction byproduct species.

5. Catalytic particles in porous regions and coatings are not necessarily electrically connected to current carrying structure, and thus, may not carry current away from the reaction sites, as intended

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