A challenge

"…discrete models of an entire monolith reactor, even a relatively small one, would require vast computational resources when the computational domains are fully discretized … by means of the finite element … method;

in fact, such simulations are not tractable with these conventional CFD methods and therefore have not yet been seen in the literature."

from F. Bertrand et al., Towards the simulation of the catalytic monolith converter using discrete channel-scale models, Catalysis Today 188 (1) 2012

Accelerating R&D with COMSOL: A Personal Account

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24-25 October, Singapore

COMSOL CONFERENCE SINGAPORE 2013

Outline

- Mathematical modeling & COMSOL
- Energy systems
  - Fuel cells (1998-present)
- Biomedical systems
  - Hydrogels (2004-present)
  - Human skin(2011-2013)
- Monolithic catalytic converter
  - New solver for weakly-compressible parabolic Navier-Stokes (2013)
- Conclusions

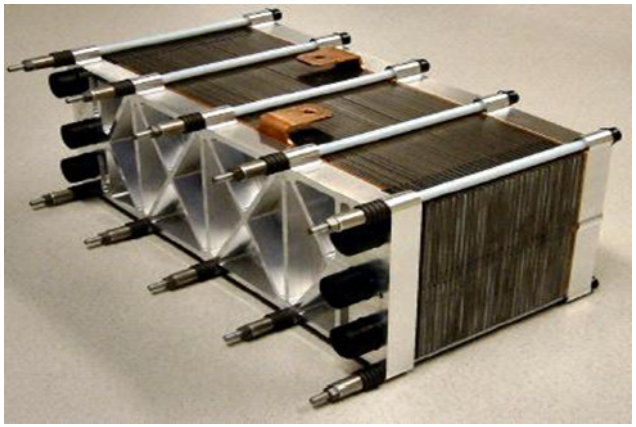
Mathematical modeling & COMSOL

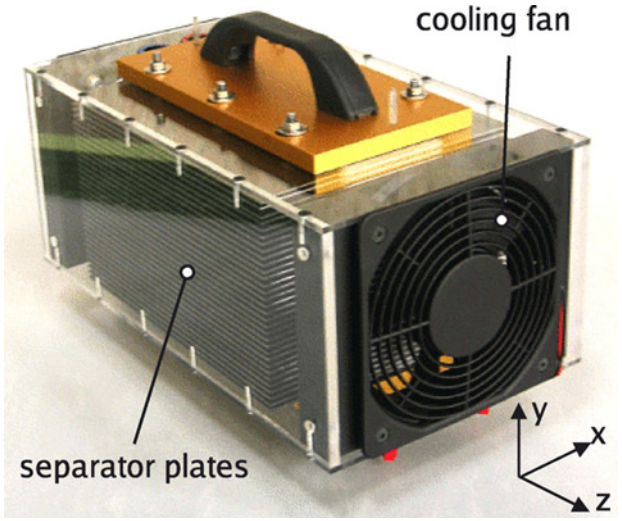
- A mathematical model and its solution need to satisfy three criteria:
  - sensible representation of the physics of interest
  - can be solved at a computational cost that is not prohibitive
  - the numerical implementation does not require too much effort in setting up
- COMSOL addresses all three criteria

Energy systems

Fuel cells

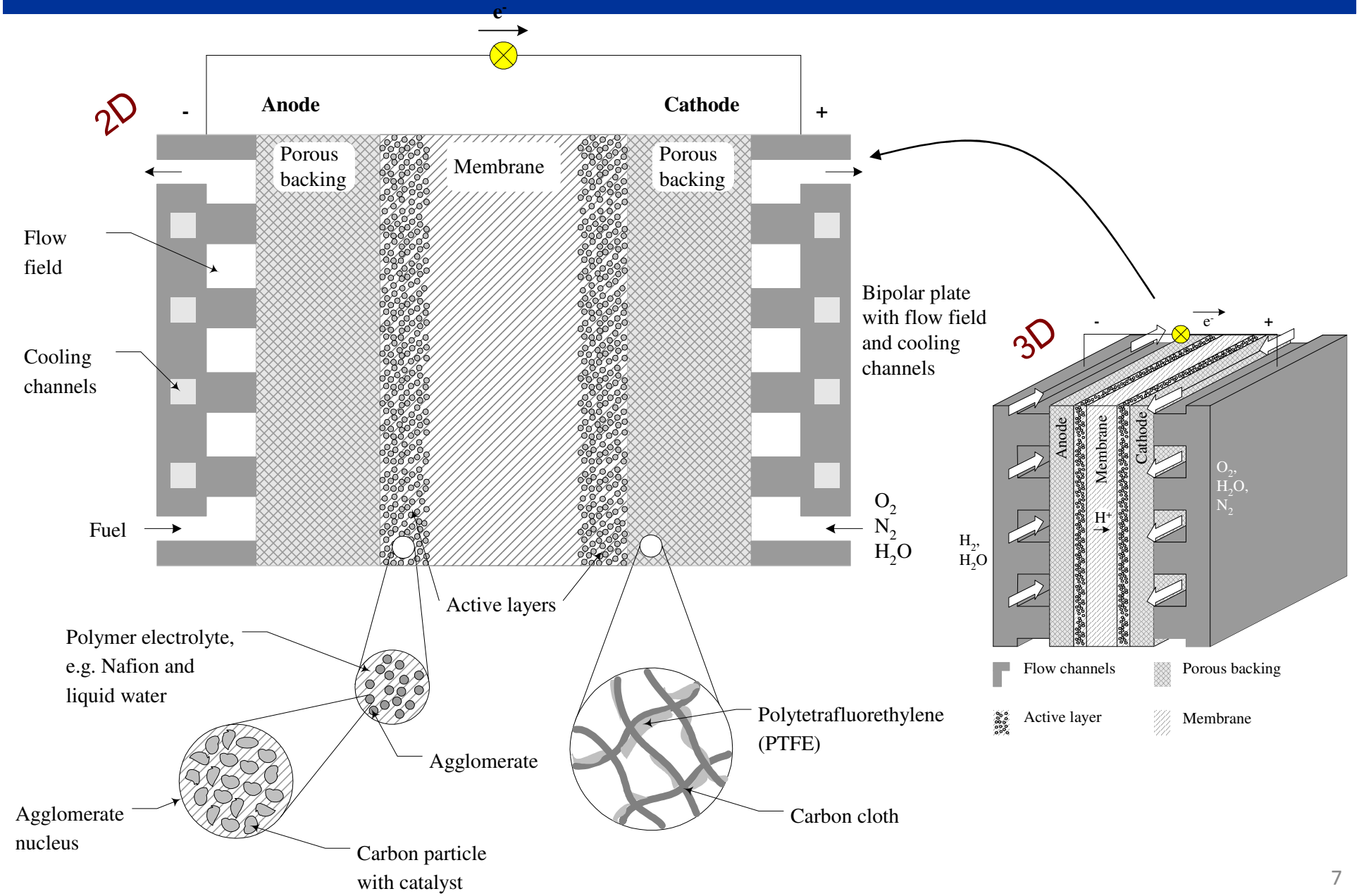
- Invented in 1839
- Advantages:
  - Chemical energy → electrical energy
  - Hydrogen + oxygen → water + energy + heat
- Characteristics:
  - Cost & complexity
  - Immaturity
  - Replacement technology
- Design issues:
  - Pressure drop
  - Distribution of reactants
  - Thermal management
  - Water management
  - Gas management
  - Cell performance





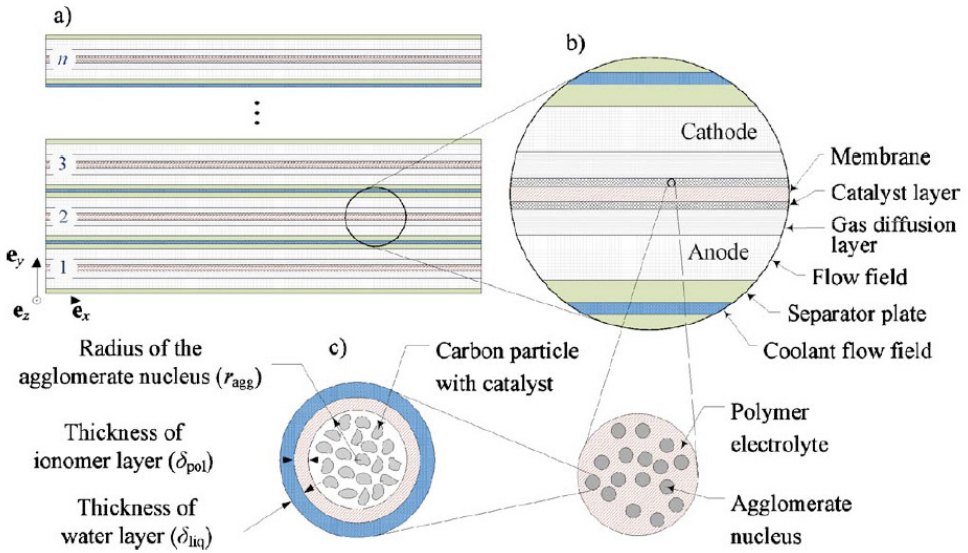
References: search for Erik Birgersson in Google Scholar
Photos: *R. Fluckiger et al. / Journal of Power Sources 172 (2007) 324–333* and Horizon fuel cells

The components of a fuel cell

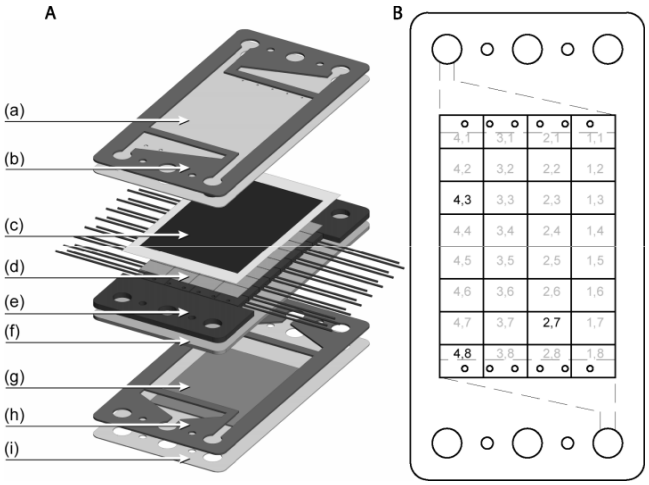


Fuel cells: Model

- Multi-physics:
  - Momentum
  - Mass
  - Species
  - Energy
  - Charge transfer
  - Two-phase flow
  - Electrochemistry
- Multi-scale:
  - Agglomerates (10^{-7} m)
  - Cell (10^{-3} - 10^{-1} m)
  - Stack (1 m)
- Automated code generation

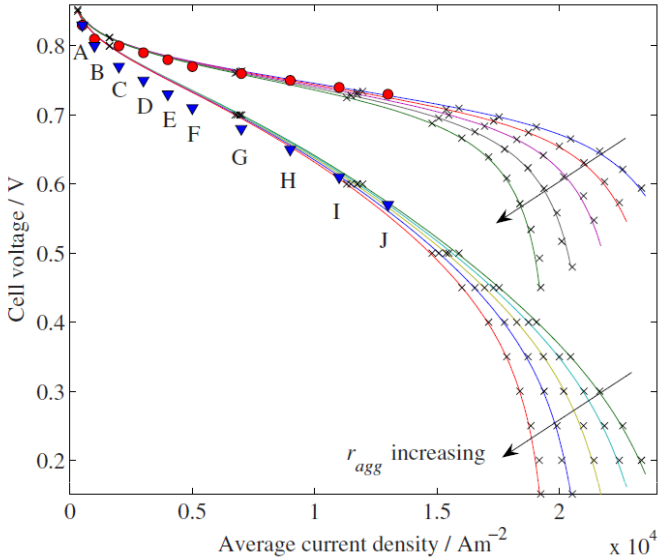


Fuel cells: Validation

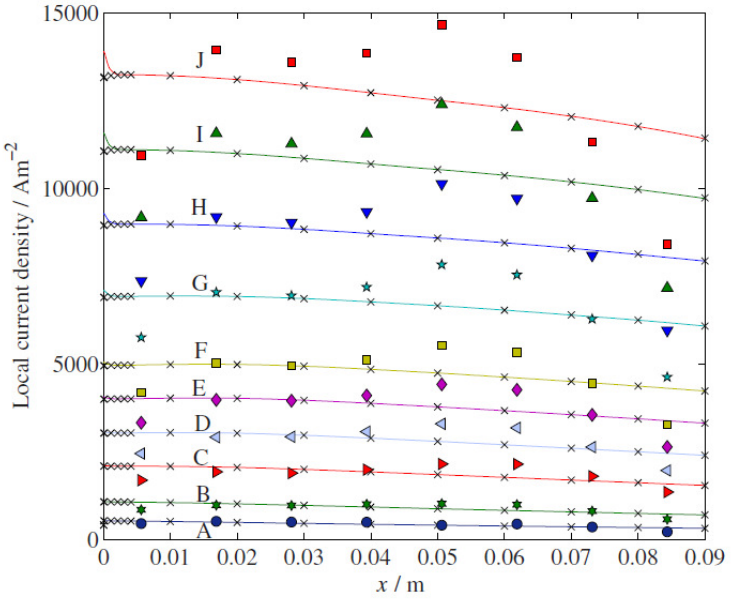


Fuel cell with segmented anode

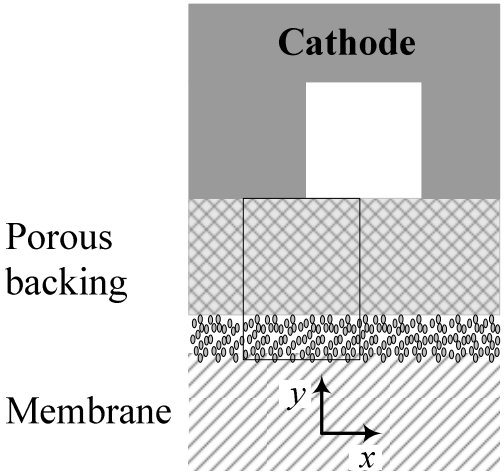
Global

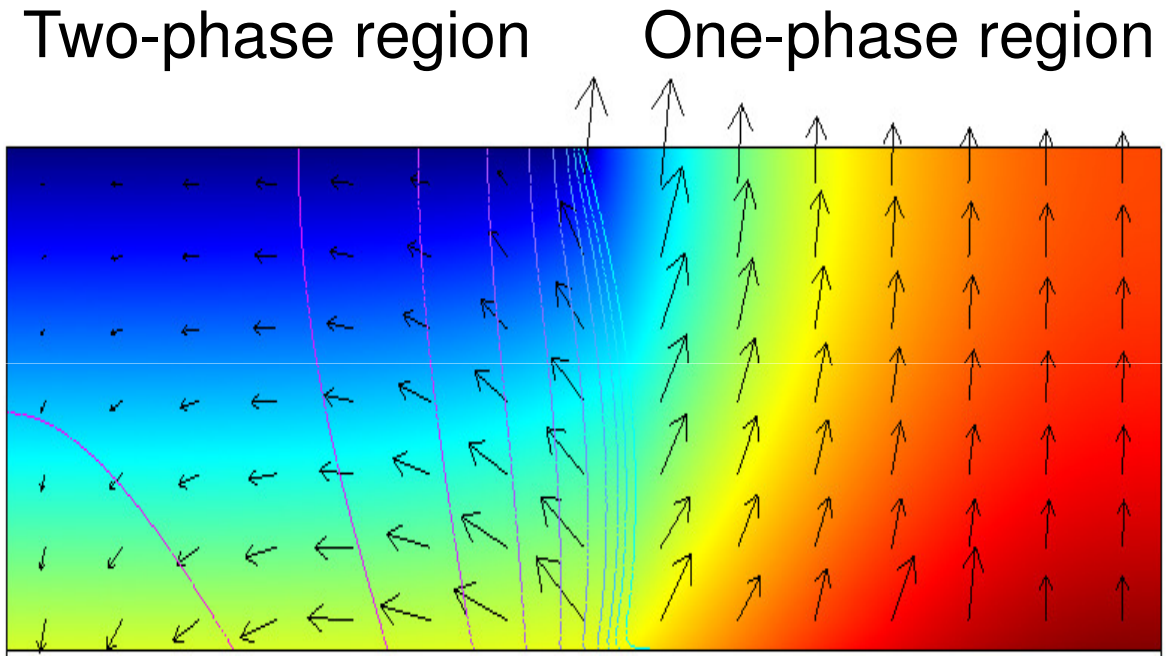


Local



Fuel cells: Results





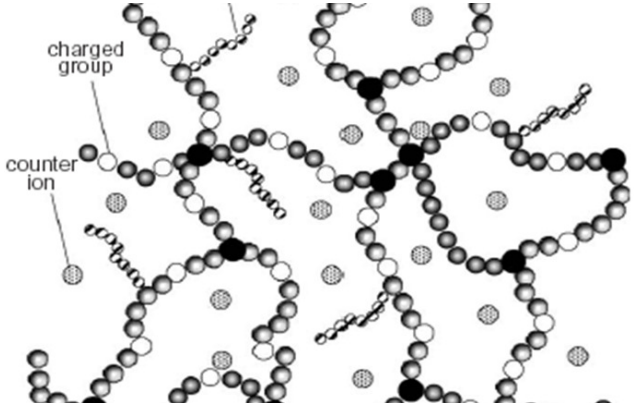
⟶ Velocity (gas) ~10^{-4} ms^{-1}

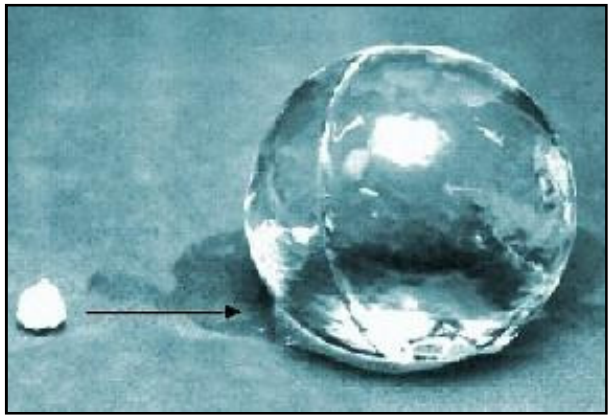
Current density ~10^{4} Am^{-2}, E_{cell}~ 0.6 V

Biomedical systems

Stimuli-responsive hydrogels

- A hydrogel comprises
  - 3D network of long polymer molecules
  - liquid
  - ions (if charged)
- Characteristics:
  - Excellent biocompatibility and biostability
  - Active sensing/actuating elements
- Stimuli:
  - pH
  - Electrical field
  - Temperature
  - Glucose
  - …

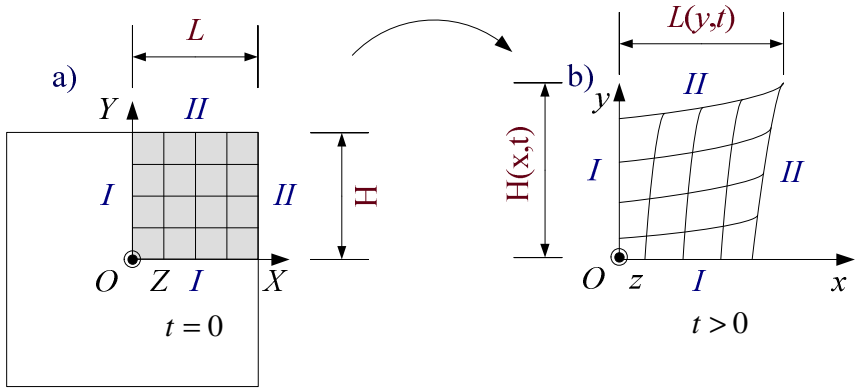


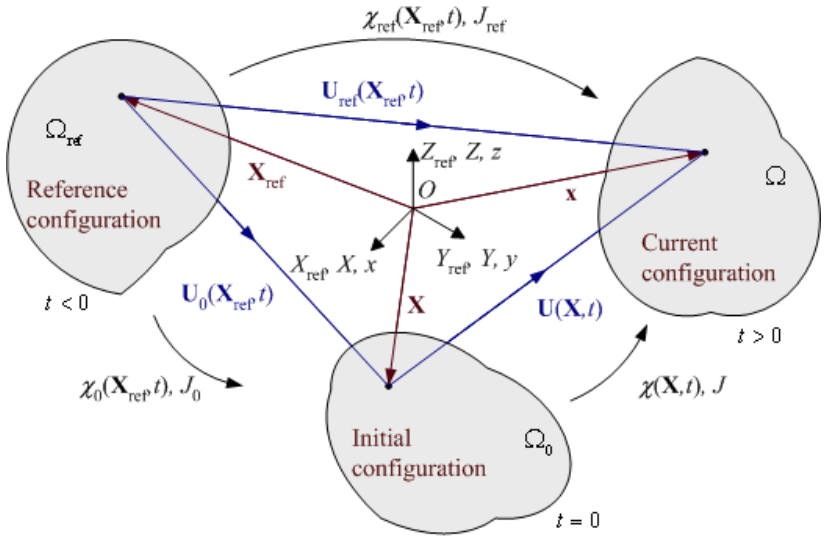


References: search for Erik Birgersson in Google Scholar
Figures from Ron Dagani, Chemical & Engineering News, June 9,1997 American Chemical Society

Hydrogels: Model

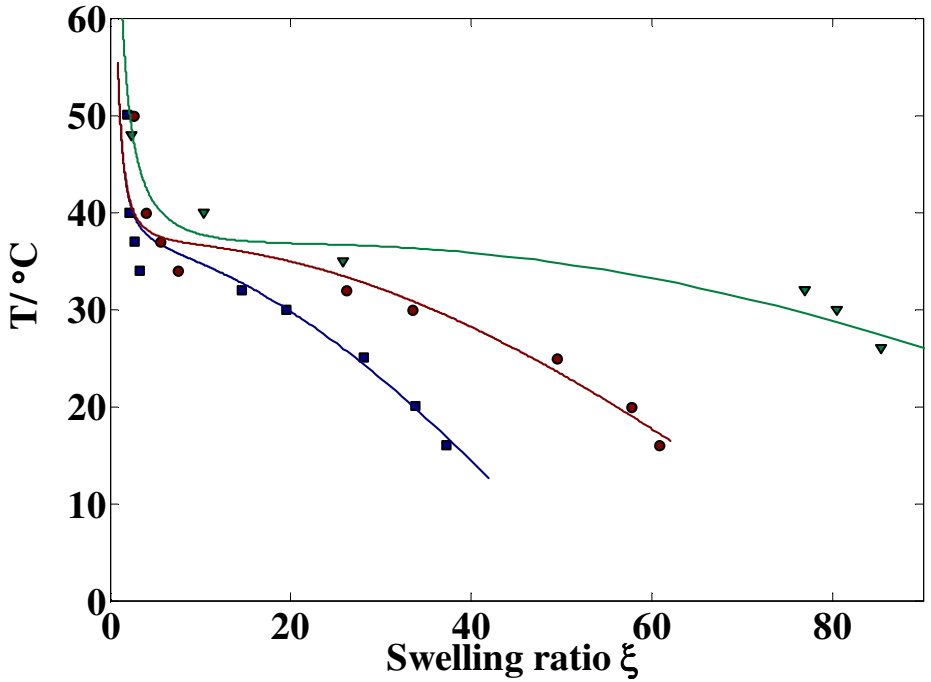
- Multi-physics:
  - Polymer phase
  - Liquid phase
  - Momentum
  - Energy
- Lagrangian description
- Arbitrary Lagrangian Eulerian (ALE) description



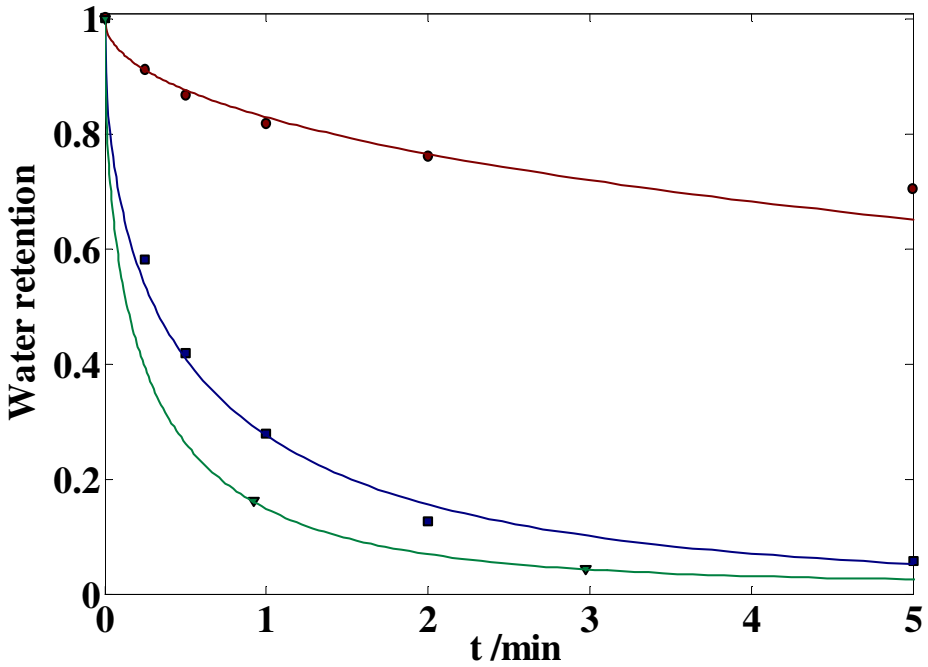


Hydrogels: Validation

Equilibrium swelling ratio



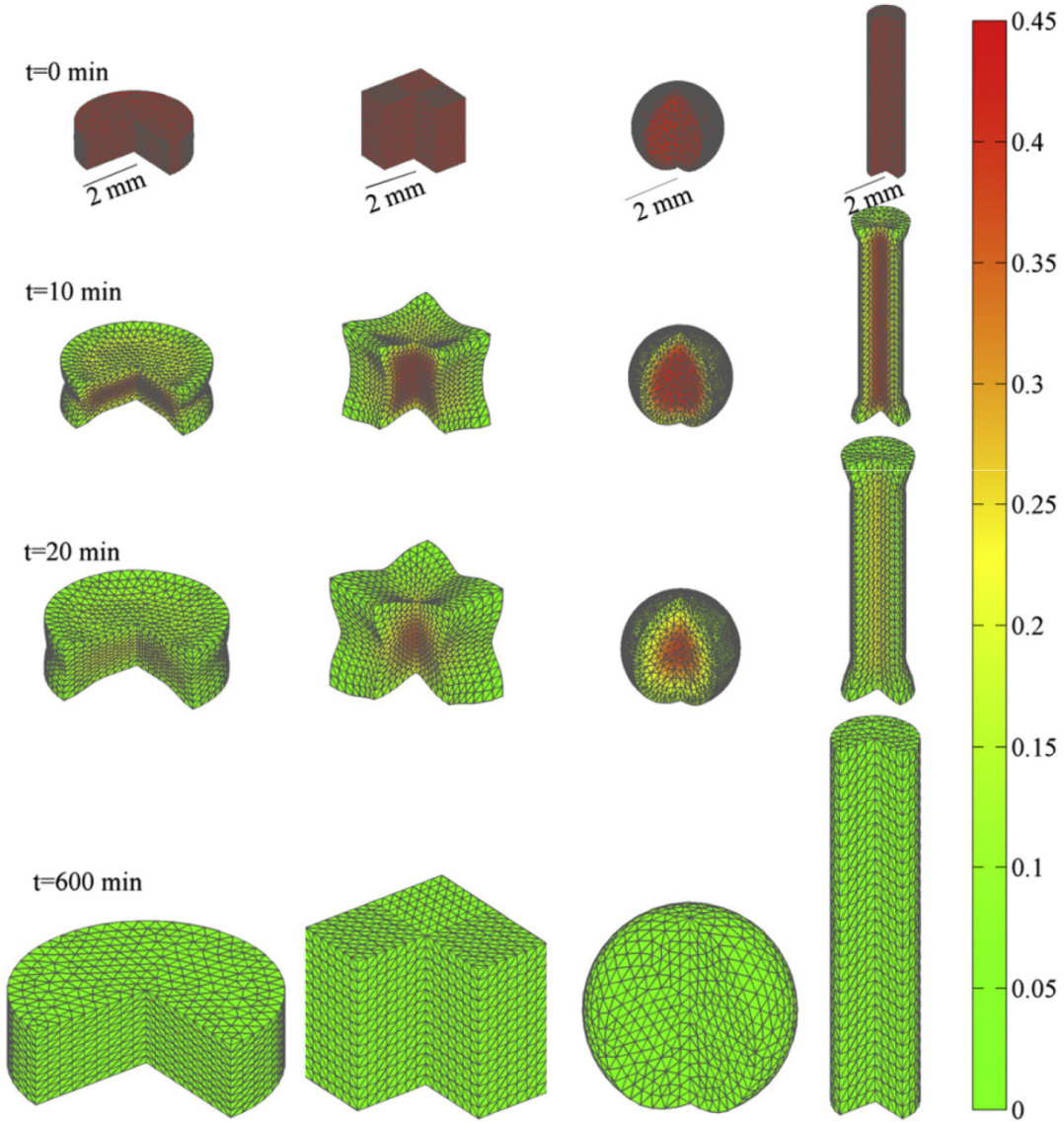
Transient deformation



(—) simulation
(■,●,▼) experiment

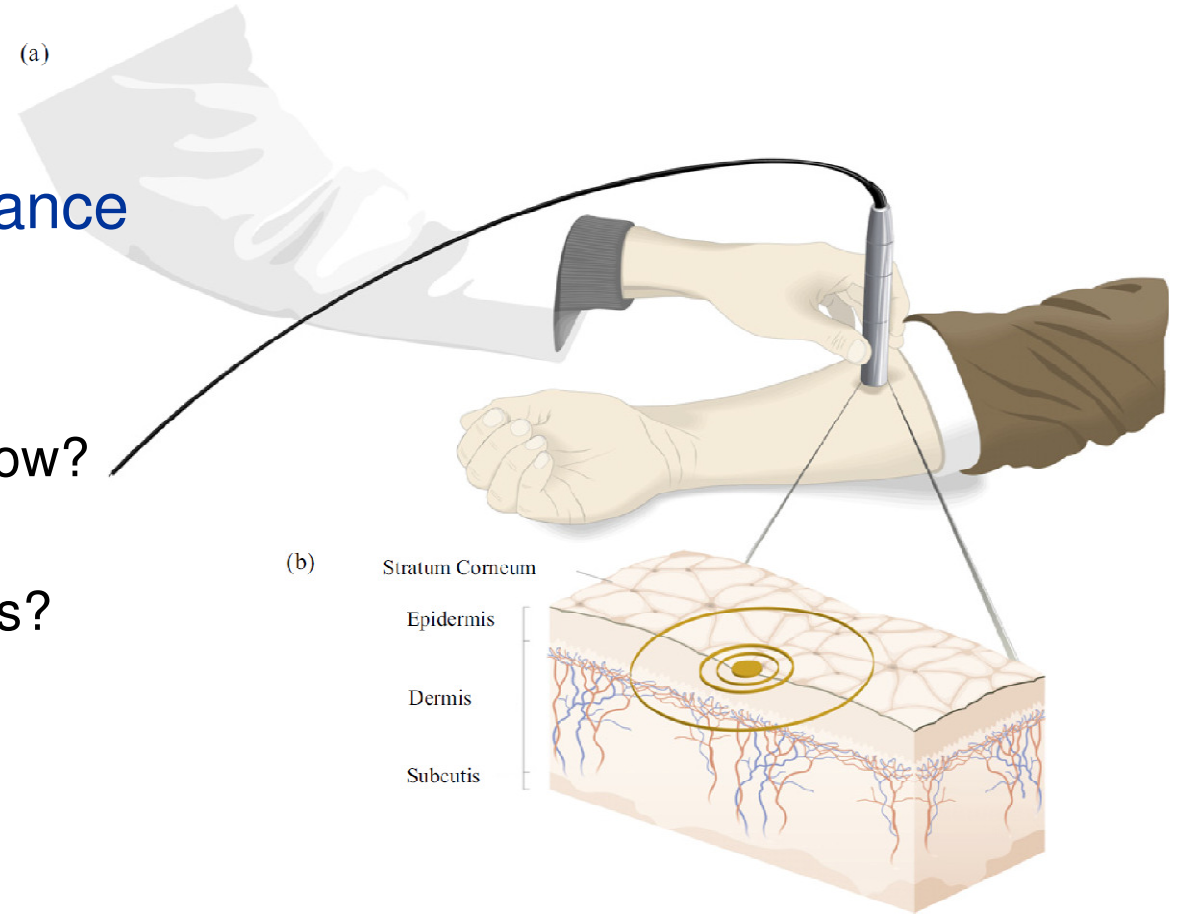
Experimental data (symbols) from: Zhang, X.Z., Zhuo, R.X., 2000, Eur. Polym. J. 36, 2301-2303; Cheng, S.X., Zhang, J.T., Zhuo, R.X., 2003, Macroporous poly(N-isopropylacrylamide) hydrogels with fast response rates and improved protein release properties, J. Biomed. Mater. Res 67 (1), 96-103.

Hydrogels: Results



Human Skin

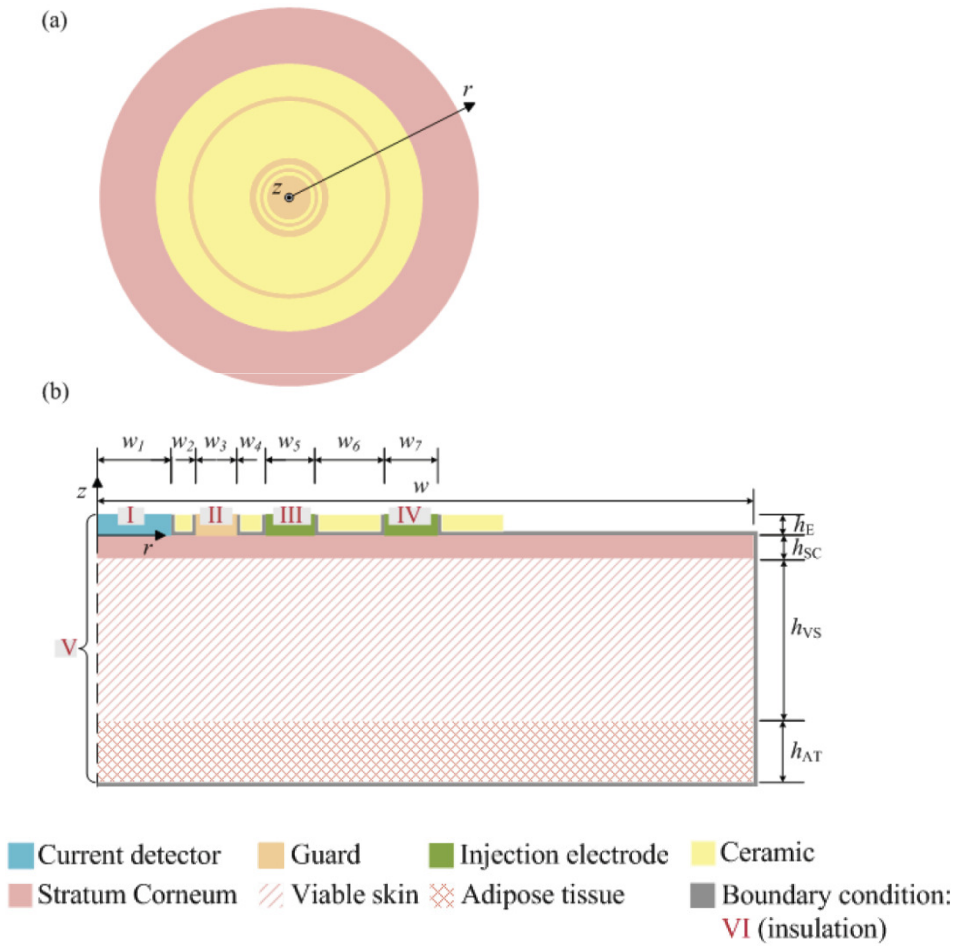
- Skin cancer
- Human skin
- Non-invasive impedance spectroscopy
- Design questions:
  - Where do currents flow?
  - Size of electrodes?
  - Number of electrodes?
  - …



U Birgersson et al., Non-invasive bioimpedance of intact skin: mathematical modeling and experiments, Physiological measurement 32, 1 2011
U Birgersson et al., Estimating electrical properties and the thickness of skin with electrical impedance spectroscopy: Mathematical analysis and measurements, Journal of Electrical Bioimpedance 3 (1), 51-60 2012
U Birgersson et al., A methodology for extracting the electrical properties of human skin, Physiological measurement 34, 723 2013

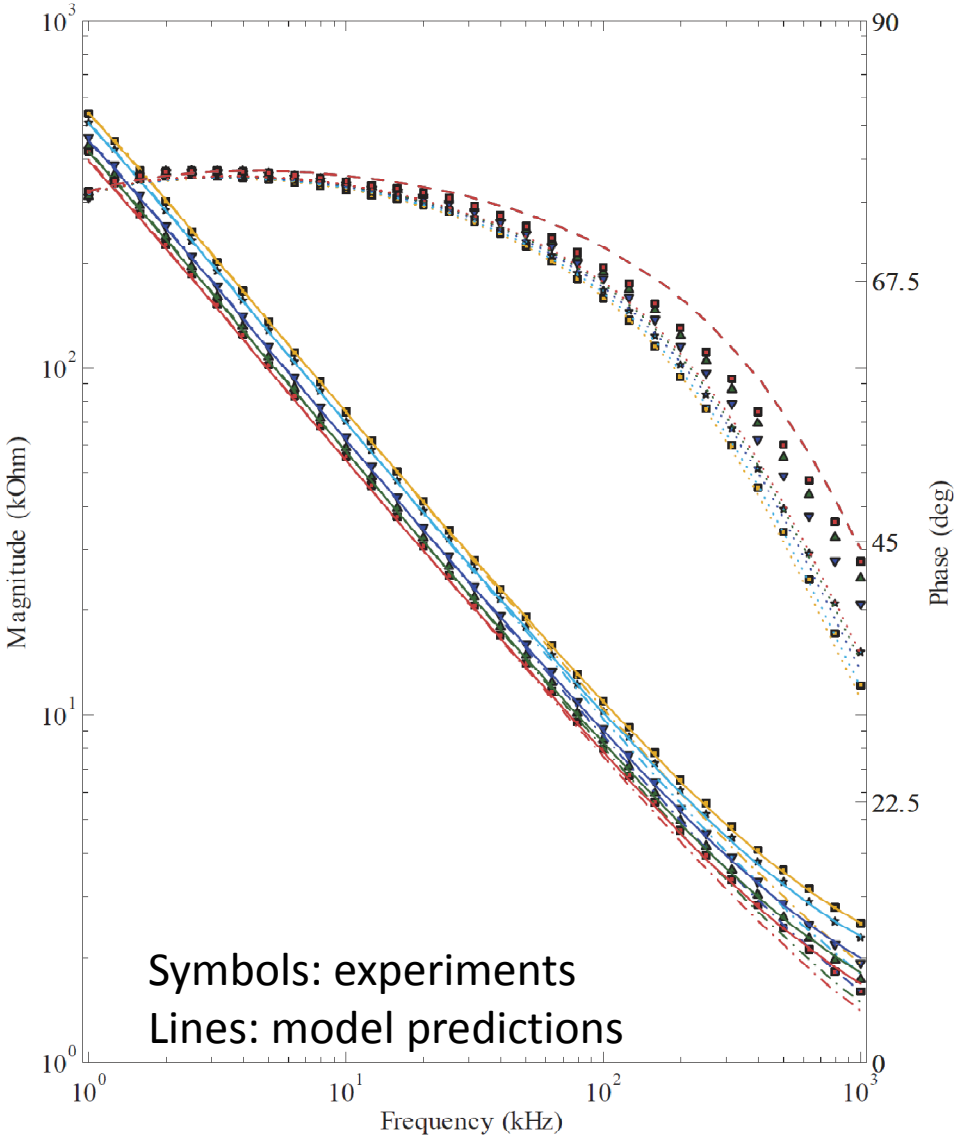
Skin: Model

- Equivalent electric circuits
- Mathematical model:
  - Impedance spectroscopy
  - Laplace equation for potential
  - Displacement and ohmic currents
- Reverse-engineer material properties
- Predict skin thickness?

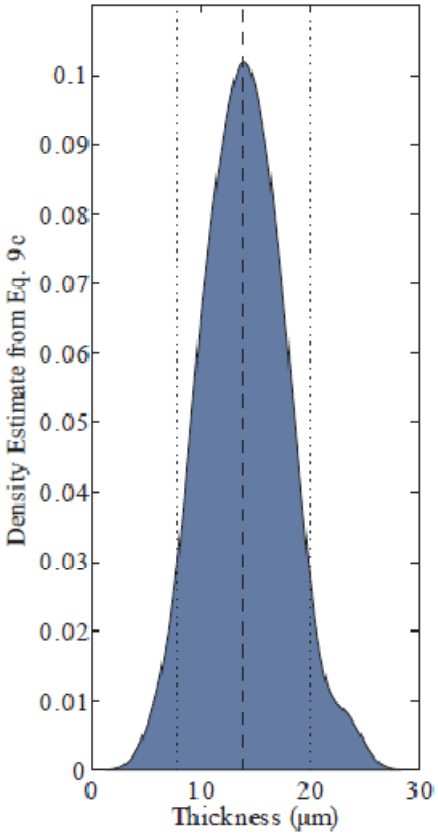


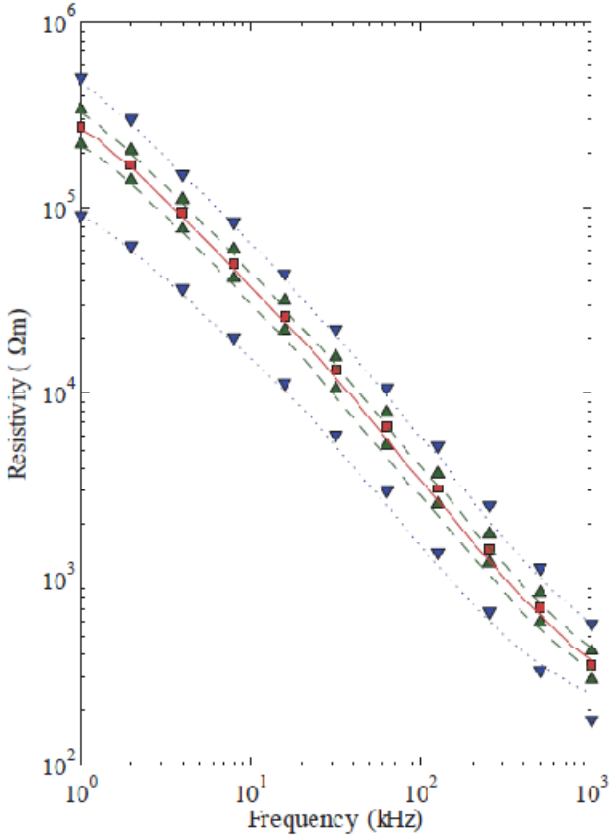
Skin: Validation

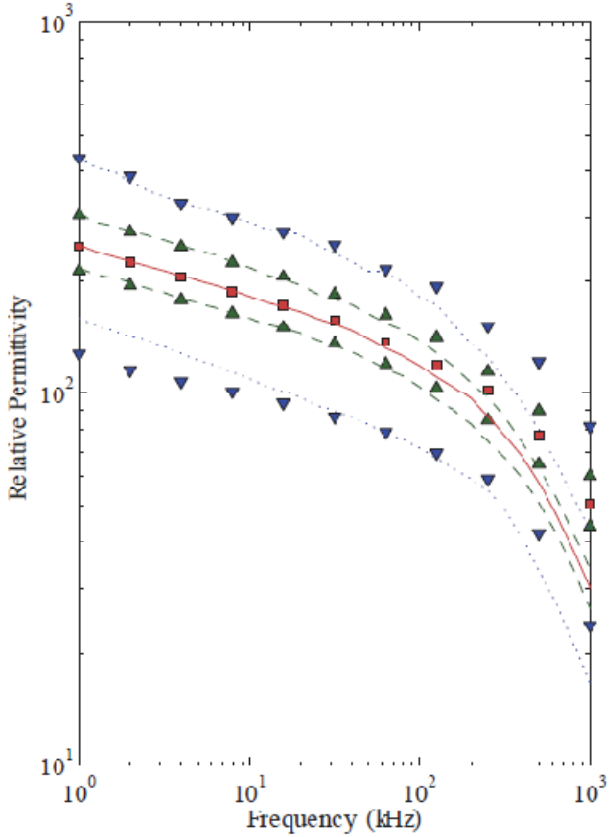
- Study with ethics approval and informed consent
- 120 young volunteers
- Equal distribution of men and women
- 24 ± 3 years of age



Skin: Results







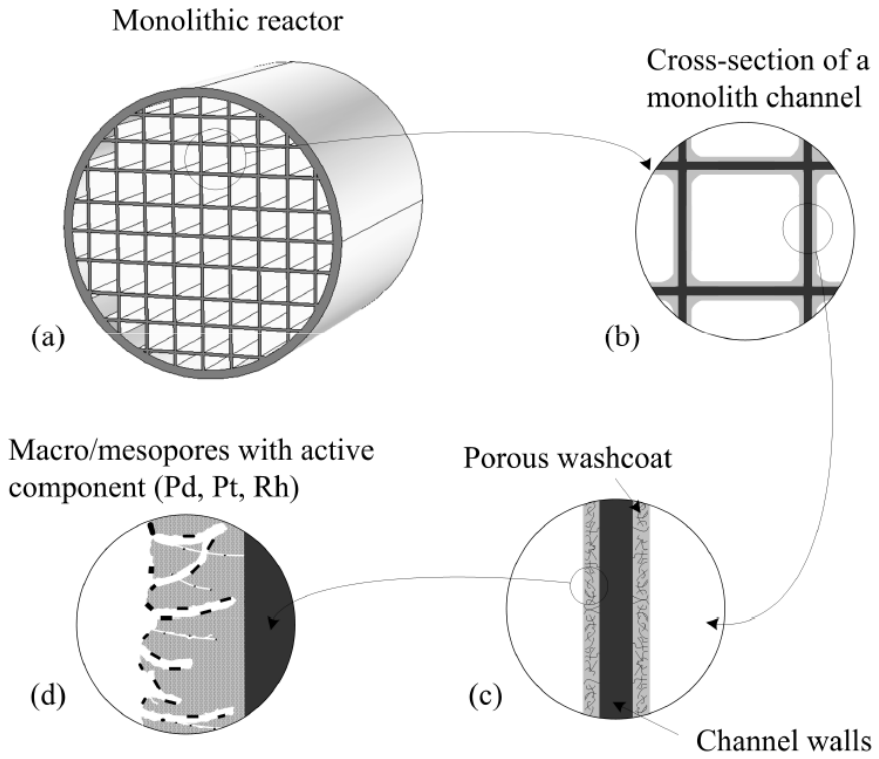
Skin thickness

Skin properties

Monolithic catalytic converter

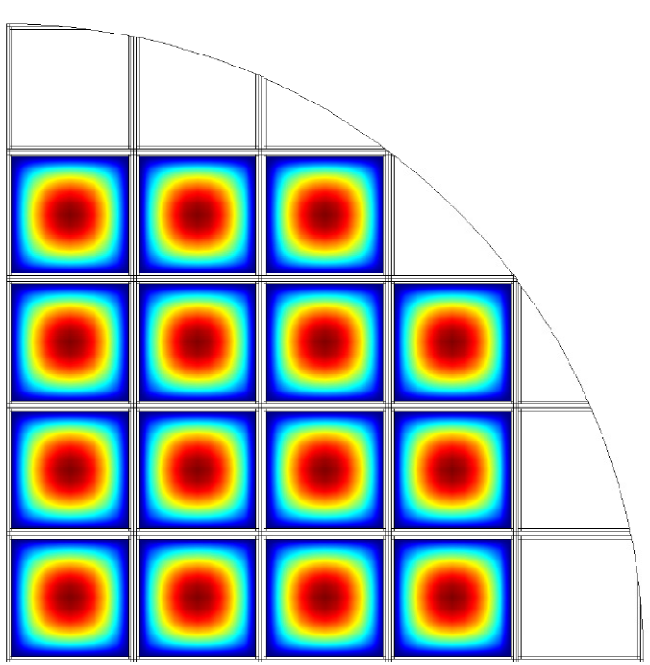
Monolithic catalytic converter

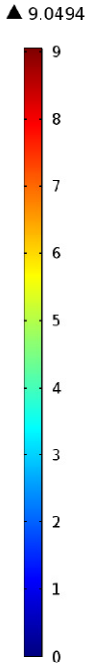
- Reduce toxicity of exhaust emissions
- Heterogeneous catalysis
- Mass, momentum, energy transport as well as reaction kinetics affect conversion
- Large number of channels
- Our solution: New weakly-compressible finite-element solver for parabolic Navier-Stokes

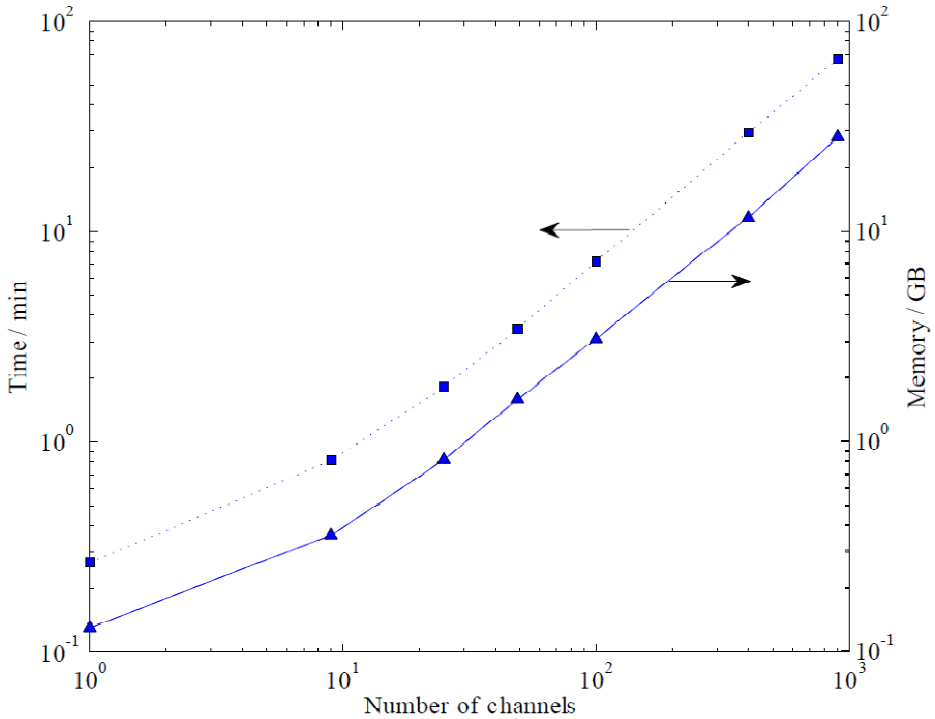


A. K. Sharma, E. Birgersson, M. Vynnycky, submitted for publication

MCC: Results







Streamwise velocity distribution

Challenge met: 1000 channels in 3D in less than 100 minutes with COMSOL

Conclusions

- An overview of mathematical modeling in different fields
- COMSOL Multiphysics:
  - Allows for a sensible representation of the leading-order physics
  - Solvers that keep on improving as COMSOL matures
  - Easy to use
  - Can be “tweaked” beyond standard formulations
- COMSOL allowed us to meet the challenge!