Liquid water transport in stochastic material of gas diffusion layers of polymer electrolyte fuel cells

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Objectives

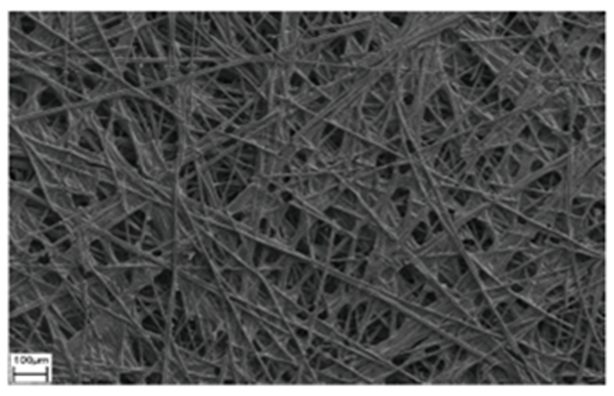
Hydrophobic and **hydrophilic** materials of gas diffusion layers affect **water transport** in PEFCs. Transport is **simulated** with the Lattice Boltzmann method in **stochastic geometries** of these layers. Droplets emerging at the **surface** are characterized with **statistical** methods.

- Gas diffusion layer design
- Application of the Lattice Boltzmann method
- Analysis of the contact angle
- Position of liquid water droplets

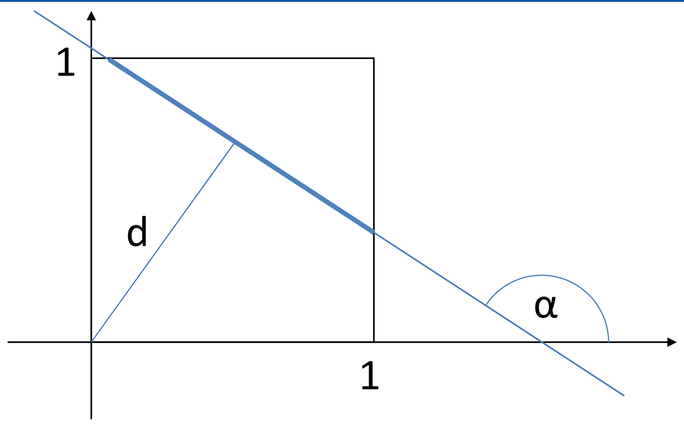
Approach

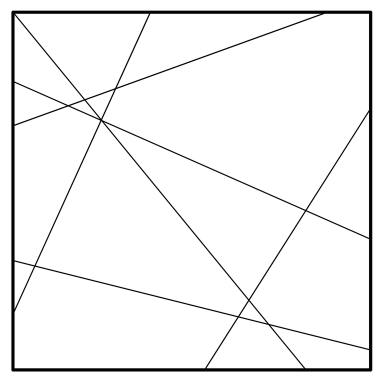
Stochastic Modelling

- Geometric characterization
- Poisson line tessellation (PLT)
- Intersecting lines in Hesse normal form
- Dilatation to fiber diameter
- Coverage by fibers related to the intensity γ of the PLT
- Validation by synchrotron images
- 25 realizations

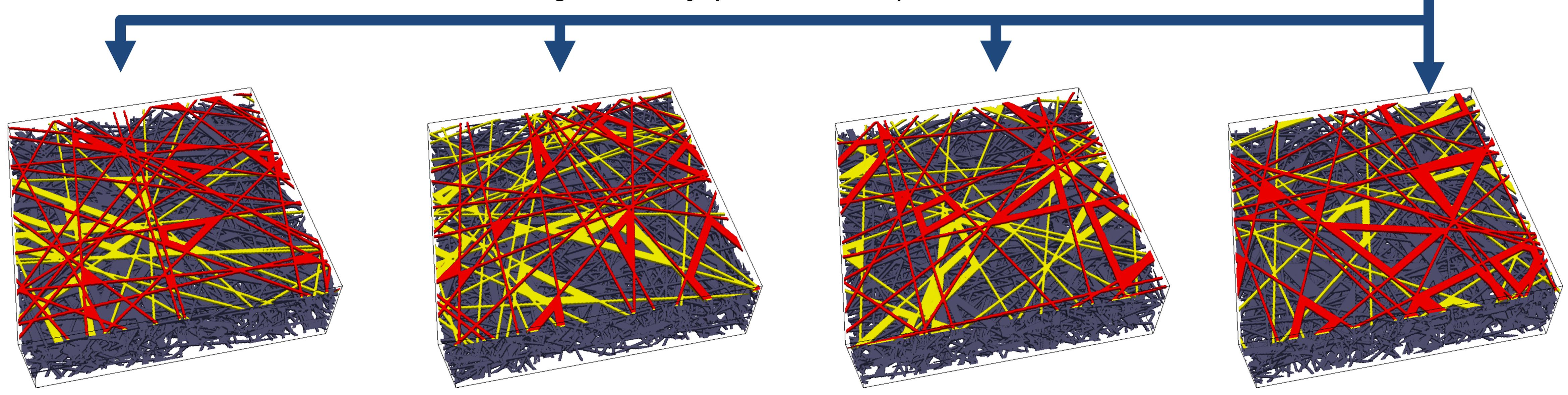


$$\gamma = \mathbb{E}\left| \bigcup_{n=1}^{\infty} \partial \Xi_n \cap [0,1]^2 \right|$$





Real structure – identification of geometry parameter γ of a Poisson line tessellation



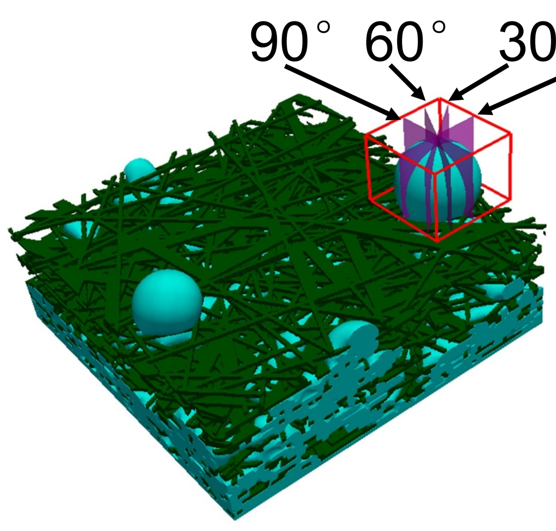
Stochastic equivalent 3D structures. 4 of 25 realizations are shown.

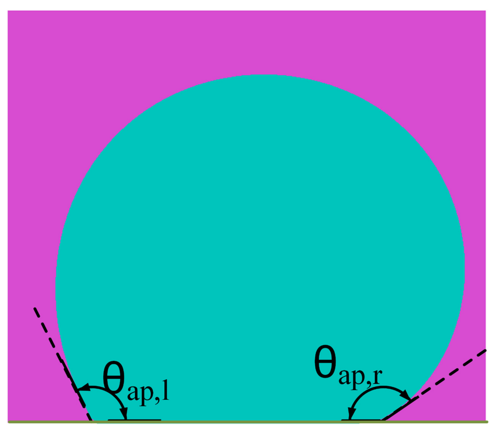
Transport Simulation

- 2-phase flow with Lattice Boltzmann
- Inherent high performance computer efficiency
- Combination of stochastic and numerical modelling

Simulation Results

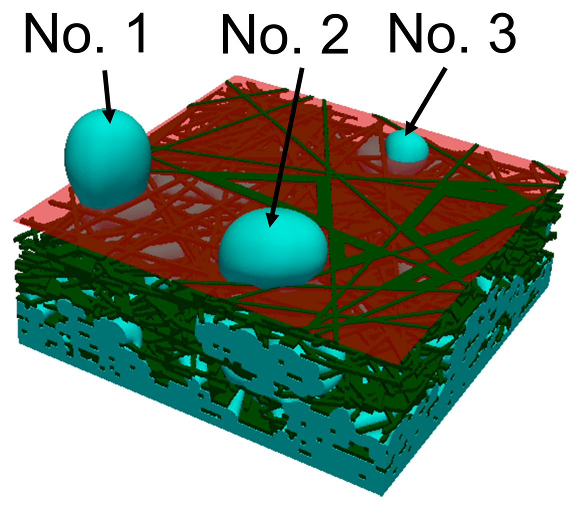
Contact Angles

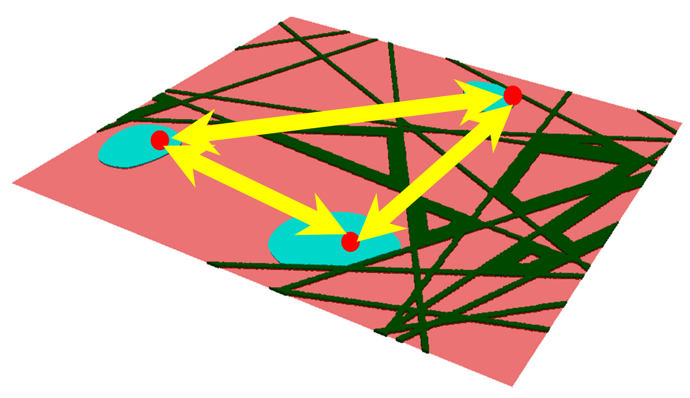




Apparent contact angles of a droplet at the rough surface

Breakthrough Point Distances





Distances between droplets emerging on the surface

- Statistic evaluation of **contact angles** and breakthrough point **distances** in **stochastic** reconstructed layer geometries
- JURECA application JIEK30: 1.4 million core hours per year

Conclusions

- Stochastic geometry turns simulation results into random variables
- Bridging the gap between micro-scale flow simulations in the GDL and macro-scale simulations in the gas channel
- Correlation between stochastic geometry and statistical distribution of the simulation results

Acknowledgements & References

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