The Lattice-Boltzmann Method for industrial, energy-related applications

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Benefits of numerical simulations

Why numerical simulations of fluid flows?

Fluid flows are found in a broad variety of industrial applications; their understanding is important for improving many technological processes.

Experiments:

- they require a great effort: e.g. the experimental set-up is one of the most difficult phase and for a second experiment one has to start from the beginning;
- they require long times to reach valuable results;
- they are expensive.

Numerical simulations:

- the set-up of a numerical “experiment” is a few kilobytes text file;
- today, with the present computational power, simulations are orders of magnitude faster than experiments;
- they are cheap.
The Method

LBM

Micro-geometry generation of:

- **ARTIFICIAL MEDIA**: e.g. fibrous materials randomly placed and oriented, innovative materials;
- **REAL MEDIA**: reconstruction of real materials (X-Ray Tomography, MRI);

**Mesoscopic model:** the proper link between Macroscopic and Microscopic world

- Two-phase Heat Equation
- **Mimic chemical properties of solid surfaces**: hydro -philic -phobic fibers

Advantages compared with traditional CFD:

1. easy handling of complex geometries;
2. simulating complex fluids;
3. massive parallelization.

Application to innovative materials

Climbing down to microscale..

Recent technologies provided new techniques to produce innovative materials which could be efficiently used as e.g. electrodes in fuel cells and energy storage systems, or innovative materials in many other industrial applications.

Platinum coated nonostructured supports, A. Arico’ et. al, Nature Materials (VOL.4) MAY 2005

Nevertheless, it is still not known how to proper design the porous microstructure in order to optimize the desired macroscopic features. How to optimally design a porous material for improving and optimizing the efficiency of such technologies?

→ LB Numerical Modelling
Energy storage materials
1. Energy storage materials for RFBs

Redox Flow Batteries: Slow species diffusion is a limiting factor. How the fibrous microstructure (orientation) affects mixing and dispersion of species?

1. **Streamwise dir:** higher dispersion when fibers are preferentially aligned along the streamwise dir.;
2. **Transverse dir:** this configuration presents the highest dispersion! (probably because particles can be carried by the flow following slightly tilted fibers);
3. **Permeability:** the same microstructure configuration presents the highest permeability.

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1. Energy storage materials for RFBs

Dispersion + Reaction efficiency

LBM applications

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1. Energy storage materials for RFBs

Maggiolo et al. 2018, En. Storage Materials, 16, 91-96
2. Fuel Cells materials
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**Fuel Cells:** slow water transport is a limiting factor. How hydro-phobic properties of fibers affect IMBIBITION and DRAINAGE process?

- **Neutral**
- **Hydrophobic**
- **Hydrophilic**
- **Two-wetting**

**IMBIBITION and DRAINAGE with Forcing**

- No wetting
- Hydrophobic
- Hydrophilic
- Double-wetting layer

Two-wetting layer: lower $\theta \approx 108^\circ$, upper $\theta \approx 72^\circ$;

Two-wetting layer promotes imbibition and drainage cycle;
2. Fuel Cells materials

Marie Curie EU Project **HyPoStruct**: 

“A key breakthrough in hydrogen fuel cells: enhancing macroscopic mass transport properties by tailoring the porous microstructure”

1. 3D GDL models will be **reconstructed with X-rays scanning**.
2. the **statistical characterisation** of fibers distribution and orientation of reconstructed GDL models
3. **simulations** with varying different microstructure properties* number, size, distribution of fibers, 
   * preferential alignment, 
   * wettability of fibers.

**GOAL**: identify the main mechanisms of liquid transport. In particular, the influence of anisotropy and hydrophobic properties of the microstructure on water transport. ⇒ Identify the **IDEAL MATERIAL**

![Statistical characterization](image)
Pharmaceutical tablets
Pharmaceutical tablets

Pharmaceutical coating of tablets. How to improve the uniformity of the coating and the efficiency of the process?

▶ LB is able to catch the microscopic dynamics of spreading and adsorption of droplets;
▶ interestingly, we found that hydrophilic tablets could help to improve the uniformity of the coating process.

Literature

LBM simulations
Self-cleaning materials
4. Self-cleaning materials

How we can protect surfaces from fouling via wetting?

The chemical composition of tar is very difficult to characterise;

- the majority of organic tar compounds is considered to have **low water-solubility**;
- over the last 20 years research efforts have been focused on **hydrophobic adsorbents**;

**Is tar hydrophobic?**

If YES, we can try to protect the plates with a **WATER FILM** induced by tuning the chemical properties of the plates as **HYDROPHILIC** so that TAR will be repelled.

source: British Glass & Glazing.co.uk
4. Self-cleaning materials

How the droplets formation is related to self-cleaning?

Looking closer we observe that:

1. **tar** shows an unexpected **tendency to attach to the droplets surface** (the liquid-gas surface). Probably because of **BENZENE-WATER AFFINITY**.

**Self-cleaning** seems to be promoted on a **hydrophobic** surface, by inducing:

1. **small droplets**; \[ \rightarrow \text{high mobility} \]
2. **large droplets surface**. \[ \rightarrow \text{large surface for tar collection} \]

Something in nature with similar self-cleaning properties?
CO2 sequestration
5. CO2 sequestration

CO2 sequestration is a complex and delicate mechanism. How LB simulations can help:

1. via two-phase flow simulations (CO2 bubble) and transport of contaminants in porous media;
2. possible characterization of real soil samples then used as input for simulations;
3. fundamental understanding at the MICROSCALE (pores) of the phenomenon.

https://eesa.lbl.gov/

The soil can be reconstructed

1. via artificial packing of spheres (figure on left);
2. via real reconstruction.
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Reynolds et al. PNAS 2017, 114 (31) 8187-8192
Other applications

- microfluidic devices (cancer research);
- bio fluid-dynamics (blood flow in complex veins);
- injekt micro-printing technologies;
- boiling phenomena in industrial processes;
- superhydrophobic surfaces for drag reduction.