Coupling Lattice Boltzmann 3D flow simulation in porous media with X-ray microtomographic imaging

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Within 2 European cross-border regions:

- **Meuse-Rhine Euregio**
  - 3 countries (BE, NL, DE)
  - 4 regions

- **University of the Greater Region**:
  - 4 countries (BE, DE, LU, FR)
  - 7 universities
  - 115 000 students
  - 6 000 professors
Liège: an attracting city

Important centre for Transport & Logistics:
- 2nd river port in Europe
- 8th freight airport in Europe
A collaborative work at LGC (*)

Chemical Reaction Engineering

Mutiphase systems

Separation technologies

Chemical processes and sustainable development

D. Toye

M. Crine

P. Marchot

A. Léonard

(*) Laboratoire de génie chimique
Flow through porous media

- A great number of unit operations, e.g.
  - Fixed bed catalytic reactors
  - Fixed bed adsorbers
  - Fibrous or granular filtration systems
  - Packed column absorbers
  - Distillation columns
  - ....

- Complex (random) porous media whose geometry and texture directly affect fluid flow hydrodynamics.

- How to deal with this complexity?
Two objectives:

1. To get a detailed description of porous media geometry
   - X-ray (micro)tomographic imaging

2. To develop a flow simulation model able to deal with the complex geometry of porous media, in terms of boundary conditions
   - Lattice Boltzmann Methods
X-ray tomography principles

- **Objective**
  - Irradiating an object with X-ray under numerous angles, using a fan beam or a cone beam configuration, to get 2D or 3D images of phase saturation distribution
X-ray tomography principles

- Theory
  - Visualization technique based on X-ray transmission:
    - Beer-Lambert law:
      \[
      \frac{dI}{I} = -\mu \, de
      \]
      \[I_0 \quad \mu \quad e \quad I\]
  
  - \( \mu \): attenuation coefficient
    - \( \mu = \text{const.}: \) homogeneous material
    - \( \mu = \text{fct.}(e): \) heterogeneous material

- \( X \)-ray intensity attenuation along one line depends on local attenuation coefficients values encountered along that line
X-ray tomography principles

- Values of the attenuation coefficient $\mu$ depends on:
  - Material properties
    - the density $\rho$
    - the atomic number $Z$
    - the atomic mass $A$
  - X-ray energy $E$

- The most important factors are:
  - The density (gas-solid; gas-liquid): $\rho^1$
  - The atomic number $\sim Z^2$ (at low energies, $Z/A \sim \text{Const.}$)

\[
\mu(E) = a \rho \frac{1}{E^n} \frac{Z^m}{A}
\]

$n$ and $m$ depends on X-ray energy range
  - At “low” energies: $m = 3.8$ ; $n = 3.2$
  - At high energies $m = 1$ ; $n = 1$
X-ray tomography allows differentiating elements with strong differences in density, e.g.:

- Gas and solid in porous material (deer antlers)
- Gas and liquid in gas-liquid contactors


Aferka et al. (2010). *Canadian Journal of Chemical Engineering* 88(4), 611-617
X-ray tomography also allows differentiating elements according their atomic numbers $Z$, e.g.:

- Adsorption of methyl iodide ($\text{CH}_3\text{I} ; Z_I = 53$) on activated carbon ($Z_C = 6$) in a gas mask filter (coll. Royal Military Academy)

Verdin, et al. (2010). 7th European Congress of Chemical Engineering (ECCE7), Prague
Tomographic image reconstruction

- Back projection algorithm

Using 3 views

Using many views

Transformation in the Fourier domain
Reconstruction time proportional to $N^3$

Blurred image
Tomographic image reconstruction

- Filtered back projection algorithm

Using 3 views

Using many views

Filtered view 1

Filtered view 2

Filtered view 3

Ramp filter

Sharper image
Microtomographic equipments

- High resolution (a few microns) visualization of small size (a few centimeters) objects
- Several commercial microtomographs, e.g.:
  - High resolution tomograph Skyscan 1172 (Skyscan, BE)
    - **X-ray ray source**
      Microfocus
      Voltage: 20-100 kV
      Current: 0-250 mA
      Cone beam geometry
    - **Detector**
      High resolution CCD camera (10 Mpixels)
      Pixel size: from 2 to 35 µm
A wide range of spatial resolutions and X-ray energies

- Microtomograph: 2 – 40 µm, 30 – 200 keV
- Synchrotron microtomograph: ≅ 0.3 µm, 6 – 150 keV
- Nanotomograph: ≅ 100 nm, 20-80 keV

A lot of applications
- Material sciences
- Electronics
- Biomedical
- Agrofood
- Geology
- ….
Macrotomographic equipments

- Macrotomography or ‘industrial’ tomography aims at visualizing much larger objects, e.g. unit operations.

- No commercial standard equipment
  - An example: the high energy tomographic facility available at the LGC
  - Main applications: visualizing hydrodynamics in distillation and gas-liquid absorption columns

**X-ray ray source**
- Focal spot: 0.8 mm
- Voltage: 30-420 kV
- Current: 2-8 mA
- Fan beam geometry (40°)

**Linear detector**
- 1280 photodiodes
- Pixel size: ~0.3 mm

A few macrotomographic images

- Gas-liquid distribution in a catalytic distillation Packing
  (Katapak™ SP12, Sulzer Chemtech, CH)

Catalytic zone

Separation zone

Liquid

Aferka, et al. (2005)
CHEMCON 2005, New Delhi
A few macrotomographic images

- Gas-liquid distribution in a structured packing
  (Mellapak Plus™ 752Y, Sulzer Chemtech, CH)

Liquid

Corrugated sheet
(Macro)tomographic applications

- Large scale high energies tomographic facilities available, a.o., at:
  - Helmholtz-Zentrum Dresden-Rossendorf (DE) (X-ray)
  - University of Texas at Austin (USA) (X-ray)
  - IIT Delhi (IN) (gamma-ray)
  - IFP-EN (FR) (gamma-ray)
  - Missouri University of Science and Technology (gamma-ray)
  - University of Washington  St Louis  (USA) (gamma ray)
Image analysis: a first example

- **Structure visualization of a open cell metallic foam**
  (RCM-NCX-1116 of RECEMAT® International, NL)

  - Material: Nickel – Chromium deposited onto open-cell polyurethane foam
  - Mean pore diameter: 1.4 mm
  - Grade number: 11 – 16 ppi
  - Specific area: 1000 m²/m²
  - Porosity: ~95 %
  - Density: ~0.6 g/cm³
2D images processing

Grey level
Binary
Filled

Hollow strut
« Filled » strut

Thresholding +
Binarization +
Erosion

Internal
« porosity »
filling
3D images processing

- **3D imaging**
  - 3D images are obtained by stacking a series of 2D cross sections
  - The grey level image is obtained by adding shadow effects on the binary image
Visualization of a structured packing used in absorption columns

(Mellapak Plus™ 752Y of Sulzer Chemtech, CH)

- Material: Embossed, perforated corrugated sheets of stainless steel
- Element height : 0.2 m
- Element diam. : 0.09 m
- Specific surface area : 510 m\(^{-1}\)
- Void fraction : 97.5 %
2D images processing

Grey level

Thresholding + Binarization

Binary
Two objectives

1. To get a detailed description of porous media geometry
   A 3D binary (gas-solid) matrix
   X-ray (micro)tomographic imaging

2. To develop a flow simulation model able to deal with the complex geometry of porous media, in terms of boundary conditions
   Lattice Boltzmann Methods
Lattice Boltzmann Models

- Fluid flow is represented by the movement of fictitious particles allowed to move and collide on a lattice.

- A triple discretization
  - Space $\rightarrow$ Lattice
  - Velocity or momentum
  - Time
The particles jump from one lattice node to the next, according to their (discrete) velocity.

- This is the **propagation phase**.

Then, the particles collide and get a new velocity.

- This is the **collision phase**.

Rules governing the collisions are designed such that the time-average motion satisfies mass and momentum conservation.
A limited number of lattices are able to cope with this constraint, e.g.:

2D: D2Q9
2 dimensions, 9 velocities

3D: D3Q19
3 dimensions, 19 velocities
Particle occupation within the lattice is described by a series of particle density distribution functions \( f_k \).

The evolution of these functions is described by a discrete form of the Boltzmann equation:

\[
\tilde{f}_k(x, t) = f_k(x, t) + \Omega_k(x, t), \quad k = 0, \ldots, q - 1,
\]

\( q \) : number of directions

\( \Omega_k \) is the collision operator: it determines the way velocities are modified after each collision.
Different ways to determine the collision operator.

They all describe a relaxation process towards equilibrium.

- **SRT**: single relaxation time approximation
  Bhatnagher-Gross-Kook (BGK) collision model
  \[
  \Omega_{k}^{BGK}(f) = -\frac{1}{\tau}(f_k - f_k^{(eq)}).
  \]

- **MRT**: multiple relaxation times approximation
  \[
  \Omega_{k}^{MRT}(x, t) = -M^{-1}\hat{R}\left[m(x, t) - m^{(eq)}(x, t)\right].
  \]
Simulation algorithm

- 3D tomographic binary image (matrix)

\[ f_k(x + e_k, t + \delta t) = f_k(x, t), \quad k = 0, \ldots, q - 1 \]

\[ \tilde{f}_k(x, t) = f_k(x, t) + \Omega_k(x, t), \quad k = 0, \ldots, q - 1. \]
Boundary conditions

- Pressure gradient between the entrance and exit faces
- Periodic boundary conditions on faces parallel to the flow direction
- Bounce back conditions (no slip) at the fluid-solid interface
LB simulations are expressed in lattice units.
The comparison with real systems implies to convert LB units into real (physical) units.
The conversion is rather tricky and different ways have been proposed.
A guideline: dimensionless variables, e.g., Reynolds number are conserved.

\[
Re_{\text{phys.}} = \frac{u_{\text{phys}} d}{\nu_{\text{phys}}} = Re_{\text{LB}} = \frac{u_{\text{LB}} d_{\text{LB}}}{\nu_{\text{LB}}}
\]

\(\nu_{\text{LB}}\) represents the kinematic viscosity in the LB domain.
It is fixed according to the value of the relaxation parameter \(\tau\).
A few examples of flow simulation

- Through a metallic foam
- Through an activated carbon fixed bed
- Through a fiber filter
- Through a structured packing
Flow through a metallic foam

- **Open cell metallic foam**
  (RCM-NCX-1116 of RECEMAT® International, NL)

  - Material: Nickel – Chromium
  - Mean pore diameter: 1.4 mm
  - Grade number: 11 – 16 ppi  → Pore aperture ~ 1.6 – 2.3 mm
  - Specific area: 1000 m²/m²
  - Porosity: ~ 95 %
  - Density: ~ 0.6 g/cm³

3D imaging of the porous texture

- Sample size
  - $176 \times 176 \times 352$ voxels $\sim 11 \times 11 \times 22$ mm
  - 1 voxel $\sim 64 \times 64 \times 64$ µm$^3$
  - Porosity: $\sim 95\%$

By stacking a series of 2D images
2D Flow visualization

- Velocity distribution in a plane perpendicular to the flow direction.

Simulation conditions
- D3Q19
- SRT (BGK) collision mode
- B.C. : - Pressure gradient
  - Periodic boundary cond.
  - Full bounce back (no slip)

Moving along the flow direction: 54 images

Preferential flow paths

« Strut »
3D Flow visualization

- Simulation conditions
  - D3Q19
  - SRT (BGK) collision mode
  - B.C.: - Pressure gradient
    - Periodic boundary cond.
    - Full bounce back (no slip)
Pressure drop

Ergun equation fitted on LB numerical simulations

\[
\frac{\Delta P}{L} = \frac{\rho \left(1 - \varepsilon\right)}{d_p \varepsilon^3} \left[ A \left(1 - \frac{\varepsilon}{Re}\right) + B \right] \cdot u_{sup}^2
\]

A = 77.9
B = 0.77
A few examples of flow simulation

- Through a metallic foam
- Through an activated carbon fixed bed
- Through a fiber filter
- Through a structured packing
Activated carbon granules synthetised from recycled PET bottles

**Pyrolysis**
700 °C, N₂ + 925 °C, N₂, 1 h

**Carbon particles**

**Crushing**

**Sieving**
Granulometry between 1 and 1.5 mm

**Irregularly shaped particles**

**Activation**
925 °C, CO₂
2D imaging of the porous texture

Images of cross-sections at three different depths separated by 2 mm

Bed porosity : ~ 78 %

- Sample size
  - Diam. : 14 mm
  - 1 pixel ~ 40 × 40 µm²

Verdin et al, 2010
FOA10, 10th International Conference on Fundamentals of adsorption
3D imaging of the porous texture

1 voxel ~ $10 \times 10 \times 10 \, \mu m^3$

2D Image

By stacking a series of 2D images

$H = 8 \, mm$

$\phi = 14 \, mm$

CA: Brown zone
Flow visualization

- Simulation conditions
  - B.C. : - Pressure gradient
    - Periodic boundary conditions
    - Full bounce back (no slip)
  - D3Q19
  - SRT (BGK) collision mode

- Sample size
  - Diam. : 14 mm
  - 1 pixel ~ 40 × 40 µm²

Solid : white zones
Pressure drop

\[ \frac{\Delta P}{L} = \frac{\rho}{d_p} \frac{(1 - \varepsilon)}{\varepsilon^3} \left[ A \frac{(1 - \varepsilon)}{Re} + B \right] \cdot u_{sup}^2 \]

Ergun equation fitted on LB numerical simulations

\[ A = 4887 \]
\[ B = 25 \]
A few examples of flow simulation

- Through a metallic foam
- Through an activated carbon fixed bed
- Through a fiber filter
- Through a structured packing
Flow through a fibre filter

- High permeability fibre filtration media
  (PST 290 of ACS Filter Mechelen, BE).

- Material: Polyester
- Grade number: G3 (EN 779)
- Fiber diameter: ~ 20 µm
- Porosity: ~ 98%

3D tomographic view

Air flow, 14 mm
2D imaging of the porous texture

- Sample size
  - 358 x 358 x 200 voxels
  - 1 voxel ~ 20 × 20 × 20 µm³

\[ Z = 20 \mu m \]

\[ Z = 1 \text{ mm} \]
Flow visualization

- Flow distribution within a series of cross-sections $\text{Re} \sim 1$
  - From the inlet of the gas flow ($Z = 20 \text{ µm}$) towards the outlet ($\rightarrow Z = 3 \text{ mm}$) of the filter

- Spreading of the gas flow within the filter cross-section
- Decrease of the maximum velocity

Max. velocity

$Z = 20 \text{ µm}$  $Z = 3 \text{ mm}$
Pressure drop

Ergun equation fitted on LB numerical simulations

\[
\frac{\Delta P}{L} = \frac{\rho}{d_p} \frac{(1 - \varepsilon)}{\varepsilon^3} \left[ A \frac{(1 - \varepsilon)}{Re} + B \right] \cdot u_{sup}^2
\]

A = 46.2
B = 0.35
Permeability of porous media

- Computed permeability

\[ K = \frac{\varepsilon^3 d_P^2}{A (1 - \varepsilon)^2} \]

<table>
<thead>
<tr>
<th>Material</th>
<th>( \varepsilon ) (-)</th>
<th>( d_P ) (m)</th>
<th>( A ) (-)</th>
<th>( K ) (m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Metallic foam</td>
<td>0.95</td>
<td>1.4 \times 10^{-3}</td>
<td>77.9</td>
<td>5.38 \times 10^{-8}</td>
</tr>
<tr>
<td>Activated carbon</td>
<td>0.78</td>
<td>1.25 \times 10^{-3}</td>
<td>4887</td>
<td>3.07 \times 10^{-9}</td>
</tr>
<tr>
<td>Fibre filter</td>
<td>0.98</td>
<td>6.5 \times 10^{-4}</td>
<td>46.2</td>
<td>2.02 \times 10^{-8}</td>
</tr>
</tbody>
</table>
A few examples of flow simulation

- Through a metallic foam
- Through an activated carbon fixed bed
- Through a fiber filter
- Through a structured packing
Flow through a structured packing

- Flow between two corrugated sheets of a structured packing

- Structured packing
  Sulzer Plastic MellapakTM 250 Y, Sulzer ChemTech, CH
  - Material: Polyethylene
  - Hydraulic diam. : 2 cm
  - Corrugation geometry
    - Triangular channel base : \( b_0 = 26\,mm \)
    - Triangular channel height : \( h = 13\,mm \)
  - Specific area: \( 250\,m^2/m^2 \)
  - Porosity: \( \sim 85\% \)
Two corrugated sheets of Mellapak 250 Y containing four triangular channels each (without perforation)
Flow visualization at low Reynolds

- Axial velocity $u_X$

Gas flows

Re = 20 (SRT-LBE)
Flow visualization

At higher Reynolds numbers: \( \text{Re} > 100 \)

**Plane A**

Re = 310

MRT-LBE

Re = 5040
Pressure drop

\[ \frac{\Delta P}{L} = \frac{\rho}{d_p} \frac{(1 - \varepsilon)}{\varepsilon^3} \left[ A \frac{(1 - \varepsilon)}{Re} + B \right] \cdot u_{\text{sup}}^{2} \]

- Stichlmair et al., (1989)
- Ergun equation fitted on CFD (NS) simulation
- Ergun equation fitted on LB simulation

\begin{align*}
LB \quad & A = 89 \\
& B = 0.54 \\
Stichl. \quad & A = 80 \\
et al. \quad & B = 0.37
\end{align*}

Two objectives

1. To get a detailed description of porous media geometry
   - X-ray (micro)tomographic imaging
   - A 3D binary (gas-solid) matrix

2. To develop a flow simulation model able to deal with the complex geometry of porous media, in terms of boundary conditions
   - A few challenges to take up
The numerical resolution of LB equation is simple and straightforward.

It however requires large execution time and massive memory access.

Two main solutions to reduce these drawbacks:
- To reduce the sample size: **image undersampling**
- To **parallelize** the computing architecture
Undersampling consists in sampling a reduced number of voxels from the original image.

- The sampling rate is defined as the ratio between the total and reduced numbers of voxels, along one direction in the space.

This modification of the gas-solid interface does not affect significantly the calculated values of pressure drop through an open cell metallic foam (RCM-NCX-1116).

- Experimental data

- Sampling rate of 7: voxel size: 224 µm
- Sampling rate of 6
- Sampling rate of 5
- Sampling rate of 4
- Sampling rate of 3: voxel size: 96 µm

The pore diameter is around 1.4 mm.
Image undersampling

This small modification can probably be explained by the absence of modification of the porous media morphology, e.g., its porosity × 32

<table>
<thead>
<tr>
<th>Number of voxels</th>
<th>~ 2 × 10⁸</th>
<th>6.4 × 10⁶</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>58³</td>
<td>67³</td>
</tr>
<tr>
<td>Sampling rate</td>
<td>7</td>
<td>6</td>
</tr>
<tr>
<td>Resolution (µm)</td>
<td>224</td>
<td>192</td>
</tr>
<tr>
<td>Porosity (%)</td>
<td>93.38</td>
<td>93.41</td>
</tr>
</tbody>
</table>
Parallel computing

- An LB simulation can hardly be executed on a single PC:
  - 10 gigabytes of memory and more than 10000 time steps are typically required
  - On a computer with a Pentium IV 3GHz processor, equipped with enough memory, it would take around 2 years to complete the simulation’s execution.

- The LB simulation can easily be executed in a distributed way
  - Using a supercomputer equipped with a great number of identical processors and a large amount of memory
  - Using a cluster of numerous desktop computers interconnected on a grid
Parallel computing

- LB codes are easily adapted to parallelization or task sharing among several computers on a grid
Parallel computing

- Lattice is decomposed into sub-lattices
- Sub-lattices can be deployed on different machines
- Data link between sub-lattices

Illustration:
- a 2D lattice decomposed into
- 16 sub-lattices
Main challenges

- Distribution on a single (multiprocessors) machine
  - **G1**: 2 Xeon dual-core
    (4 cores), 2.0 Ghz, 4 Mo cache, each with 16 GB of RAM
  - **G2**: 6 Xeon dual-core
    (12 cores), 2.0 Ghz, 4 Mo cache, each with 16 GB of RAM

**Speedup**:  
\[
\frac{\text{CPU time}_1}{\text{CPU time}_2} = \frac{11.5}{4.1} : 2.80
\]

**Efficiency**:  
\[
\frac{\text{Speedup}}{\text{Processor number}} = \frac{2.8}{3} = 0.93 \sim 1
\]

Efficiency almost equal to 1  
No time lost in data exchange

Marchot et al., 2007, ECCE6; Copenhagen
Main challenges

- Cluster of Pentium Celeron 2.4 Ghz processors inter-connected by a switched-ethernet 100 Mbits network
  - Celeron 2.40 Ghz, 128 ko cache, each with 512 MB of RAM

200 times steps on:

- ∇ 64-MRT : 64×64×64 sites lattice and a MRT-LB model
- 64-SRT : 64×64×64 sites lattice and a SRT-LB model
- 32-SRT : 32×32×32 sites lattice and a SRT-LB model

Efficiency markedly smaller
Depends on sample size et model complexity

Dethier G., et al., 2011
Procedia Computer Science
Load balancing

The efficiency of parallel computing in heterogeneous distributed systems (computers of different computational power and memory size), depends strongly on proper load balancing among the computers.

- *A priori*: static load balancing
  
  depends on processor parameters, memory available,…

- *During computation*: dynamic load balancing
  
  depends …

Computing architecture

- *Locality*: data associated to addresses that are close in memory address space should be accessed at close moments in time

Network latency and bandwidth
Two phase flow LB models

- LB models provide are promising tools to describe complex fluid flow in porous media.

- Existing models are based on SRT (BGK) equations applied to the two fluids:

  \[ f_k^\alpha(x, t) = f_k^\alpha(x, t) + \Omega_k^\alpha(x, t) \]  
  \[
  \text{Phase } \alpha
  \]

  \[ f_k^\beta(x, t) = f_k^\beta(x, t) + \Omega_k^\beta(x, t) \]  
  \[
  \text{Phase } \beta
  \]

- All these models rely on one or several modifications of the BGK collision operator \( \Omega_k \)
Two phase flow collision operators

- Introduction of 2 relaxation parameters

\[
\Omega_k^\alpha = - \frac{1}{\tau^\alpha} \left( f_k^\alpha - f_k^\alpha (eq) \right)
\]
\[\tau^\alpha : \text{relaxation parameter for phase } \alpha\]

\[
\Omega_k^\beta = - \frac{1}{\tau^\beta} \left( f_k^\beta - f_k^\beta (eq) \right)
\]
\[\tau^\beta : \text{relaxation parameter for phase } \beta\]

- Modification of distribution functions at equilibrium to account for fluid-solid and fluid-fluid interactions.

- Up to now, surface properties (surface tension and wetting) have been included.
Thank you for your attention