EFFICIENT TOPOLOGICAL AND MORPHOLOGICAL CHARACTERIZATION OF POROUS MICROSTRUCTURES

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POROUS NETWORK CHARACTERIZATION
3D POROUS MEDIA CHARACTERIZATION (ALUMINA SUPPORT)

- Standard geometrical descriptors:
  - Porous volume fraction
  - Specific surface area
  - Granulometry
  - Average curvature
  - Maximal included ball

- Not sufficient*
- New descriptors are needed
  - Quantifying topology and accessibility
  - A single scalar value

Electron tomography reconstructions, size = 500 nm

GEOMETRICAL TORTUOSITY*

Which answer can we give to this question:
Is it easy to go through a given porous media?

- Purely geometric calculation, notion of flux, no consideration of chemical / surface interaction
- Accessibility: easy or not
- Diffusion: at a given constant speed, time to go from one location to another

Difference between:

GEOMETRICAL TORTUOSITY

Definition: need two points, ratio of two distances

\[ \tau_{n,m} = \frac{D_g(p_n, p_m; X)}{D(p_n, p_m)} \]

Difference between:

\[ \tau_{n,m} = 1 \quad \tau_{n,m} \gg 1 \]
TORTUOSITY FOR A “CUBIC SAMPLE”

- A and B being fixed parallel planes, computation of
  - 3D tortuosity map$^a,b$
  - Distribution considering all paths$^c$
  - Average or minimal path$^d$

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b. M. Moreaud et al., Analysis of the accessibility of macroporous alumino-silicate using 3D-TEM images, Material Science and Technology 2008 conference, Pittsburgh USA.
How to define two planes or points?
How to be representative?
M-TORTUOSITY a,b,c

a. J. Chaniot et al., Tortuosimetric operator for Complex Porous Media Characterization, Stereology, Spatial Statistics and Stochastic Geometry, Prague, Czech Republic, June 25th, 2018

b. J. Chaniot et al., From Tortuosity to Narrowness: Straightforward Porous Media Characterization, Workshop in Honor of Dominique Jeulin "Physics and mechanics of random structures: from morphology to material properties", Oléron, June 18th – 22th, 2018

STOCHASTIC TORTUOSITY

Random sampling of two points, and calculation of tortuosity

Not representative...

Several points are needed, but how to combine them?
M-TORTUOSITY

- Random sampling of points
- For each point:
  - Tortuosity calculated for each pair
  - Weighted average by respective geodesic distances*:
    - Gives less importance to nearby points, where the tortuosity is often equal to 1
- Combination of all points:
  - Weighted average with respect to center of mass:
    - Gives more importance to points nearby outer border

Proper random sampling is important!

Uniform distribution introduces a bias: dense porous areas are given more weight

Volumic distribution: same importance for all areas
M-TORTUOSITY*: FORMULATION

\[ \tau_{n,m} = \frac{D_G(p_n, p_m; X)}{D(p_n, p_m)} \]

\[ C_n = \frac{\sum_{m=0, m \neq n}^{N-1} D_G(p_n, p_m; X) \tau_{n,m}}{\sum_{m=0, m \neq n}^{N-1} D_G(p_n, p_m; X)} \]

\[ \tau_M = \frac{\sum_{n=0}^{N-1} (1 + D(p_n, c)) C_n}{\sum_{n=0}^{N-1} (1 + D(p_n, c))} \]

* J. Chaniot et al., Tortuosimetric operator for complex porous media characterization, Image Analysis and Stereology, accepted, 2019
MULTIPLE COMPONENTS CASE

How to deal with disconnected components?

- Undefined standard combination for infinite tortuosities
- Our solution: consider inverse geometric tortuosity*

\[
\tau_{n,m} = \frac{D_G(p_n, p_m; X)}{D(p_n, p_m)}
\]

\[
C_n = \frac{1}{N-1} \sum_{m=0, m \neq n}^{N-1} \frac{1}{D_G(p_n, p_m; X) \tau_{n,m}}
\]

\[
\tau_M = \frac{1}{N-1} \sum_{n=0}^{N-1} \frac{1}{1 + D(p_n, c)}
\]

\[
D_c(p_n, p_m; X) = \infty
\]

* J. Chaniot et al., Tortuosimetric operator for complex porous media characterization, Image Analysis and Stereology, accepted, 2019
M-TORTUOSITY, ILLUSTRATION
ILLUSTRATION ON MOFS CHARACTERIZATION*

Complementary to the classical descriptors

ZIF-68

ZIF-CN

M-tortuosity discriminates distinct topologies, unlike usual descriptors

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<th>ZIF-CN</th>
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<td>0.51</td>
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<tr>
<td>$r_{max}$</td>
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<td>15</td>
</tr>
<tr>
<td>$\tau_M$</td>
<td>1.30</td>
<td>1.20</td>
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ILLUSTRATION ON MOFS CHARACTERIZATION*

- Fills a large gap in the classical descriptors

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M-tortuosity is the only descriptor that singles out the topological similarity

CONCLUSION AND PERSPECTIVES

- **M-tortuosity new descriptor**
  - Mixture of geometrical tortuosity and narrowness
  - Applicability to complex microstructures and disconnected components
  - Scalar value containing topological information

- **M-Tortuosity** gives a thorough characterization of alumina supports and zeolites

- **Work in progress: extension to gray-level microstructures**
  - No segmentation needed

*One more thing...*
plug im!
Software platform for

Signal, Image and Volume processing
Simple interface for advanced and state-of-the-art algorithms from industry or academic worlds

plug im! has been used since 2010 by hundreds of people, mainly non-experts in signal and image processing. Its initial design has been deeply modified by their feedbacks.
Create new plugin using your favorite programming language

C, C++, C#, java, Fortran...

or prototyping software:

EXE stand-alone executable

+ XML GUI description
Efficient Topological and Morphological Porous Microstructures Characterization
Johan Chaniot, Maxime Moreaud (maxime.moreaud@ifpen.fr), Thierry Fournel, Jean Marie Becker, Loïc Sorbier

M-Tortuosity available soon under plug im!
Thank you for your attention!

www.plugim.fr