Spatial statistical analysis of micro-structures of nano silica particle gels

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Content

Nano silica particle gels
  RLCA process

Spatial Statistical Analysis
  Spatial summary statistics
  RLCA parameter estimation

Conclusion and Outlook
Motivation: Mass transport

- Mass transport: Diffusion and flow
- Nano silica particle gels as test bed for mass transport
Nano silica particle gels

STEM micrograph of 90nm thick silica particle (20nm) gel
Goal: 3D reconstruction of micro-structure

500x500 nm section of micrograph

3D reconstruction based on mass thickness estimation
RLCA process

• Reaction limited cluster aggregation (RLCA)

• Particle diffusion according to Brownian motion

• Sticking probability: $P_{stick} \in [0, 1]$

• The larger the cluster the smaller the diffusion coefficient
Sticking probability: $P_{\text{stick}} \in [0, 1]$
Spatial summary statistics

Task: Find suitable spatial summary statistics to characterize different particle configurations

Three first candidates:
- Pair-correlation function
- Empty space function
- Cluster function
Pair-correlation function

Ripley’s K-function

\[ K(r) = \lambda^{-1} \mathbb{E}_o(\Phi(b(o, r)) \setminus \{o\}) \quad r \geq 0 \]

with expectation w.r.t. Palm distribution given a point exists in \( o \)

Pair-correlation function

\[ \rho(r) = \frac{d\mathbb{E}(\Phi(b(o, r)))}{dr} / \frac{\lambda d\nu_d(b(o, 1)) r^{d-1}}{r \geq 0} \]
Pair-correlation function

- data
- p=1
- p=0.1
- p=0.01
- p=0.001
- p=0.0001
- CSR

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Empty space function

\[ F(r) = \mathbb{P}(\inf\{\|o - x\| : x \in \Phi\} \leq r) \]
\[ = 1 - \mathbb{P}(\Phi(b(o, r)) = 0) \quad r \geq 0 \]
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Empty space function

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Theo(r) - Est(r)

r
Cluster function

\[ c(r) = \frac{1}{n} \sum_i \frac{\sum_{j,k \in \partial(i)} \mathbb{I}(\|X_j - X_k\| \leq r)}{|\partial(i)| \binom{2}{r}} \quad r \geq 0 \]

for \( n \) points and neighborhood \( \partial \) defined via \( \| \cdot \| \leq r \)
Cluster function

c(r)

r
Sticking probability estimation

LS-type approach:

\textbf{for} \ i \ \textbf{in} \ \text{grid}

1. Generate RLCA reconstruction with $P_{\text{stick}} = p_i$
2. Compare to real data by calculating

$$S_i = \omega_1 S_1 + \ldots \omega_k S_k$$

for features $S_1, \ldots, S_k$ describing the spatial structure of the particles

\textbf{end}

\textbf{Find} \ i_{\text{min}} = \arg\min_i (S_i) \ \textbf{and select} \ P_{\text{stick}} = p_{i_{\text{min}}}$
Conclusions and Outlook

Goal: Estimate RLCA sticking probability using spatial statistics

• Current step: Finding spatial summary statistics
  - Normalize real and simulated data
  - $k^{th}$ nearest neighbors
  - Develop gray scale based summary statistics

• Next step:
  - Validation of concept in a simulation study
  - Analyze 3D data
References


Thank you very much for your attention!