Modeling and Experimental Evaluation of Structured Powder Dissolution

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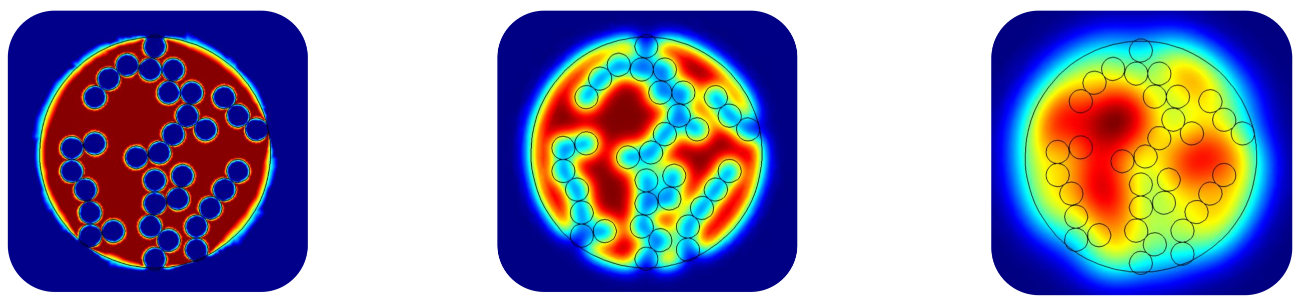
Introduction

The **dissolution behaviour** of powders is an important factor when evaluating their applicability for customer and industrial use. In this study, the effect of **particle size**, **porosity** and proportion of **soluble and insoluble materia**l on dissolution speed was investigated.



t = 0 s   t = 0.3 s   t = 2 s

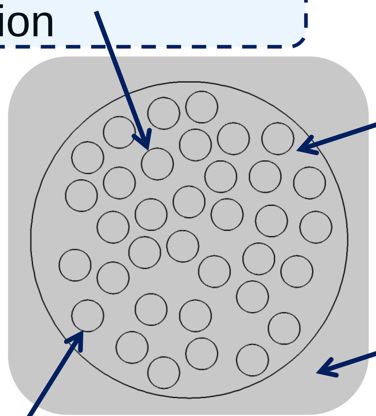
Computational Methods

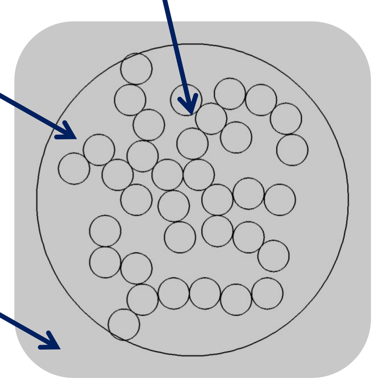
The **model geometry** was created using **LiveLink™ for MATLAB®**. The pores or areas containing insoluble material were placed at random coordinates following a **uniform distribution** inside the powder particle.
The **model physics** were set up using the **Chemical Reaction Engineering Module** with the **Transport of Diluted Species interface**.

Thin diffusion barrier at surface of closed pores. Diffusion coefficient is zero until the surrounding concentration is lower than a threshold concentration

Initial concentration in powder:
$$c = 1\,\frac{\mathrm{mol}}{\mathrm{m}^3}$$

Open pores are initially filled with water





Initial concentration in water:
$$c = 0\,\frac{\mathrm{mol}}{\mathrm{m}^3}$$

Thin impermeable barrier at surface of insoluble material

Diffusion of soluble material:
$$\frac{dC}{dt} = D\left(\frac{d^2C}{dx^2} + \frac{d^2C}{dy^2} + \frac{d^2C}{dz^2}\right)$$

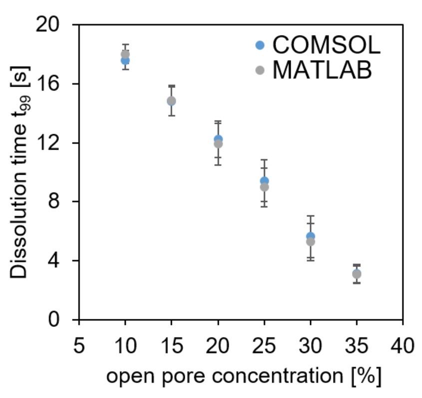
The results of the COMSOL Multiphysics® simulation were compared to results obtained by implementation of the Finite Difference Method in Matlab®.

Results

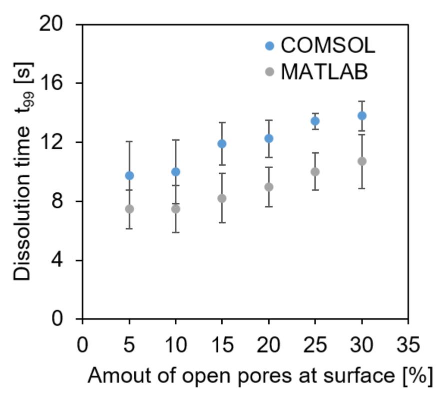
Parametric Study

The impact of particle size, porosity and proportion of soluble and insoluble material was investigated in a parametric study

Open pores

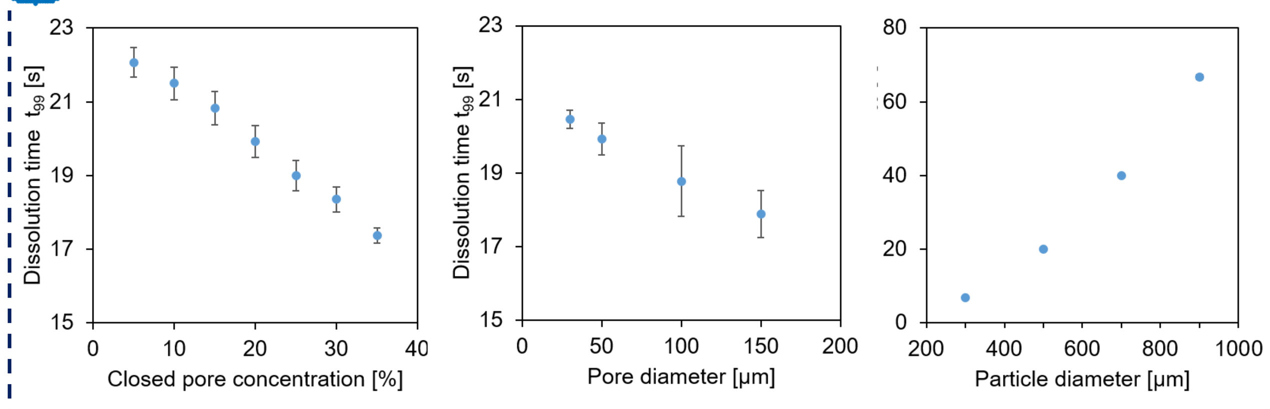


→ Faster dissolution with increasing open pore concentration (less material to dissolve)



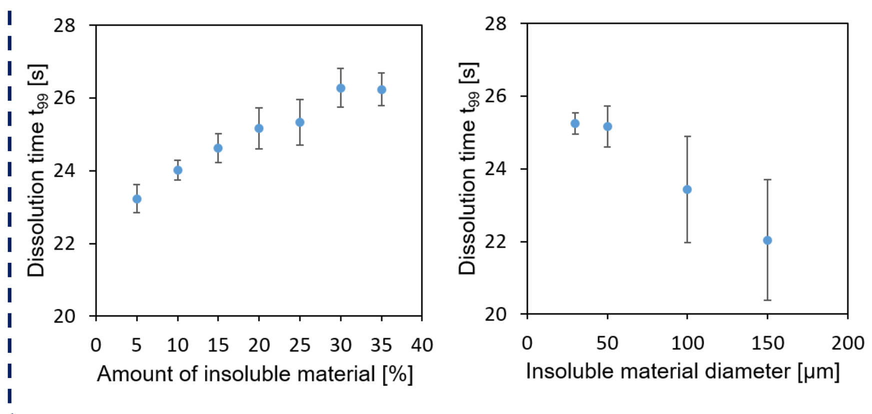
→ Faster dissolution with decreasing amount of surface pores (Surface area enlargement)

Closed pores



→ Faster dissolution with increased pore concentration and size (less material to dissolve)
→ Slower dissolution for larger particles

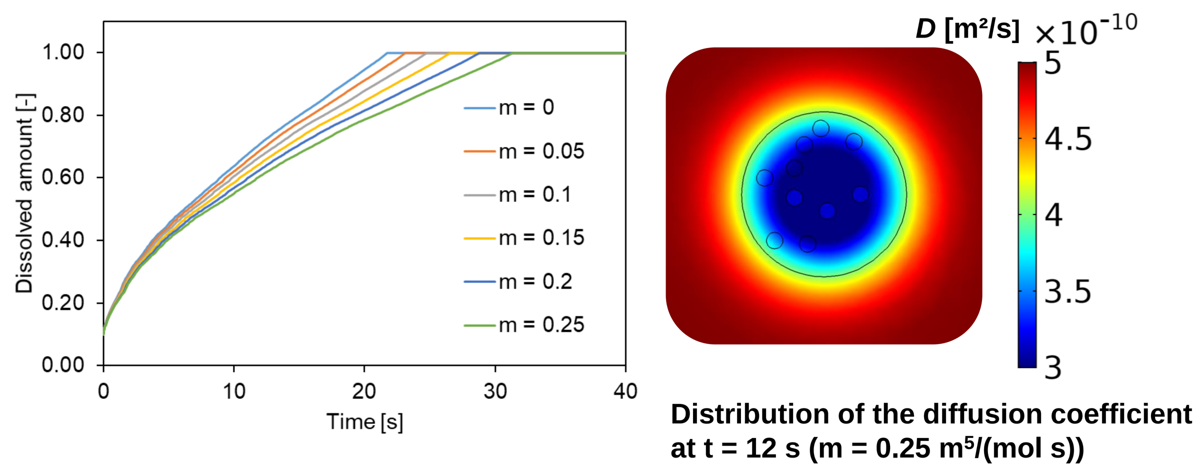
Soluble and insoluble material



→ Slower dissolution with higher amount and diameter of insoluble material
→ Diffusion pathways are blocked by insoluble areas

Influence of a concentration dependent diffusion coefficient

The influence of a concentration dependent diffusion coefficient was investigated by a linear decrease (with slope m) of the diffusion coefficient with concentration.

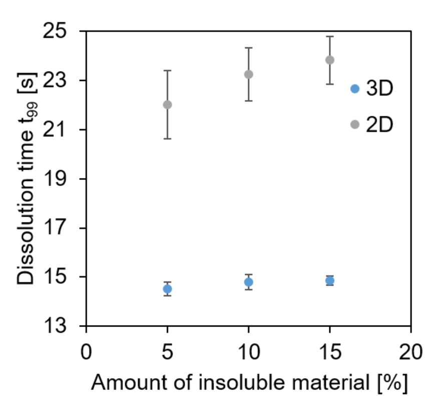


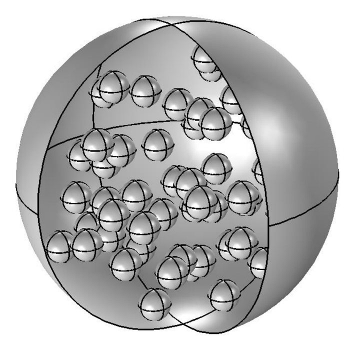
Distribution of the diffusion coefficient at t = 12 s (m = 0.25 m⁵/(mol s))

→ An increasing concentration dependency slows diffusion and thereby dissolution

Comparison of 2D and 3D Simulation

Model setups were solved in both 2D and 3D to evaluate the impact of the neglected dimension.





→ Results from 2D and 3D showed similar trends
→ Faster dissolution in 3D – less hindrance of diffusion due to insoluble material
→ 3D with higher computation times and meshing difficulties

Conclusion

Increasing porosity leads to faster dissolution. This effect is more pronounced for open porosity and for low amounts of pores directly connected to the surface due to surface enlargement.
An increasing amount of insoluble material as well as small insoluble particles lead to a slower dissolution due to longer diffusion pathways.