Oxygen Based Diffusion Modeling of Oxidation Behaviour of Encapsulated Lipids

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Introduction

Nutritionally beneficial unsaturated fatty acids are susceptible to oxidation. Encapsulating oil droplets inside a matrix of carbohydrates protects lipids against environmental oxygen by forming a **diffusion barrier**. It is assumed that **oxygen diffusion** and **surface oil** play a major role for oxidative stability. The aim of the study is to quantify the impact of the particle structure.

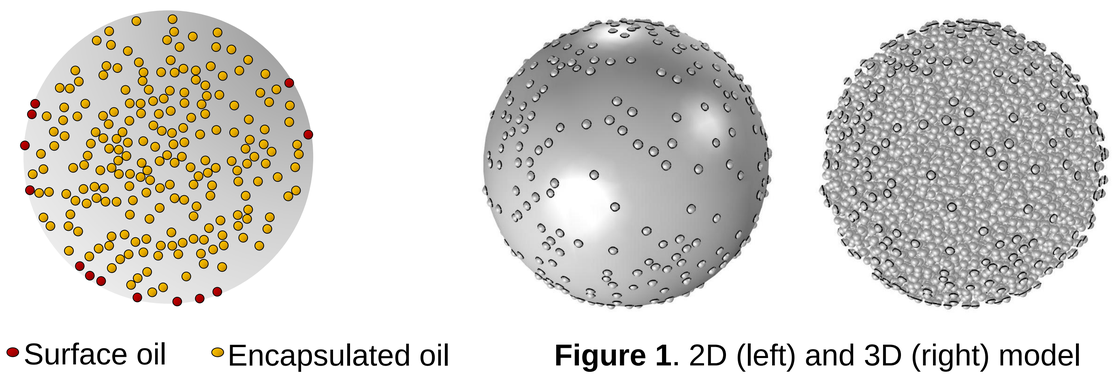

Figure 1. 2D (left) and 3D (right) model

Computational Methods

The **model geometry** was created using **LiveLink™ for Matlab®**. The oil droplets were placed at random coordinates following a **uniform distribution** inside the powder particle.

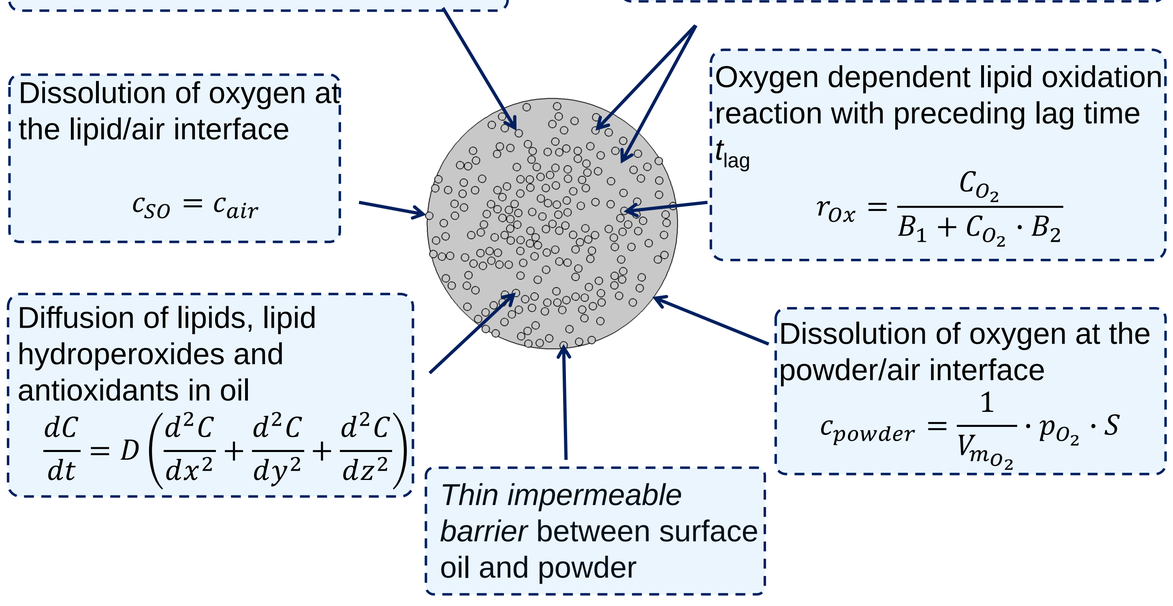

Figure 2. Physics and boundary conditions

The **model physics** were set up using the **Chemical Reaction Engineering Module** with the **Chemistry** and **Transport of Diluted Species interfaces**.

Oxidation Kinetics

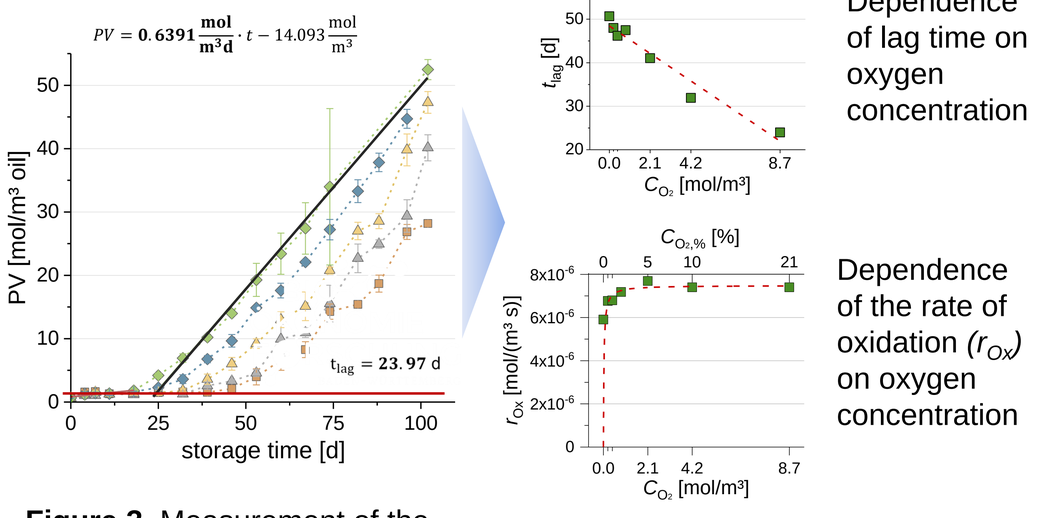

Figure 3. Measurement of the reaction kinetics

Results

Parametric Study and Validation

The impact of the particle structure was studied in a 2D model.

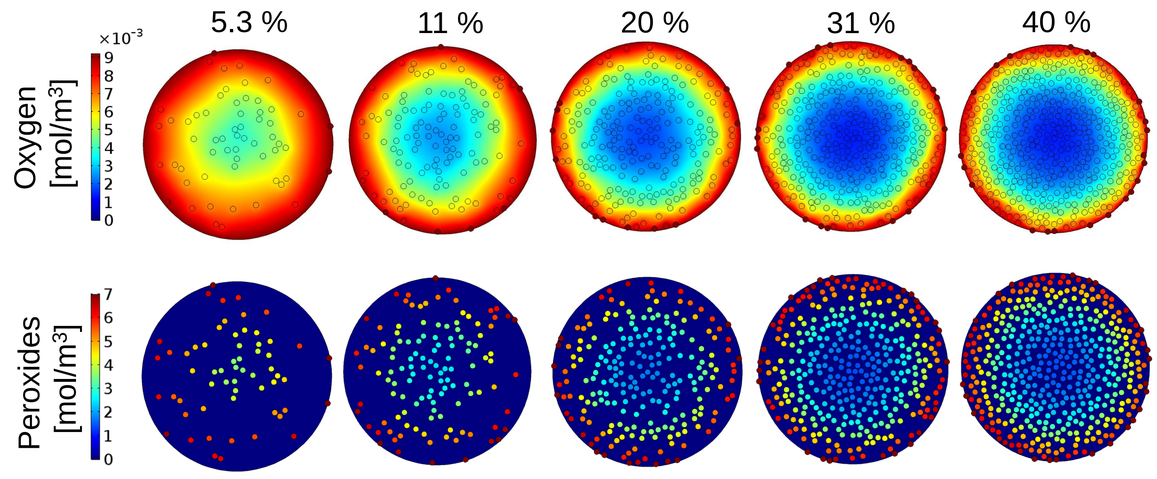

Figure 4. Variation of oil content

Each variation was solved 9 times. The average hydroperoxide concentration was evaluated after 100 days and compared to experimental data of linseed oil encapsulated in maltodextrin.

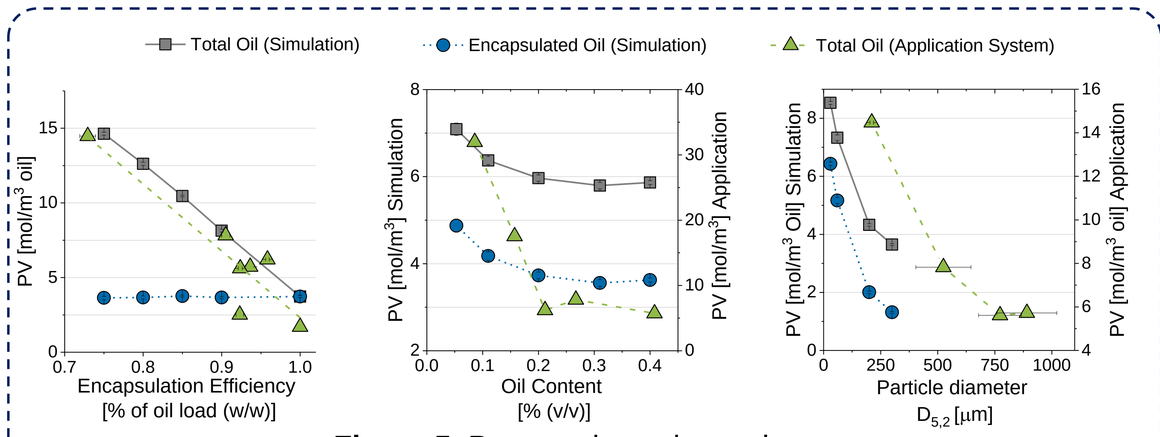

Figure 5. Parametric study results

Comparison of 2D and 3D Simulation: Four model setups were solved in both 2D and 3D to evaluate the impact of the neglected dimension.

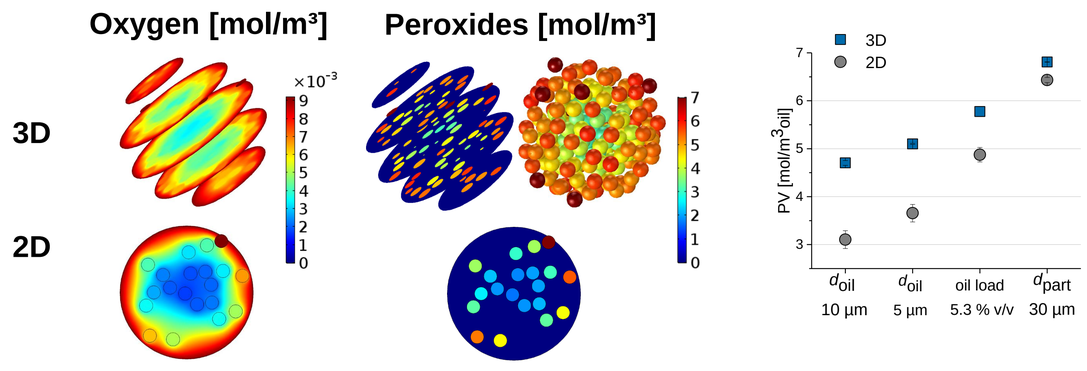

Figure 6. Comparison of 2D and 3D

The average hydroperoxide concentration was generally higher in the 3D model. Running the parametric study in 3D was not feasible due to **high computation times** and **meshing difficulties**, especially at large differences in scale between powder and oil droplets.

Conclusions

A low oil load, more surface oil and smaller particles increase lipid oxidation. The model and experimental trends were similar. 3D simulation was difficult due to high computation times and meshing problems. For future work, the mesh should be manually adapted to increase the meshing stability and decrease computation times.

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