

Master – Thesis

09.02.2026

CFD Simulation of an air or flue gas cleaning process by means of enzymatic catalysis

Description

The aim of this research is to use an enzymatic formulation that generates catalytically active surfaces for the detoxification of harmful halogenated alkanes. Toxic gases that cannot be captured by standard filtering technics such as fluorochlorohydrocarbons (CFCs) are converted into products that are harmless to the environment and health by means of enzymatic catalysis.

A continuous flow reactor (CFL) is simulated in Ansys Fluent to derive velocity and concentration fields. The active surface is modelled by appropriate methods like “porous media” in Ansys Fluent. Validation parameters have to be defined (e.g. pressure loss, break through time) and compared with lab data. Different geometry developments should be compared regarding the most homogeneous concentration distribution of substrates on the active surface aiming for the size of the necessary active surface.

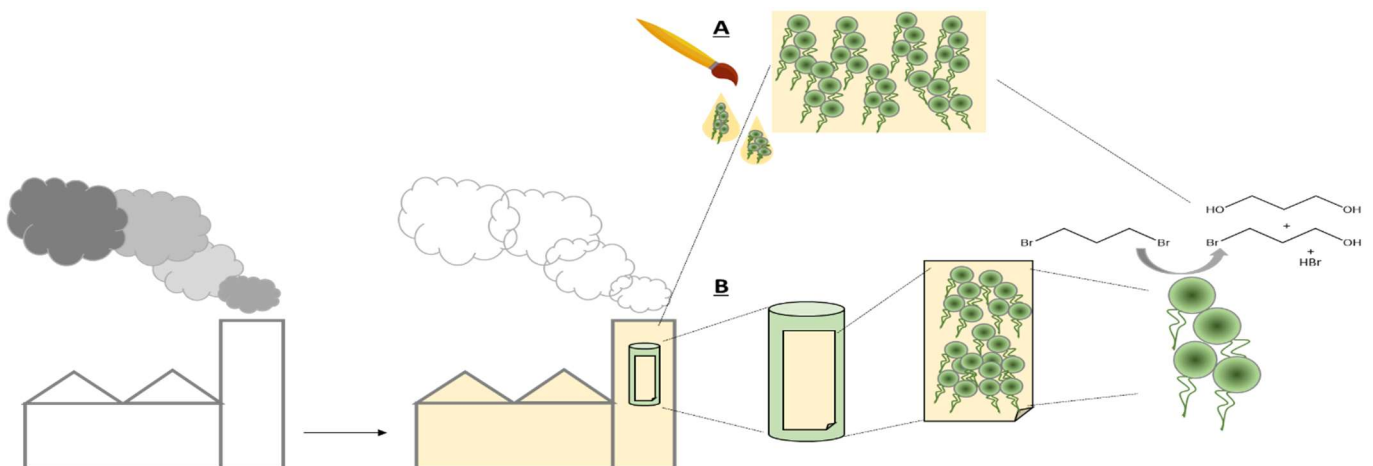


Figure 1: exhaust air cleaning from contaminations with halogenated alkanes by enzymatic catalysis Left: Exhaust air without bio-hybrid room and exhaust air treatment. Center/right: schematic representation of room air/exhaust air purification using bio-based wall coatings (A) or modular filter cartridges (B).

Tasks

- Literature research
- Physical modelling
- Definition of target parameters
- Definition of CFD methods
- CFD Simulation of various catalytic filter designs
- Post processing and data analysis
- Validation results by provided experimental data

Requirements

- Basic knowledge of reaction kinetics
- Basic knowledge of Ansys Fluent
- Basic programming skills (Matlab, Python, C..)
- Interest in bringing basic research and engineering together

Start: March 1st, 2026

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