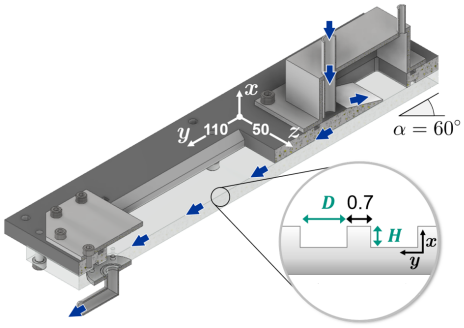
Interfacial Mass Transfer Enhancement in Falling Films: Adjoint Topology Optimization with Volume-of-Fluid Method

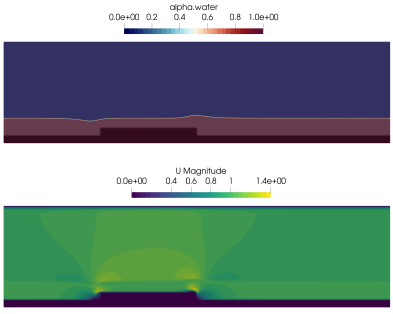
Wiebke Schrader[1] * David Müller[1] Andrea Düll[2] Thomas Häber[3]
Alexander Stroh[1]
[1]Institute of Fluid Mechanics (ISTM),
[2]Institute for Chemical Technology and Polymer Chemistry (ITCP),
[3]Institute of Catalysis Research and Technology (IKFT),
Karlsruhe Institute of Technology (KIT)

The reduction of anthropogenic greenhouse gas emissions requires carbon capture from exhaust gas streams as well as its utilization and storage. One promising technology for capturing the greenhouse gas is carbon dioxide (CO_2) absorption in gas-liquid contactors with falling film absorbers. In fluid film absorbers a thin, gravity-driven liquid film is in contact with a concurrently or countercurrently flowing exhaust gas stream while falling down a vertical or inclined plate. Through the modification of the surface structure of the absorber's backplate, the capturing performance can be improved by introducing eddies into the film to enhance mixing. Thus, the interfacial mass transport between the involved phases is intensified.

To assess the optimization potential, a simplified geometry is analyzed using an in-house code, based on the OpenFOAM Volume-of-Fluid (VoF) library *TwoPhaseFlow* introduced by Scheuffler *et al.*[1]. Thereby, the liquid film and gaseous CO_2 are modeled and the two-phase interface is captured with the VoF Methode. An appropriate model for the interfacial mass transfer is implemented into the existing code [2]. The corrugations on the backplate of the absorber are modeled using the Immersed Boundary Method (IBM) enabling the application of the adjoint optimization method to the given problem. The adjoint method is derived based on the time-averaged flow equations, so the temporal fluctuations are considered for the primal equations only and their derivatives are neglected for the computation of the adjoint variables. The sensitivity map computed from the primal and adjoint variables provides information on the change of the surface structure with respect to the chosen objective and constraints. In the conference contribution we will present the details of simulation setup and optimization tool and also report on the preliminary results of the optimization application.



(a) Experimental Setup [3]



(b) Preliminary numerical results for periodic domain

References

[1] H. Scheufler et al., *TwoPhaseFlow: An OpenFOAM based framework for development of two phase flow solvers*, https://doi.org/10.48550/arXiv.2103.00870, 2023.

[2] F. Özkan et al., *Numerical investigation of interfacial mass transfer in two phase flows using the VOF method*, Eng. Appl. Comput. Fluid Mech., 2016, **10**(1), pp. 100–110, 2015.

[3] A. Düll et al., *Influence of surface structure modification on CO2 absorption characteristics of a falling film absorber*, 14th European Congress of Chemical Engineering and 7th European Congress of Applied Biotechnology, 2023.

*Email: wiebke.schrader@kit.edu