



Aufgabenstellung für die Diplomarbeit

im Studiengang: Verfahrenstechnik und Naturstofftechnik
in der Studienrichtung: Chemieingenieurtechnik
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Thema: **Numerical simulations of radial $A + B \rightarrow C$ reaction fronts**

$A + B \rightarrow C$ reaction fronts can describe various natural or technological systems that combine specific dynamics, namely: Reaction, Diffusion and Advection (RDA). In this context, the study of the simple $A + B \rightarrow C$ reaction in a circular geometry, where reactant solution A is injected radially into solution B at a constant flowrate in a vertically confined system, provides valuable data for a variety of technological applications such as in microfluidics or in reactive mass transfer in porous media. This work consists of a two-dimensional numerical study of such fronts and aims to add to the existing knowledge by providing insights of the early-time regime, for which experimental outreach is not possible. Various temporal metrics are analyzed, such as the front position, the production rate and the front width. Adjusting geometrical, flow or physical property parameters, the effect on reaction and mass transfer can be studied to enhance understanding of the dynamics present in such fronts in early times and their contribution in shaping the front for later-time stages.

Task description:

- Literature research on radial $A+B \rightarrow C$ reaction fronts and their technological applications.
- Setup of the two-dimensional numerical simulations: mesh design, calculation methods, post-processing, parallel computing.
- Mesh dependency study and validation of the numerical code with the use of preexisting experimental results.
- Rendering of detailed 2D-views of early-time reaction fronts, otherwise non-accessible through experiments.
- Variation of flow field geometry.
- Parametric study of the front's response to changes in the flow conditions and the fluid properties.
- Comprehensive discussion of the results regarding the product formation rate, the front width and other relevant reaction front metrics in radial reactors.
- Discussion of current limitations and future directions of the work.

Die von der Studienrichtung erlassenen Richtlinien zur Anfertigung der Diplomarbeit sowie die Prüfungsordnung sind zu beachten.

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