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Towards generalized and improved criteria for gas-liquid reactions in the instantaneous regime modeled by non-stagnant interphase mass transfer

Aim

Validating and generalizing the newly proposed improved criteria for the so-called instantaneous regime for gas-liquid reactions as derived for the stagnant film model, using the physically relevant penetration and surface renewal mass-transfer models implemented in a CISTR and PFR model.

Justification

The classic criteria for gas-liquid reactions to be operating in the "instantaneous regime" can be found in many chemical engineering textbooks and have been derived for the well-known stagnant-film model with a reaction plane near the gas-liquid interface (Eq. 1 and Figure 1).[1]

$$Ha_A > 2 \; and \; Ha_A \gg E_{A\infty} - 1 \qquad \textbf{(1)}$$

However, for the selective reactive removal of an impurity B, present in a liquid product stream P, by a gas-phase component A in which the interface concentration C_{Ai} is substantially higher than the bulk-liquid concentration C_{Bb}, these criteria were found to be needed but not sufficient.

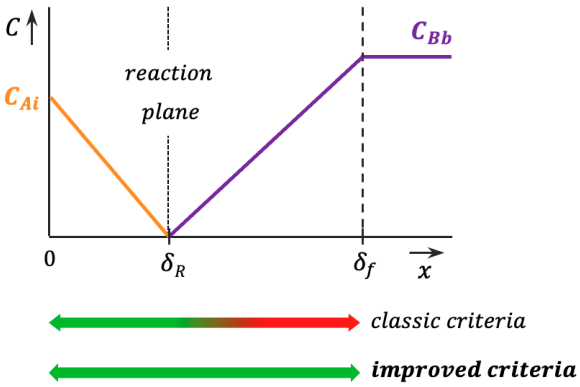

Figure 1 Qualitative concentration profiles in the film model for the instantaneous regime and the validity of the classic and improved criteria. The classic criteria are needed but not sufficient to identify the instantaneous regime if the location of the reaction plane shifts towards the liquid film-bulk boundary.

$$\boldsymbol{A_L + B_L \xrightarrow{k_1^{(1,1)}} C_L} \qquad \boldsymbol{A_L + P_L \xrightarrow{k_2^{(1,1)}} X_L}$$

This represents for example the selective oxidation or chlorination of organic product streams that contain small amounts of impurities, e.g. in a falling film reactor. Consequently, the reaction zone is not limited to the liquid film and the breakthrough of the gas-phase component into the bulk-liquid volume should be accounted for during reactor design.
The root cause of this breakthrough was recently traced back to the location of the reaction plane (δ_R).[2] These criteria were improved to extend their validity throughout the entire liquid film, and subsequently generalized to systems of N parallel reactions.
Although often used for engineering purposes, the stagnant film model inherently holds limited physical meaning. To cope with these shortcomings, Higbie and Danckwerts developed the penetration and surface renewal models respectively. The main research question in this proposal is centered around the validity of the aforementioned improved criteria using these more realistic mass transfer models which tentatively may yield qualitatively different results for our specific reaction system.

Program

- Literature review on continuous reactor models with alternative G/L mass transfer models.
- Develop and implement these mass transfer models in CISTR and PFR type reactor models.
- Compare the results of the stagnant film model with the penetration and surface renewal models and validate whether or not they yield opposite predictions in the limiting cases and whether or not the newly proposed criteria remain applicable.
- Further improve the criteria if needed, or extend the scope of the considered reactions for:
  - multiple gas-phase reactants
  - unequal diffusivities and non-unitary partial reaction orders

1. Westerterp, K. R., van Swaaij, W. P. M., Beenackers, A. A. C. M. & Kramers, H. *Chemical reactor design and operation*. (Wiley, 1991).
2. Janssens, P. Improved and generalized criteria for the instantaneous regime for multiple parallel gas-liquid reactions. (Ghent University, 2020).

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