

A CFD hybrid approach to simulate liquid-phase chemical reactors.

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Highlights

- A novel CFD approach for simulate liquid reactions is proposed.
- The model is based on spectral density functions for concentration variance dissipation.
- A batch to continuous process is analyzed as case-study.

1. Introduction

A detailed description of reacting systems is an effective tool for designing chemical reactors where productivity and safety aspects are relevant. Mixing, along with chemical reactions and energy transfer, can be described using methods developed in the frame of computational fluid-dynamics (CFD). If a chemical reaction is present in the system, the non-linear production terms in the equations involved in the CFD approach have to be computed using a turbulence-kinetics interaction (TKI) model. Many TKI models have been developed in the past [1, 2], mainly for gaseous phase reactions (that is, conditions characterized by the Schmidt number, Sc , ~ 1), while liquid systems (characterized by $Sc > 1$) have not been much considered. This unbalance is mainly due to historical reasons: TKI has been introduced to describe fuel oxidation in internal combustion engines and burners, where homogeneous gas phase reactions occur. Application of these models to liquid reacting systems generally leads to a poor description of real systems. Baldyga [3] has proposed an interesting solution for liquid systems, based on spectral density functions for concentration variance dissipation, the so-called MTS (multiple time scales) model, which is supposed to work properly when $Da \gg 1$ (being Da the Damköhler number), that is, for turbulence controlled systems; when $Da \ll 1$ (that is, kinetic controlled systems), the average reaction rate equals the reaction rate computed at the average scalar values and the simple Laminar Rate (LR) TKI model can be used. The aim of this work was to develop and test a new TKI approach, which combines MTS and LR methods to effectively account for intermediate situations where neither MTS nor LR models are expected to work properly in the whole integration domain. The proposed approach was implemented in a commercial CFD code and validated by comparison with several experimental data from the literature. Finally, a case-study that involves a continuous reactor design for a batch process was used to show the potentialities of the proposed approach with respect to the standard ones.

2. Methods

Liquid reactions are mainly influenced by concentration gradients rather than temperature gradients. A measure of the variance of local concentration is therefore an index of unmixedness and strongly affects reaction rates. In this contest, a spectral density function of concentration distribution becomes useful and can be divided into three ranges: inertial-convective (1), viscous-convective (2), and viscous-diffusive (3). Assuming that variances (σ_i^2) in these subranges are transported as generic scalars, together with the so called mixture fraction f , an overall variance ($\sigma_s^2 = \sigma_1^2 + \sigma_2^2 + \sigma_3^2$) can be computed [3] and then used to estimate the value of turbulence characteristic time, $\tau_T = f(\sigma_i, Sc)$. Comparing the turbulence characteristic time with the chemical one, the local value of the Damköhler number can be computed in each cell of the computational domain and used to decide whether MTS ($Da \gg 1$) or LR ($Da \ll 1$) is more suited to represent TKI in that cell. The proposed hybrid approach (in the following referred to as MTS/LR) is based on the same principle, computing the local reaction rate as the smallest value between MTS and LR reaction rates; therefore, the production rate of species k can be computed as:

$$\bar{\Omega}_k = \sum_j v_{kj} \min(\bar{\Omega}_{MTS}, \bar{\Omega}_{LR})$$

where v_{kj} is the stoichiometric coefficient of species k in reaction j . As it is possible to observe this approach is very useful when $Da \sim 1$.

3. Results and discussion

The proposed MTS/LR approach was validated using several experimental data from the literature [4, 5], and the results were also compared with other TKI models already presented in the literature. A sensitivity analysis on the turbulence model used was also carried out. As application, a case-study involving a process used to produce a species E through a series of two reactions:



was used. In particular, two concentric tubes are positioned along the main tube axis; A is fed from the largest tube, D from the smallest one, and B from the outer corona.

As shown in Figure 1a and Figure 1b, we can see that also in this simple case using different TKI models can lead to quite different yield values at the reactor exit.

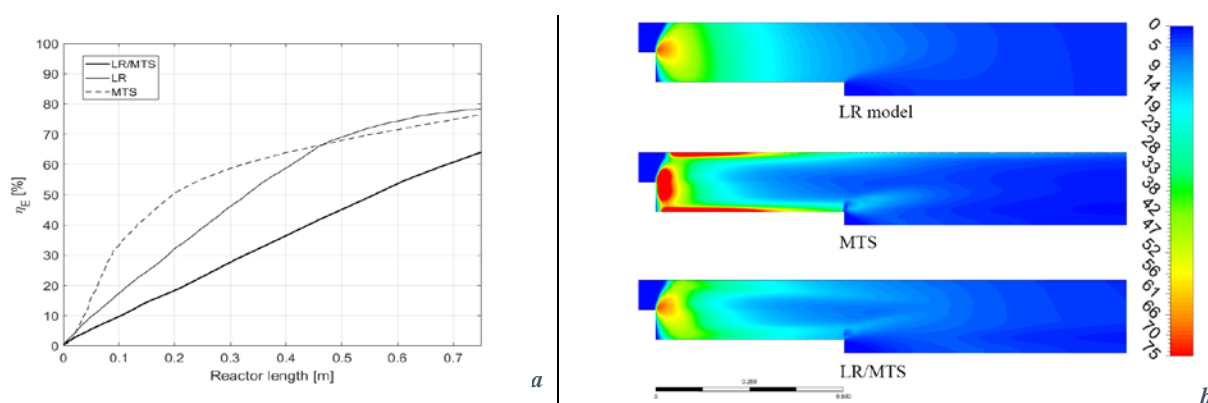


Figure 1 Final product yield as function of reactor length from the second entrance according to different TKI models (a), reaction 1 rate distribution [$\text{mol m}^{-3} \text{s}^{-1}$] (b).

4. Conclusions

The aim of this work was to develop a new TKI model for CFD simulations of liquid-phase reacting systems where Da is neither much larger nor much lower than one. The novel MTS/LR approach can be considered an effective tool able to deal with liquid-phase reactions under a wide range of reaction condition, filling the gap of previously proposed TKI models.

References

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Keywords

Computational Fluid Dynamics; Turbulence-Kinetics Interaction; Multiple Time Scales; Batch to continuous process;