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Editorial

Industrial Chemistry Reactions: Kinetics, Mass Transfer and Industrial Reactor Design (II)

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1. Introduction

Due to the success of the first edition of the Special Issue "Industrial Chemistry Reactions: Kinetics, Mass Transfer and Industrial Reactor Design" in terms of both the quantity and quality of the published papers, we thought it would be prudent to announce a second edition.

Recently conceived, powerful calculation methods have enabled the development of more sophisticated approaches to catalysis, kinetics, reactor design, and simulation. It is well known that many chemical reactions of a large scale and of great interest for industrial processes require information related to topics ranging from thermodynamics and kinetics to transport phenomena related to mass, energy, and momentum. For reliable industrial-scale reactor design, all these pieces of information must be incorporated into appropriate equations and mathematical models that facilitate accurate and reliable simulations for scale-up purposes. One challenge in this regard is to collect, in a memorable volume, the main advances and trends in the field of industrial chemistry that have been brought about by the contributions of various champions of scientific and technological progress by reviewing their past activity in the field or providing, through original manuscripts, examples of modern approaches to the investigation of industrial chemical reactions.

Therefore, the aim of this Special Issue is to collect worldwide contributions from experts in the field of industrial reactor design pertaining to kinetic and mass-transfer studies. The call for reviews and original papers solicited research in the following areas:

- Kinetic studies of complex reaction schemes (multiphase systems);
- Kinetics and mass transfer in multifunctional reactors;
- Reactions in mass-transfer-dominated regimes (e.g., fluid–solid and intraparticle diffusive limitations);
- Kinetics and mass transfer modeling with alternative approaches (e.g., stochastic modeling);
- Pilot plant and industrial-size reactor simulation and scale-ups based on kinetic studies (e.g., the lab-to-plant approach).

This Special Issue collected eleven papers that could be framed within different macro areas and whose distribution is depicted in Figure 1.

As depicted, the distribution is well-balanced among the five different macro areas, namely,

(i) kinetics for complex reaction schemes;
(ii) multifunctional reactors;
(iii) reactions in mass-transfer-dominated regimes;
(iv) modeling with alternative approaches;
(v) scale-ups.

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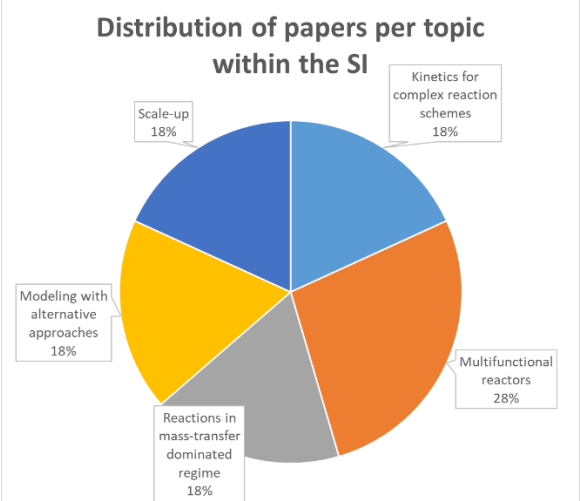
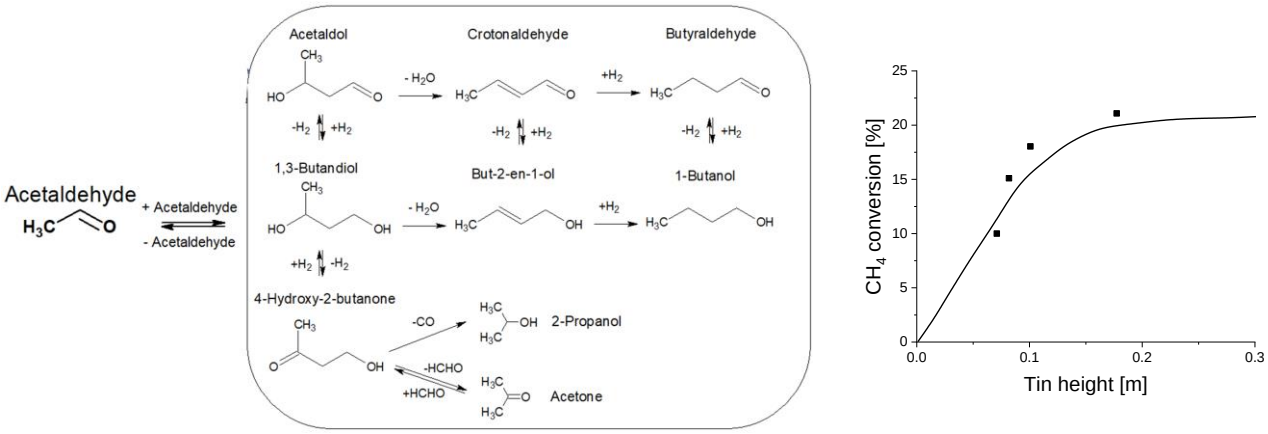


Figure 1. Statistical information related to the Special Issue, "Industrial Chemistry Reactions: Kinetics, Mass Transfer and Industrial Reactor Design (II)": distribution of papers per macro area.

In the following sections, the main achievements published in this SI will be reviewed and summarized, highlighting the points of novelty with respect to each macro area.

2. Kinetics for Complex Reaction Schemes

Two articles were published in the field of kinetics for complex reaction schemes. Santacesaria et al. [1] reviewed and analyzed the possibility of using ethanol as a liquid organic hydrogen carrier (LOHC), analyzing in detail both the main and side reactions (see Figure 2A for the latter), finding that the main rate expressions can be strongly dependent on the adsorption phenomena with regard to the surface reaction mechanisms.



(**A**) (**B**)

Figure 2. (**A**) Detailed reaction scheme of acetaldehyde condensation [1]. (**B**) CH_4 conversion versus reactors' axial coordinates for 6.0 cm ID reactor [2].

Palo et al. proposed a kinetic model of thermal methane cracking on molten metal [2] that correctly described the experimental data collected using a pilot plant even when using simplified ideal packed bed reactor models (see Figure 2B).

3. Multifunctional Reactors

Three papers were published in the field of multifunctional reactor technologies. Alqahtani et al. [3] explored the possibility of using a membrane reactor for hydrogen production, specifically with respect to its modeling and simulation. Figure 3A shows the

hydrogen concentration profiles along the residence time, illustrating that the model can also predict instability regions for the operation, making it a valuable tool in reactor design.

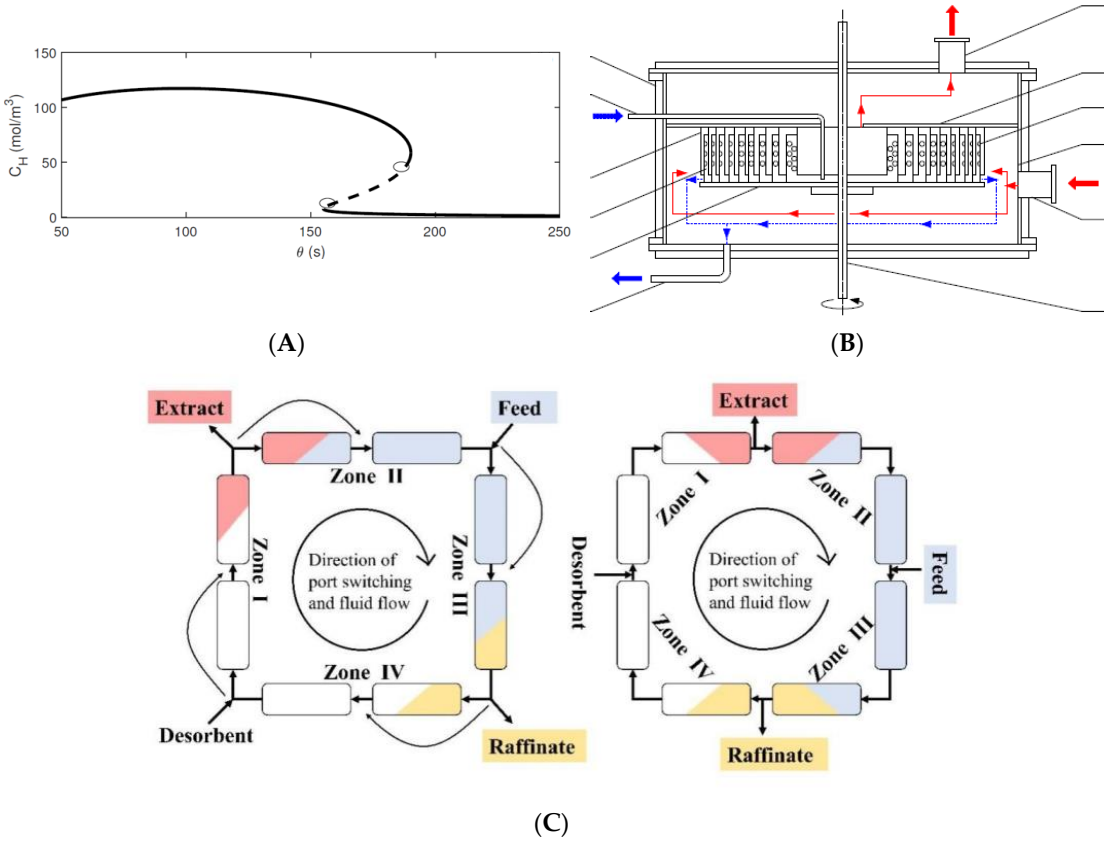


Figure 3. (**A**) Variations in hydrogen concentration with residence time in a membrane reactor [3]. (**B**) Diagram of a rotating zigzag bed [4]. (**C**) Simulated moving bed reactor [5].

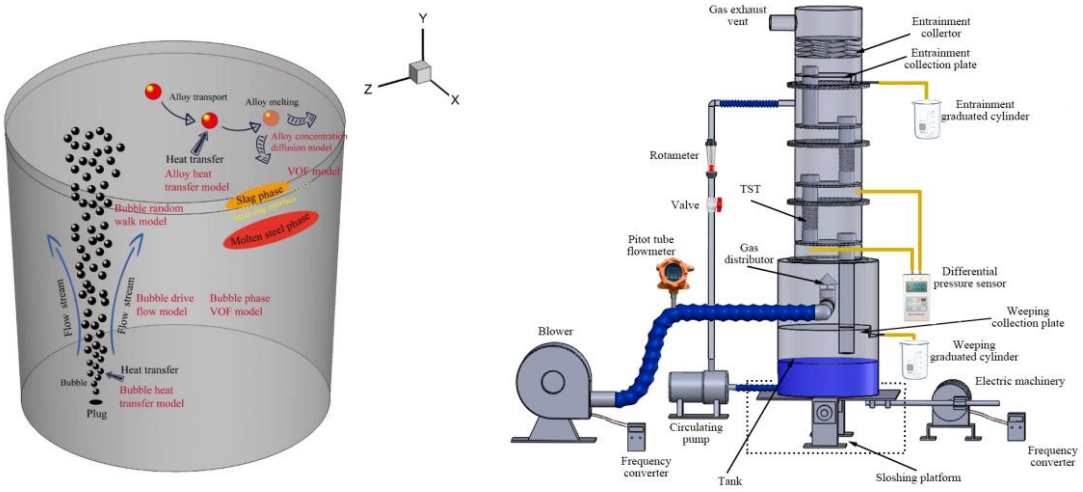
Liu et al. proposed a rotating zigzag bed reactor for a modeling and experimental study on CO_2 absorption using NaOH solution [4], adopting the experimental apparatus sketched in Figure 3B. The authors managed to measure and simulate the gas–liquid mass transfer interfacial parameters with high precision.

Finally, Zhang et al. reviewed both the classical and the most recent technologies in relation to simulated moving bed reactors (see Figure 3C) [5], reviewing the possibility of using such technologies in specific applications.

4. Reactions in Mass-Transfer-Dominated Regimes

Two articles were published in the field of chemical reactions in the presence of mass-transfer limitations. Hua et al. published a paper on a Multiphysics numerical simulation model related to an argon-stirred ladle [6]. As revealed in Figure 4A, the model accounts for the mass transfer aspects involved in the overall reaction network, paying particular attention to the diffusion of the chemical components between the involved phases. The results were promising and in line with the collected experimental data.

Tao et al. explored the hydrodynamic performance of a countercurrent total spray tray under sloshing conditions [7]. The influence of the main experimental conditions, including gas velocity and rolling-induced sweeping, on pressure drops, entrainment, and plate fluctuations was determined, thereby retrieving information for a better physical understanding of the system under investigation (see scheme reported in Figure 4B).

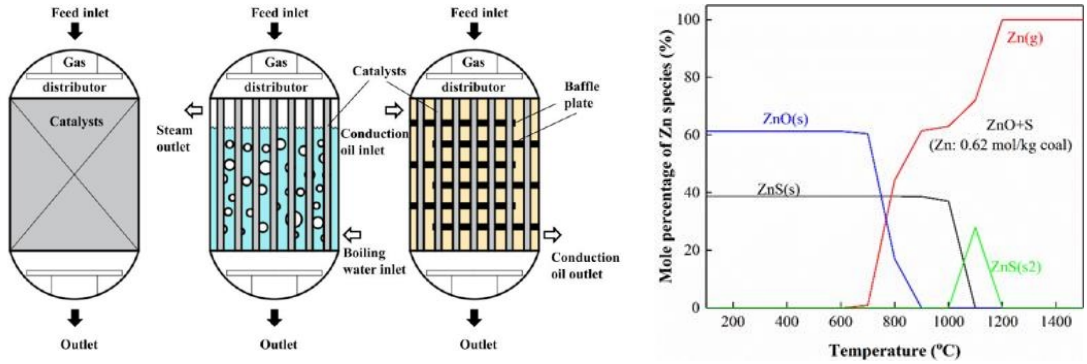


(**A**) (**B**)

Figure 4. (**A**) Diagram of the simulation model applied to the argon-stirred ladle [6]. (**B**) Experimental setup used by Tao et al. to investigate the hydrodynamic performance of a countercurrent total spray tray under sloshing conditions [7].

5. Modeling Using Alternative Approaches

The research groups of Huang and Lan published two articles on the topic of modeling using alternative approaches. Huang et al. conducted a model-based analysis of ethylene carbonate hydrogenation in industrial tubular reactors [8], comparing the performances of different reactors operating in adiabatic or heat-exchanged modalities (see Figure 5A). They identified the optimal operation-condition-related windows within which to optimize both the conversion and selectivity of the process.



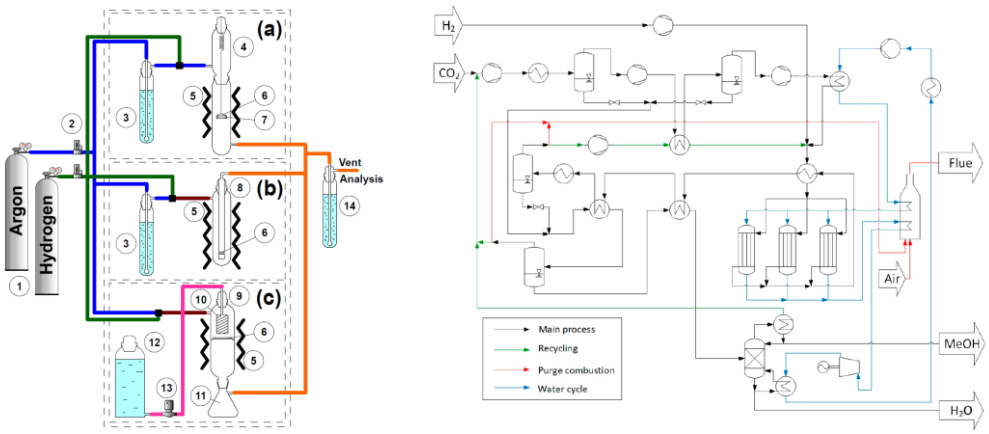
(**A**) (**B**)

Figure 5. (**A**) Different industrial tubular reactors modeled in the work conducted by Huang et al. [8]. (**B**) Thermodynamic equilibrium distribution distributions of Zn when S and Zn coexist in the coal [9].

Lan et al. investigated the effects of S and mineral elements (Ca, Al, Si, and Fe) on the thermochemical behavior of Zn during the co-pyrolysis of coal and waste tires [9]. The authors conducted an in-depth experimental and thermodynamic analysis to model the mentioned system, allowing them to predict the chemical composition of the mixtures obtained at different temperatures after thermal treatment (Figure 5B). Undoubtedly, this study yielded information required for the further scale-up of the operation.

6. Scale-Up

Finally, two articles were devoted to the scale-up process. Wang et al. studied the scaling-up of the catalytic decomposition of chlorinated hydrocarbons [10]. A dedicated experiment (see device in Figure 6A) was conducted to prove the concept, analyzing the quality of the products obtained for the future scaling-up of the process.



(**A**) (**B**)

Figure 6. (**A**) Experimental setup of the catalytic decomposition of chlorinated hydrocarbons: (**a**–**c**), reactors (**b**); 1 gas cylinders; 2 flow mass controllers; 3 saturator; 4 quartz reactor; 5 heating zone; 6 catalyst sample; 7 foamed quartz basket; 8 lab flowthrough quartz reactor; 9 scaled-up quartz reactor; 10 evaporator; 11 carbon collector; 12 vessel; 13 pump; 14 alkali trap. [10]. (**B**) One-step process flowsheet [11].

Lacerda de Oliveira Campos et al. proposed a process and techno-economic analysis of methanol synthesis from hydrogen and carbon dioxide with intermediate condensation steps [11]. The authors proposed a detailed flowsheet (see Figure 6B) that was designed to optimize the operation conditions of the whole plant.

7. Conclusions

Due to the success of the first edition, the second edition of this Special Issue on Industrial Chemistry Reactions: Kinetics, Mass Transfer, and Industrial Reactor Design (II) was launched and received significant attention. Part of the success of this second edition was due to the great variety of options that can be obtained when chemical reactions, catalysis, kinetics, transport phenomena, and multiphase systems are considered. The high quality of the collected papers, together with the highly interdisciplinary approach, allowed for the production of relevant papers in this sector, which will surely serve as a reference for future research.

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