

Editorial

# Special Issue on “Industrial Chemistry Reactions: Kinetics, Mass Transfer and Industrial Reactor Design”

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The impressive developments in commercially available technologies, in terms of new equipment and faster computers, allow us to solve ever-more complicated chemical and technical issues within industrial chemistry and reaction engineering fields. More sophisticated approaches to catalysis, kinetics, reactor design and simulation have been developed thanks to the newly available powerful equipment and calculation methods. It is well known that many chemical reactions are of great interest for industrial processes and must be conducted on a large scale to obtain the necessary information in thermodynamics, kinetics, and transport phenomena related to mass, energy, and momentum. The aim of this Special Issue, entitled “Industrial Chemistry Reactions: Kinetics, Mass Transfer and Industrial Reactor Design”, was to collect worldwide contributions from recognized experts in the field of chemical reaction engineering. The following areas/sections were covered by the call for original papers:

- Kinetic studies for complex reaction schemes;
- Mass transfer aspects in multifunctional reactors;
- Reactions in mass-transfer-dominated regimes (fluid–solid and intraparticle diffusive limitations);
- Kinetics and mass-transfer modeling with alternative approaches.

The interest in the topics could be verified by considering the information extracted from the Scopus database, related to the number of publications per year, as demonstrated in Figure 1A.



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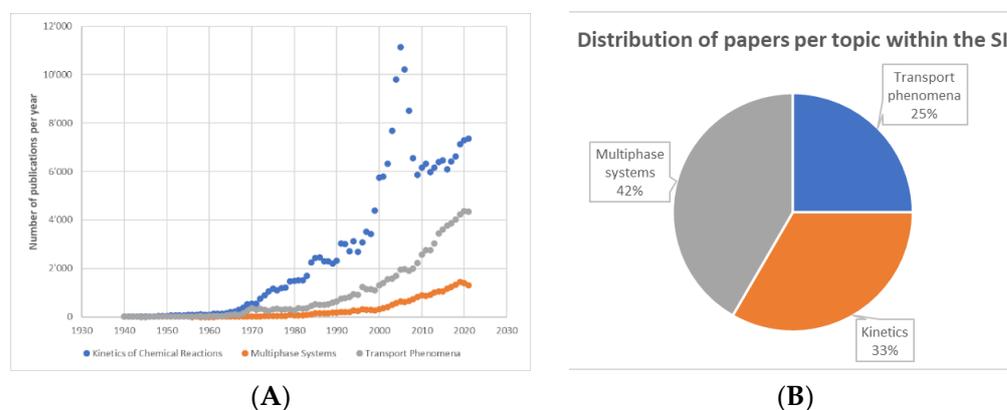
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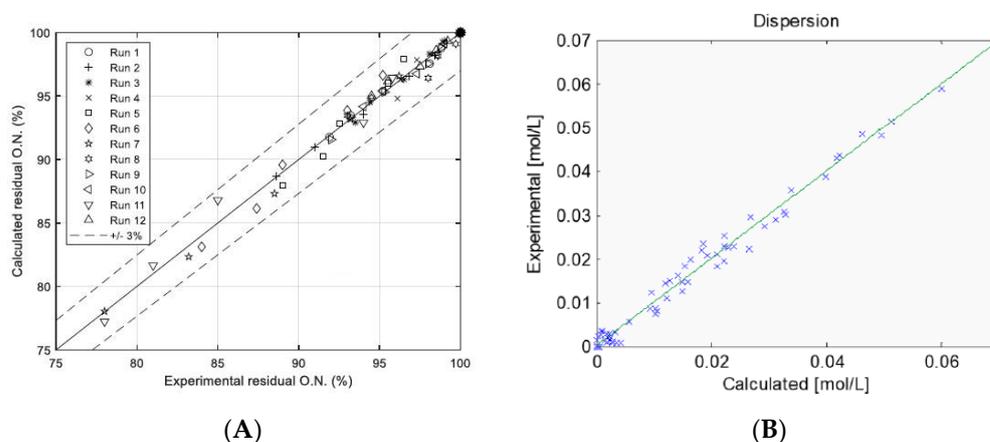
**Figure 1.** Statistical information related to the Special Issue “Industrial Chemistry Reactions: Kinetics, Mass Transfer and Industrial Reactor Design”. (A) Number of publications per year related to each specific macro area (Scopus Database). (B) Distribution of papers per macro area.

The Special Issue collated twelve papers, which could be framed within different macro areas, whose distribution is depicted in Figure 1B. As revealed, the trends are all

exponentially increasing, proving the effective scientific interest in the selected topics. Moreover, the distribution is well-balanced along three different macro areas, namely: (i) transport phenomena; (ii) kinetics; and (iii) multiphase systems. In the following sections, the main contributions published in the SI are reviewed and summarized, highlighting the novelty for each macro area.

Four articles devoted to the kinetics of chemical reactions have been published in this Special Issue. The first article, published by Tapio Salmi et al. [1], proposes a robust method for the estimation of kinetic parameters for systems including slow and rapid reactions. These systems require the solution of differential–algebraic equation systems. The authors simplified the approach by converting all the equations to a system of ordinary differential equations, enabling easier determination avoiding problems of numerical stability in the kinetic parameters by mathematical regression analysis. Two examples illustrate the method in practice, showing the good performance of the developed numerical strategy. A second article by Santacesaria et al. [2] examined the kinetics of epoxide ring opening reactions in detail. These are side reactions in the epoxidation of unsaturated vegetable oils, reducing the yields of the industrial process. All the factors affecting the reaction have been considered and experimentally tested, while a reliable kinetic model has been developed for simulating all the performed kinetic runs (Figure 2A).

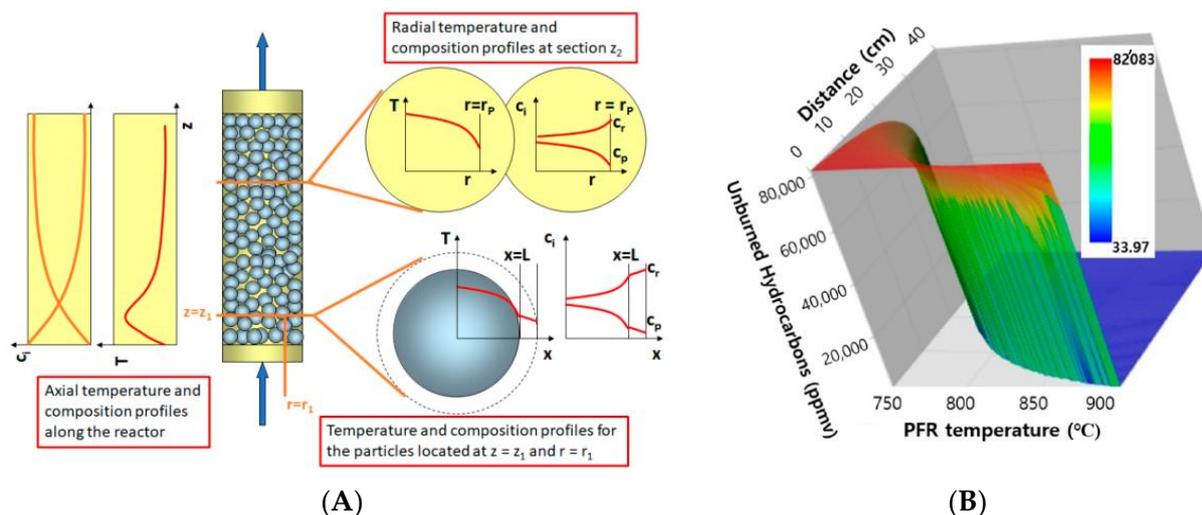
Linda Nikoshvili et al. [3] studied a polymer-Pd nanocatalyst deactivation in the Suzuki–Miyaura cross-coupling reaction. This reaction is widely applied in industry for C–C bond formation. The authors found methods for increasing the catalyst stability. The last article of this topic written by Rosengart et al. [4] deals with the hydrogenation of trans, trans-muconic acid to bio-adipic acid promoted by Pd/C 5% (wt). The authors studied the reaction in batch conditions and developed an LHHW kinetic model for interpreting all the experimental kinetic data. The most reliable reaction mechanism was individuated and discussed, resulting in a proper description of the collected experimental data (Figure 2B).



**Figure 2.** Parity plots for: (A) epoxidized soybean oil ring opening tests in the presence of sulfuric acid as catalyst [2]; (B) hydrogenation of trans, trans-muconic acid to bio-adipic acid promoted by Pd/C 5% (wt) [4].

Three articles of the Special Issue were devoted to problems of transport phenomena. First of all, Tesser and Santacesaria [5] published a brief review on the role of mass and heat transfer in gas–solid catalytic reactions, updating the knowledge on this topic by considering the considerable progress in computing power has occurred in the last 20 years. This progress has favored the use of numerical methods in the simulation of complex systems involving kinetics and mass transfer, as in gas–solid catalytic reactions, starting from a generic treatment of the multiphase system (see the sketch in Figure 3A). Somchart Chantasiriwan [6] published a study on sugar juice evaporation, aiming to increase the energy efficiency and decrease the sucrose inversion loss through modification of the conventional method. Finally, Hee-Chul Yang [7] investigated the two-step thermochemical

treatment of carbonization and halogenation for the removal of radionuclides from spent cation-exchange resins, developing a reliable model useful to describe the dependence of unburned hydrocarbon content as a function of both reactor temperature and length (Figure 3B).

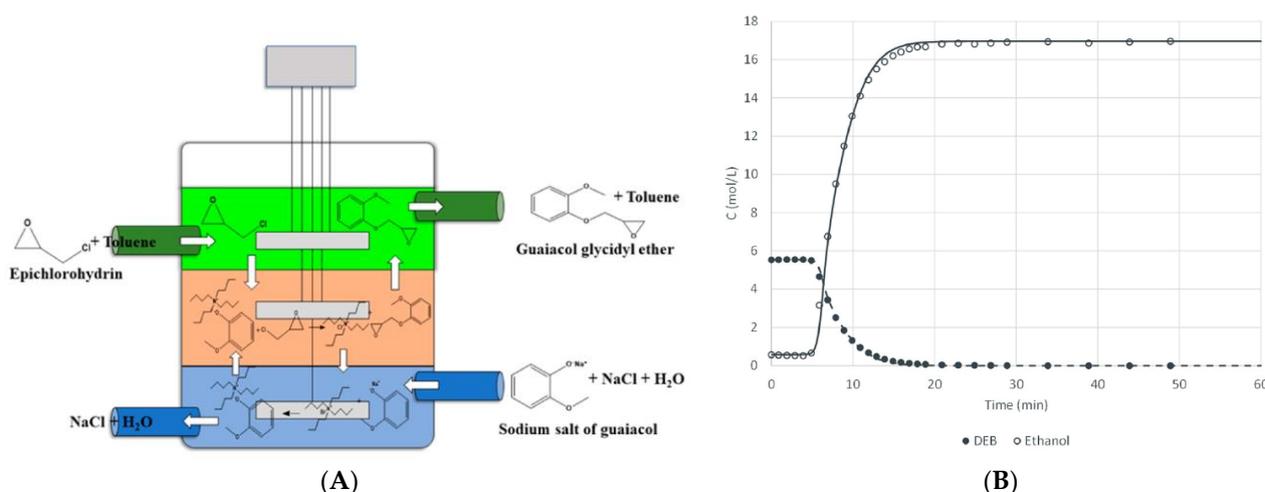


**Figure 3.** (A) Sketch concentration and temperature gradients along both the catalyst particle radius and reactor length [5]. (B) Unburned hydrocarbon concentration at the center of the reactor as a function of the plug flow reactor length and temperature [7].

Finally, five articles of the Special Issue were devoted to the study of multiphase systems. In particular, Margi and Yadav [8] published research on the design and development of a novel continuous flow stirred multiphase reactor, by studying the phase transfer catalyzed reaction of guaiacol with epichlorohydrin to obtain guaiacol glycidyl ether.

Figure 4A is a singular example of liquid–liquid–liquid phase reaction conducted in a novel continuous reactor, as proposed by Margi and Yadav.

Yu et al. [9] studied a system gas–liquid–solid with a numerical approach to define the bubble of gas rising in channels saturated with liquid. A mathematical model avoiding numerical instability has been proposed by the authors. Ravisut Vitidsant et al. [10] studied the transesterification of triolein, containing solid CaO particles, with methanol. The oil and solid particles were injected through an ultrasonic spray into an atmosphere of methanol. This three-phase reactor produced methyl ester with yields higher than the conventional reactors. Spitters et al. published an article concerning the optimization of the production of 1,1-diethoxybutane (DEB) by a simulated moving bed reactor (SMBR) [11], showing that this approach results in a high level of productivity and high purity of the desired product. The data collected were described quantitatively with sophisticated models (Figure 4B). The last study of this section, by Zemeng Zhao et al. [12], is devoted to the removal of dissolved oxygen from water by stripping with nitrogen coupled with vacuum degassing in a novel rotor–stator reactor. The performance of the mentioned reactor has been carefully determined and interpreted.



**Figure 4.** (A) Liquid–liquid–liquid reaction system in a continuous flow stirred reactor [8]. (B) Break-through curve between ethanol and DEB within an SMBR [11].

As it can be seen, although high in quality, the studies published in this first edition of the Special Issue entitled “Industrial Chemistry Reactions: Kinetics, Mass Transfer, and Industrial Reactor Design” are rather heterogeneous for their contents. This is due to the many different options that can possibly be obtained when chemical reactions, catalysis, kinetics, transport phenomena, and multiphase systems are considered without focusing on a single aspect. On the other hand, to have an open view on all the mentioned subjects is useful to be ready to understand what the best approach for any possible system could be: gas–solid, liquid–solid, liquid–liquid, gas–liquid–solid, etc., both in chemical regimes and limited by transport phenomena. The multiple approach of this Special Issue is, therefore, useful when presenting the approaches followed by eminent scientists in studying the kinetics of different reactions in many different situations. It would be desirable to further enlarge the casuistry of possible examples under study. For this reason, a second edition of this Special Issue with the same title has been recently launched.

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