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Editorial

Special Issue on “Thermal Safety of Chemical Processes”

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Chemistry plays an essential role in our modern society. The shift from fossil to biomass/renewable materials continues to increase rapidly industrial chemical activities and to generate more accidents. Such accidents can create a shortage in the supply of essential chemicals or deteriorate the financial situation of a chemical plant until bankruptcy.

Safety analysis [1] and management [2] are essential to avoid major chemical accidents. Chemical accidents can be provoked by leakage, fire, explosion, or thermal runaway [3]. Two studies have shown that approximately 25% of chemical accidents are originated from a thermal runaway [3,4]. Runaway can be defined as a rapid, uncontrolled rise in temperature during a chemical reaction and occurs in non-isothermal mode.

In this Special Issue, “Thermal Safety of Chemical Processes”, we aim to present the relevance and diversity of this research area. In particular, the issue proposes some research in the field of thermal parameters measurement [5], in the prediction of lithium-ion battery thermal runaway [6], and in thermal analysis of vacuum resistance furnace [7] or dust explosion [8].

Thermal runaway is the most common failure mode of lithium-ion battery which may lead to numerous safety incidents, because lithium-ion batteries are commonly used in portable electronic devices due to their high capacity and voltage properties. In particular, heat transport processes cause thermal runaway propagation from each battery to its neighboring batteries and may lead to the cascading failure of the whole energy storage system. The authors in [6] developed a model to predict the thermal runaway propagation for large-scale applications. For this purpose, kinetic aspects are combined with heat transfer modelling.

In [7], the authors proposed a numerical approach to study the effect of insulation thickness in a vacuum resistance furnace. They showed, with simulation, that the heating efficiency was improved by around 70% through controlling the heat flow at the insulation face. The authors consolidated these results with experimental measurements. The study using numerical methods will help design better and upgraded furnaces with more significant energy savings. In addition, the application of numerical methods is proposed as an effective design and performance prediction tool during manufacturing and operational activities.

In [8], the authors developed an inherent safety-based approach to mitigate risks associated with dust explosions in industries that either process or handle combustible dust. Such an approach consists in adding an inert material to a highly combustible material in order to decrease its ignition sensitivity. The authors studied the case of a combustible polyethylene dust and compared four inert powders (NaHCO₃, Na₂C₂O₄, KHCO₃, and K₂C₂O₄) to limit the ignition sensitivity.

The study in [1] is an in-depth investigation and analysis on a catastrophic hazardous chemical accident involving domino effects in China. The authors studied triggers and roots of the incident at the individual and organizational levels and summarized several useful lessons to avoid similar mistakes. The proposed case study provides a practical



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procedure for accident investigation and analysis, and thus, preventive measures can be made according to various causations at different levels.

The work proposed in [2] is about the assessment and analysis of chemical production safety management based on the evolutionary game theory. The proposed model uses the evolutionary game theory to construct a strategic interactive payoff matrix between the management department and the chemical plant. The approach analyzes strategic interactions and reveals the evolution of behavioral strategy selection. The application of this model provides an effective safety management basis and recommendations for the management of chemical plants, providing a foundation for the safe production and healthy development of chemical plants.

Rimmar et al. [9] evaluated the performance of the stagnation elimination of solar thermal systems. Such stagnation increases thermal risk leading to the overheating and evaporation of the heat transfer medium. The authors experimentally verified the usability of a thermal collector's tilting system to eliminate the thermal stagnation of the system. Their fully automatic method can eliminate the stagnation of thermal systems.

To assess thermal risks of a chemical process, the knowledge of kinetics and thermodynamics is vital. Thermal parameters such as specific heat capacities or thermal conductivity play an important role in the energy balance. There are several articles on the evolution of thermal properties of chemicals with temperatures. However, the measurement of heterogeneous catalyst specific heat capacities is seldom. Lu et al. [5] measured these values at different temperatures for several common heterogeneous catalysts.

CFD (Computational Fluid Dynamics) calculation can significantly contribute to understanding the development of thermal runaways in chemical reactors. In this Special Issue, Egedy et al. [10] have studied hydrodynamics during the carbonation of epoxidized vegetable oils. A 2D CFD model, based on the combination of the k - ϵ turbulence model and component material balances considering spatial inhomogeneities on the performance of a reactor, was used. Their study can be considered as the first step to predict the behavior of runaways for such reaction.

Ozawa–Flynn–Wall, Kissinger–Akahira–Sunose, and Friedman methods are frequently used to estimate kinetic constants from thermal analysis systems. Zhang et al. [11] used these methods to understand the kinetics of the thermal degradation of medical waste infusion bags and nasal oxygen cannulas. Such studies are essential to find reliable kinetic constants, thus understanding thermal runways.

Processes valorizing biomass can imply new risks such as dust explosion. The hydrogenation of levulinic acid, a platform molecule issued from cellulose hydrolysis, presents a significant risk of thermal runaway. Risk analysis of chemical processes requires the knowledge of the operating conditions of all the different units. For the valorization of levulinic acid, Garbetti et al. used the ARAMIS method, which was developed for petroleum refineries. It is essential to understand the separation process. In this Special Issue, Errico et al. [12] proposed an intensified alternatives for the purification of levulinic acid from lignocellulosic biomass.

To conclude, one should consider the question from a societal perspective. Can chemical accidents change the way the society accepts chemical industry? One should remember that Japanese public opinions on nuclear power generation became negative after the Fukushima accident. Hence, it is possible that the ultimate consequence of such industrial accidents could lead to the end or reduction of chemical activities.

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