Heat management in chemical reactors-Solved and unsolved problems.

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Proper management of the heat generated in chemical reactors is essential for the safe operation, start-up and control of any chemical reactor. Lilenroth, a DuPont employee, pointed out already in 1922 that the heat generation in a chemical reactor may lead to multiple steady states, some of which correspond to a runaway. Since that pioneering work, significant advances have been made in gaining an understanding of the impact of start up policy or transient perturbations on the dynamic behavior, stability and sensitivity of chemical reactors. A particular large body of knowledge and understanding of this has been generated by Neal Amundson and his collaborators in Minnesota. Some dynamic features of chemical reactors, such as the wrong-way behavior (a temporal temperature increase caused by a sudden decrease of the feed temperature to a packed bed reactor), are counterintuitive. To circumvent these undesired and unexpected transient temperature rise the design a special has to be applied which incorporate the ability of predicting this complex dynamic response.. The interaction between the temperature change and the fluid properties can have a major impact on the behavior of some reactors and in some cases the reaction rate. One noted example are polymerization reactors in which a change in a temperature induced change in the fluid viscosity affects the ratio between the rate of polymerization initiation, propagation and termination reactions. This in turn, may lead to a drastic undesired change in the properties of the produced polymer. Temperature induced change of the physical properties can lead to thermoflow multiplicity in multi-tube reactors, i.e., cause a nonuniform flow rate in the many catalyst packed tubes of a multi-tube packed bed reactor. This can have a deleterious impact on the yield of the desired product and cause non-uniform deactivation of the catalyst in the various tubes, requiring a early regeneration. The self-ignition of coal piles is another example of the interaction between transport phenomena, physical properties and runaway.

A reliable heat management of a chemical reactor is essential for the safe start, operation and control of a chemical reactor. Most existing rules and insightful guidance about heat management of chemical reactors rules are concerned with continuous-flow reactors. However, many industrial highly exothermic reactions are carried out in batch and semi-batch reactors. There have been many reported cases f reported explosions and runaway in these reactors, including some early ones at the DuPont company during the production of explosives. There is a need to develop similar design rules for the optimal safe feed of reactants to these reactors, i.e, what should be the proper feed rate of the various reactants and the temporal change of the coolant temperature that will lead to safe and optimal production at the desired products.

Proper design of heat management is critical for the reliable operation of autothermal chemical reactors in which the heat generated by the chemical reaction is utilized to preheat the feed to the reactor. It is well known that these reactors ma attain in certain case rather different steady states and it is essential to use a proper start up procedure in order to attain the desired one and apply a proper control to maintain it. In some applications a periodic operation may enhance the energy utilization of the process. For example, a reverse flow operation enables circumventing the need to add fuel during the catalytic combustion of feeds containing a low concentration of pollutants. This reactor may attain different periodic states and it is important to devise the proper start up and operation procedure. In some cases this reactor attains a complex periodic motion, such as a preriod-n or even chaotic operation, rather than the simple period-1 operation. A remaining important unsolved challenging problem is how to use reverse-flow operation to conduct an endothermic reaction using the heat generated by an exothermic one.

The local overheating may lead to major operation problems in industrial reactors. There is an important need to enhance our understanding and ability to predict and to circumvent the formation of local hot zones in a catalytic reactors, in which the overall heat management predicts safe operation. For example, it has been reported that local overheating of single catalytic pellet may occur in fluidized bed reactors during the polymerization of polyolefins. This overheating may lead to local melting of the growing polymer particle and subsequent formation of polymer “sheets”, requiring shut-down of the reactor. It is still not established what exactly causes this undesirable events, a knowledge needed in order to circumvent their occurrence. It is also well established that local hot spots ay form in large diameter packed bed reactors under conditions that the average temperature is closely controlled. When these hot zones form in the center of the reactor they cause local melting of the catalyst and formation of clinkers. However, when these small hot zones form next to the reactor, they can decrease the wall strength ad lead to eventual leaks of hot reactant mixtures, which lead to explosions. Special local wall control procedures have to be used to detect such local hot zones.

Another important yet unsolved problem is how to circumvent the destruction of diesel particulate filters (DPFs) due to formation of local excessive hot regions. The DPF is a multi-channeled ceramic filter. The exhaust gases flow through the porous ceramic walls and exit from the surrounding channels, while the PM is deposited in the channels and has to be periodically removed by combustion. The combustion often generates moving high temperature waves, the temperature of which may exceed in some cases the melting temperature of the DPF channels, damaging the DPF. Significant research is currently being conducted to develop regenerating procedures which avoid the destruction of the DPF by local melting.