INHERENTLY SAFER REACTOR DESIGN FOR ALKYL-PYRIDINES N-OXIDATION

Alba Pineda

Despite the fact that reactors are the heart of chemical processes, there are still many that are empirically designed, since the properties of materials and reactions involved are barely known. These reactors, where a sophisticated control system is difficult to implement, can lead to a runaway scenario. This is due to the lack of kinetic and thermodynamic data, which is necessary to ensure the thermochemical safety of the process. Another issue arising from the empirical design of reactors is that some of the strategies to improve safety lead to increased by-products, which results in an increase of energy and utility requirement for separations as well as a higher environmental impact.

The goal of this project is to develop an inherently safer continuous reactor based on scientific knowledge. This is done by integrating calorimetric studies, computational fluid dynamics, computational chemistry and reaction engineering. The object of study will be the N-oxidation of alkylpyridines, which is a complex and challenging process. The oxidant employed for the reaction is hydrogen peroxide, which has been the cause of several accidents. Hydrogen peroxide also decomposes producing oxygen, which poses a hazard of overpressure in the reactor. Furthermore, hydrogen peroxide decomposition is favored by the phase separation in the reaction mixture.

Some of the issues to be addressed in the development of the design of the reactor are the following: elimination of hydrogen peroxide decomposition, use of heat of reaction for feed preheating, separation and reuse of the catalyst, elimination of the neutralization step of the current approach by eliminating the excess of hydrogen peroxide in the reaction and water removal among others.