Prediction of inherently safer conditions for the *N*-oxidation of alkylpyridines

The risks of the chemical reactions carried out in the industrial processes are associated with the hazardous properties of the compounds employed, and the hazardous situations that can be developed under abnormal conditions. Because of these safety concerns, adequate hazard assessments as well as proper identification of the properties and the normal operating conditions of the chemicals involved are required to prevent incidents. For example, the catalytic *N*-oxidation of alkylpyridines using hydrogen peroxide as an oxidizing agent and phosphotungstic acid as catalyst presents some hazards related to the undesired reaction of hydrogen peroxide decomposition, the flammable properties of alkylpyridines, and the phase separation, which reveal the need for an inherently safer process. The oxygen generated in the decomposition of hydrogen peroxide can cause an overpressurization of the reaction vessel; and when combined with the flammable properties of alkylpyridines, can cause serious explosions and fires. In addition, the presence of two liquid phases in the reaction mixture favors the hydrogen peroxide decomposition over the *N*-oxidation, thus increasing the possibility of a hazardous situation occurring. In order to overcome these concerns, thermodynamic and calorimetric studies are combined. Thermodynamic studies will be used to investigate the phase diagrams of the reaction mixture, and calorimetric studies using adiabatic and isothermal calorimeters will be carried out to assess safety parameters and evaluate the reaction at different conditions. The purpose of this work is to find a set of operating conditions where the phase separation and hydrogen peroxide decomposition are suppressed. The selection of the new conditions is based on three important aspects: the viability of performing the operation at an industrial scale, the efficiency of the reaction, and the safety of the operation.