One number to rule them all: a reactor management strategy

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The latent thermal potential behind any exothermic reactive system is what makes a process dangerous. Under normal operating conditions, this potential remains inactive and controlled. However, under cooling failure or equipment malfunction, this potential may be unleashed and lead to a temperature increase that may trigger secondary reactions and gas formation. The evolution of gaseous products may result in a pressure increase and, ultimately, in the reactor burst if no measures are applied before the point of no return.

In fed-batch operation, this thermal potential is generally caused by the accumulation of unconverted reactants especially in the case of the production of hazardous materials. The management in such situations is profoundly related to the properties of considered reaction system, the reactor dynamics as well as the defined operating conditions [1]. Henceforth, it becomes essential to evaluate and control the thermal potential along the process course.

An approach has been developed, aiming in better characterization of the overall system and its different dynamics, predicting its behaviour under normal and abnormal conditions, and helping in preventing incidents from occurring. For that purpose, a dimensionless number has been proposed: the normalized thermal potential θ_{Gu}. This number characterizes the current process operating regime and is based on the reaction system kinetics, the reactor dynamics as well as safety limits. It also allows to define the optimal temperature profile a reactor should follow to be inherently safe as well as productive.

The proposed approach was simulated, investigated and implemented on-line for a hypothetic reaction system where a synthesis reaction may trigger a secondary autocatalytic reaction in case of failure [2]. The simulated reaction system is described as following:

$$A + B \rightarrow C + D$$
$$C \rightarrow E$$
$$C + E \rightarrow 2E$$

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