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Analysis of chemical process response to the deviation of multiple input parameters

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Modern chemical industry uses more sophisticated units and equipment. These units allow us to produce complex products with less emissions emitting and more effective energy consumption. However, using more complex units creates challenges in design, control, analysis, process safety, and economics. Chemical processes behavior is naturally nonlinear, and this behavior is mainly shown during malfunctions. The behavior of complex units is harder to predict and can hide more nonlinearities in process out parameters. Nonlinear behavior can be detected in small or wide working range of input parameters, in some cases, it can appear due to specific combinations of input parameters. Nonlinear response can occur in other pieces of equipment of unit than where input parameter deviation appears. Dangerous behavior created by combination of independent input parameters can be overlooked during hazard analysis, e.g. HAZOP. The nonlinear system response can be detected as oscillatory behavior, domino effects or high sensitivity to change in input parameters (fast change in temperature, pressure or runaway effect). Identification of nonlinear behavior can be applied to the unit with input parameter deviation from design value, but it can be applied also to connected units and equipment. Analysis of the unit with deviation and connected units can find domino effects, nonlinear response only at connected unit etc. Usage of mathematical modeling supported hazard analysis can detect more potentially dangerous scenarios, which are hardly predictable because of complex units and processes.
System response to multi-input parameter deviations is analyzed via Morris sensitivity analysis (1991). This methos is used to analyze defined range of possible deviation values. It uses one-at-time sampling method for analysis. Results of Morris analysis are parameter influence on system response and nonlinear effect and/or interactions with other analyzed inputs. Analysis is performed on propylene glycol production case study. Aspen Plus Dynamics® was used as a simulation tool for the chemical plant and Matlab® was used to evaluate Morris method. The analysis was performed in two modes: durations of deviations were shorter than one hour and infinity duration of deviations. Deviated input parameters were propylene oxide flow, water flow, cooling water flow and temperature of cooling water. The chemical plant consists of the continued stirred tank reactor and two columns. Analyzed output parameters are reactor temperature, condenser temperature of both columns and reboiler temperature of both columns. Water flow has the strongest influence on system response and nonlinear effect. Analysis including deviation duration shows also strong influence of duration of water flow deviation but decrease influence of propylene oxide flow deviation.

Morris, Max D. 1991. “Factorial Sampling Plans for Preliminary Computational Experiments.” Technometrics 33 (2): 161–74