Validation of Feasible Operating Region in Chemical Processes

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Studies on process safety and flexibility are two major issues for chemical process design. Analysis of process safety that can be ensured within some operating space is mathematically the same as analysis of process feasibility being maintained in certain operating boundaries. Therefore, although they are usually treated separately in research and practice, they share a basic feature: searching feasible operating space from possible design space.

At present, with classic methods, it is impossible to identify the accurate feasible region when the region is in a shape other than hyper-rectangle. To solve the problem, this work begins with the identification of a new modelling relationship, region to region, and then a new concept of region model framework against traditional point model framework for the new relationship is proposed. The basic component in the new framework is a simple region that is a hyper-cube formed by range values of the considered process variables and parameters. The dimensions of a region is mathematically represented by interval vector. The new model also has other advantages such as uncertainty information description and non-linear process behavior modelling.

Secondly, methodologies for region simulation are proposed. One main feature is the proposed bounding strategies. Unlike point simulation, which is done by solving differential and algebraic equations, region simulation is performed through the proposed bounding strategies. For example, for linear problems, natural inclusion of interval analysis is directly applied for region bounding.

The other main feature is the region transition model. Hybrid systems appear commonly in chemical processes especially when closed loop controllers are employed. In a point model, this is dealt with hybrid state transition network. In the region model, as sets of conditions rather than point conditions are considered, new features are introduced. The region transition model is devised in the work to deal with these new features.

Thirdly, based on the concept of region and methodologies of region simulation, an algorithm for searching the feasible space in possible design space is devised. It is illustrated by several case studies that with this new model we are able to get the accurate shape and size of feasible region within acceptable tolerance. Since closed-loop controller application is one of the main features in chemical processes, fourthly, strategies for dealing with dynamic process disturbances and modelling of closed-loop controllers in the region model are proposed.

Finally, an optimisation formulation is proposed for maximising the size of feasible region by tuning control parameters. As shown in case studies, quantitative process safety analysis and flexibility studies are unified in the new model. Since the model is able to identify accurate feasible region, it facilitates inherent safe process design. The framework has been implemented in an object-oriented architecture that makes it easier to represent a system than the equation-oriented approaches.