243t On Dimensionality of the Ar Construction

Wen Zhou and Vasilios I. Manousiouthakis

Geometric targeting procedure, based on geometric interpretations of reactions and mixing, constructs the AR by recursive application of the necessary conditions the AR must obey. Besides the unanswered question: "since the resulting candidate AR only satisfies the necessary conditions, is it indeed the true AR?", the limitations arise when the geometric targeting procedure is applied for three or even higher dimension problems. The difficulty comes from two facts: first, it is difficult to graphically visualize the procedure in high dimension space; second, even there exit a technology to graphically visualize the procedure, the procedure may be endless long to succeed.

Most recent research efforts on the AR focus on the computational construction. The IDEAS framework is applied to reactor network synthesis, and the AR boundary is calculated pointwisely. Abraham and Feinberg (2004) presented a sufficient condition for a region to be eliminated from consideration of being included in the true AR. Manousiouthakis et al. (2004), based on the mathematical formulation of IDEAS to reactor network synthesis problem, presented, a necessary and sufficient condition for a point in concentration space to belong to the AR, which is then employed to develop so-called Shrink-wrap algorithm guaranteed to approximate the true AR to an arbitrary degree of accuracy. These computational efforts, especially the proposed Shrink-warp algorithm, overcame the graphical visualization part of the difficulty of the traditional geometric targeting procedure for the AR construction. However, as the dimension of the AR construction problem increases, the computational burden increases tremendously, which may still prevent the proposed methodologies from being applied to real industrial size reaction systems.

As we know, the AR for A and B component in the Van De Vusse reaction scheme can be constructed in only two dimension space instead of four because of the independence of their generation rates on other component concentrations. However, we will going to show, even under the condition that generation rates of interested components do involve other components, it is still possible to draw the AR in lower dimension space. Our main goal here is to focus on the dimensionality of the AR construction problem, that is, to establish and mathematically prove the nature underlining the dimension of the AR construction. Knowledge of how these properties could be derived systematically is provided and proved. These properties can then be used to reduce the dimension of concentration space within which the proper AR is constructed. This work may be used to overcome the difficulty preventing the AR methodology being used for real industrial size problems.

Keywords: Dimensionality, AR, Reactor Network Synthesis, IDEAS