Design and control of recycle systems by nonlinear analysis

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Summary

This thesis provides valuable new contributions in the field of design and control of recycle systems by non-linear analysis. These could be summarized, by chapters, as follows:

I. Chapter 1 introduces the type of non-linear behaviour encountered in recycle systems and makes a comparison with stand-alone reactors. Two basic plantwide control structures are shortly reviewed: A. Self-regulation of component inventory: this conventional control structure consists of setting one or more fresh reactant streams on flow control. B. Regulation by feedback control: the component inventory is measured and an appropriate feedback control system is implemented. Feed policy of the reactants is the main difference between these two control strategies. The conventional strategy, based on the concept of self-regulation, offers more advantages but one must be aware of the non-linear behaviour when designing such systems. When stand-alone units are coupled via mass recycle, the system may exhibit state multiplicity even when the stand-alone units have a unique stable state. The non-linear behaviour of recycle systems depends on stoichiometry. A relatively simple methodology is provided for the design of recycle systems.

II. Chapter 2 investigates the multiplicity behaviour of six reaction systems of increasing complexity, from one-reactant, first-order reaction to chain-growth polymerisation. Below a critical value of the plant Damkohler number, $Da < Da^c$, the only steady state involves infinite flow rates. Feasible steady states become possible only if the critical value is exceeded. In case of one-reaction systems, one stable steady state is born at a transcritical bifurcation. For consecutive-reaction systems, including polymerisation, a fold bifurcation can lead to two feasible steady states. Moreover, the transcritical bifurcation is destroyed when two reactants are involved. If the gel-effect is included, a maximum of four steady states is possible. When multiple steady states exist, the achievable conversion is constrained by the instability of the low-conversion branch. This has practical importance for polymerisation systems when the radicals' quasi-steady state assumption is not valid or the gel-effect is significant.
III. Chapter 3 explores the non-linear behaviour of isothermal and non-isothermal PFR – separator – recycle systems. The steady state behaviour of six reaction systems of increasing complexity, from one-reactant first-order reaction to chain-growth polymerization, is investigated. In PFR – separator – recycle systems feasible steady states exist only if the reactor volume exceeds a critical value. For one-reaction systems, one stable steady state is born at a transcritical bifurcation. In case of consecutive-reaction systems, including polymerization, a fold bifurcation can lead to two feasible steady states. The transcritical bifurcation is destroyed when two reactants are involved. In addition, the thermal effects also introduce state multiplicity. When multiple steady states exist, the instability of the low-conversion branch sets a lower limit on the conversion achievable at a stable operating point. A low-density polyethylene process is presented as a real plant example. The results obtained are similar to CSTR-separator-recycle systems. This suggests that the behaviour is dictated by the chemical reaction and flowsheet structure, rather than by the reactor type.

IV. Chapter 4 addresses the design and plantwide control of Reactor-Separator-Recycle systems implying multi reactions. The study presents results of the non-linear analysis for two recycle systems involving consecutive/parallel reaction: S1. \( A + B \rightarrow P; A + P \rightarrow R \) where both reactants are recycled together; and S2. \( A + B \rightarrow 2P; 2A \rightarrow P + R \) where reactants are recycled separately. The non-linear analysis, conducted in terms of dimensionless numbers, ensures a large range of applicability. Two industrial case studies corresponding to each system are presented. It is demonstrated that plantwide control relying on self-regulation manifests regions of state multiplicity or unfeasibility. Ignoring the steady state multiplicity can lead to control difficulties or even un-operable plant. Nonlinear analysis is a way to identify and avoid such dangerous situations at an early stage of design. This chapter provides basic guidelines that are useful for the design and control of such systems.

V. Conclusions of this study and author’s comments and suggestions for further research are presented. Due to the strong nonlinear behaviour, designs near bifurcation varieties such as folds, should be avoided. The original contributions presented in this thesis cover an important area of the design and control of recycle systems. Nevertheless, there is more to explore in future studies. Further research could consider other reactor types, applicability of chemical reaction network theory, heat-integration, optimised selection of control alternatives.