Integration of design and control by nonlinear analysis
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Citation for published version (APA):
Bildea, C. S. (2001). Integration of design and control by nonlinear analysis

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Chapter 8. Conclusions and Suggestions for Further Research

The goal of this thesis was to investigate the integration between design and control of chemical plants. In contrast with the traditional methodology, where first several design alternatives are developed and afterwards their controllability is analysed, a method to generate only easily controllable designs was sought.

Due to the complexity of the problem, a systemic approach emerged. More precisely, the activity of conceptual design is viewed as selecting and assembling building blocks (called Basic Flowsheet Structures, BFS) in such a way that a system with required functionality is obtained. When this point of view is adopted, the main objectives of the plantwide control are achieved by coordination of the (local) BFS control. This way, distinction is made between local and plantwide control. Consequently, research of integration between design and control should proceed along two lines:

1. **Design of controllable BFS.** There is a lot of industrial experience regarding the design of unit operations having good controllability properties. However, in many cases, the interaction between some units is so strong that they must be considered as one system (BFS). Heat-integrated distillation and heat-integrated reactors are examples that have been analysed in this thesis. Other systems, as thermally coupled distillation systems, reactive distillation, azeotrophic distillation with solvent recycle, are possible subjects for further research.

2. **Couple the BFS in a controllable flowsheet.** In this thesis, it is shown that the main task of the plantwide control is to maintain the mass balance of the plant, by avoiding accumulation / depletion of all chemical species involved in the process. Because the chemical reactor is the place where species are formed / consumed, it plays an important role in the plantwide controllability. Hence, study of reactor-separator-recycle systems can provide valuable insights into design of controllable flowsheet. In this thesis, the steady-state behaviour of several isothermal reactor-separator-recycle systems has been analysed, and implications on control have been discussed.
Although necessary, good steady-state controllability is not sufficient. Therefore, the dynamic aspects should also be introduced. This raises the subject of development of dynamic models to be used in the early stages of conceptual design.

Further research can be also directed towards reaction systems with a more complex stoichiometry, where more than one reactor might be necessary. Moreover, including the heat effects (no-isothermal reactors) may add more complexity.

The author of this thesis considers that the interaction between design and control can be revealed only by mathematical models that take into account the nonlinearities existing in every chemical process. This does not exclude the use of linear models, but requires the linearisation to be performed around several operating points. The use of nonlinear analysis during design can be summarised as follows: divide the space of the design parameters into regions with different steady-state and dynamic bifurcation diagrams, and identify desirable regions of operation and potential stability or operability issues. Avoid operation near bifurcation varieties.

However, there might be situations when high-performance requires operation near bifurcation points. In this cases, because of unavoidable disturbances and design parameter uncertainties, the control system must ensure that possible bifurcations are supercritical, that is they do not lead to a catastrophic change of system's behaviour. This is an active field of mathematical research.

The classification methodology presented in this thesis can be applied to one state-variable problems. Although many chemical systems fall in this category, this is a hypothesis that should always be checked. Systems with more than one state-variable may exhibit very complex steady-state and dynamic behaviour whose complete classification, unfortunately, has not been achieved.

Finally, the following steps are recommended to integrate design and control:

1. Non-linear analysis: choose / identify the design variables; formulate controllability criteria; classify the operating points according to controllability criteria; identify feasible / unfeasible regions.
2. Generate design alternatives, using any available methodology.
3. Perform linear controllability analysis for the design alternatives
4. Select a suitable design