

Design and Control Structure Integration from a Model-Based Methodology for Reaction-Separation with Recycle Systems

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Abstract

This contribution presents the latest results of a systematic model-based methodology for the design and analysis of processes with a Reaction-Separation with Recycle (RSR) structure. The methodology subdivides the problem into three main stages, where the first two stages identify a common set of design and process (control) related variables and their role in design and operation of the process using simple but appropriate models for the specific analysis tasks. Based on this analysis, the methodology determines the design-operation targets, the design-process variables that can attain these targets and the operational ranges for a stable operation. The main features of this model-based methodology is presented and illustrated through a case study involving the Tennessee-Eastman (Challenge) Problem.

Keywords: Integrated Design, Model-based analysis, Reaction-Separation-Recycle.

1. Introduction

Integrated process and control (structure) design aims to satisfy simultaneously, the increasing demands for the development of environmentally benign, economically profitable yet technically operable processes. In order to achieve this, the recycle of mass and energy within the process, which introduces new challenges to modelling, design and control of the process, need to be considered (Luyben, 1994; Morud and Skogestad, 1996). Also, Russel, et al. (2002) highlighted the roles of models in the simulation, design and control of chemical processes and suggested a more intelligent use of models in an *advice* role to solve process engineering problems related to synthesis, design and control. Several approaches deal with process design or control issues. A very well known approach is the hierarchical-based method of Fisher, et al. (1988), which principally relies on experience and heuristic based rules. Bildea et al. (2000) utilize mainly a nonlinear analysis of the models where the control structure proposed is already selected at the start. Therefore, it is more like a trial-and-error approach. Optimization-based approaches (Mohideen, et al. (1996)) involve large NLP or MINLP problems in order to find an optimal design of the process. However, through a systematic model-based parametric sensitivity analysis of the RSR structure, some of

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the complex interactions in the non-linear behaviour of the processes can be understood helping to characterize them. The objective of the parametric sensitivity analysis is to identify a common set of design and process (control) variables that affect the decisions related to the design as well as control (structure) of the process, the desired values for these variables and their upper and/or lower bounds without necessarily formulating an optimization problem. Since these variables affect the design and control related decisions, their effect can therefore be evaluated through the behaviour of the process measured in terms of a set of performance criteria. Therefore, integration of aspects of design and control of a chemical process with an RSR structure can be achieved in the early stages of the design process if the model-based analysis is performed simultaneously with the conceptual design calculations.

The objective of this paper is to present some of the new features of the model-based methodology developed earlier by Ramírez and Gani (2004) and highlight its application through the well-known Tennessee Eastman Challenge Problem (TE).

2. Methodology Overview

The model-based methodology comprises of three successive stages where special purpose models are used for parametric sensitivity analyses in the first two stages and validation in the third stage. Since integration of design of the process and its control structure involves simultaneously solving these two problems in the early stages of the design process, it is necessary to use appropriate models representing specific features (operation, behaviour) of the process and the variables which may affect them.

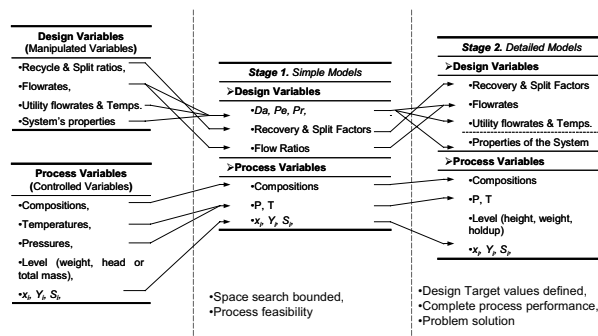


Figure 1. The roles of design and process variables in Stages 1 and 2.

Figure 1 highlights the roles of a class of design and process (control) variables typically found in processes with an RSR structure and are listed on the left hand side of Fig. 1. In *Stage 1*, some of the design variables are combined together into coupled parameters or dimensionless numbers (such as Da , the Damköhler number). The models in *Stage 1* are therefore based on these coupled variables and the objective is to find the values of these variables where the process has the optimal behaviour. Therefore, for different values of the design variables (listed in Fig. 1), the model equations are solved to obtain values of the process variables (listed in Fig. 1), which are then used to estimate the variables that determine the process behaviour (performance). This helps to decide target values for the coupled (design) variables (corresponding to the desired process performance), the operational limits (in terms of the process variables) and

desired (target) of the process behaviour. All these variables, affect the design of the process as well as the design of the control structure.

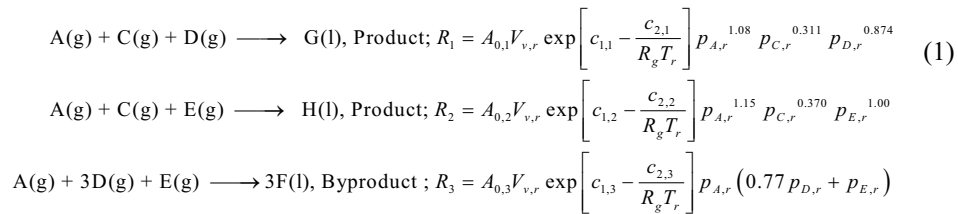
In *Stage 2*, the coupled parameters or dimensionless numbers are decoupled, generating therefore, a new model, which obviously, is more complex than the model in *Stage 1*. The objective here is to find the design variables (listed under *Stage 2* of Fig. 1) that can match the process behaviour (defined by the process variables) and the target values of the *Stage 1* design (coupled) variables. If the *Stage 1* design targets cannot be matched, new targets are set until a match is found. As highlighted in Fig. 1, the results from the model-analysis determine the operational feasibility of the process as well as the search space for the design-process variables. In *Stage 2*, the overall design targets are set and the values for a minimum set of design and process variables that matches this target is found. This means that all the design-control structure related decisions needed to make in the early stages of the design process has been made. The process can be described in terms of the performance it will give, the values of the design variables that can achieve it and values of the process variables that will be attained by the process. From a control structure point of view, these process variables will need to be controlled by manipulating the identified design variables. Also, these calculated values correspond to the set points for the manipulated and controlled variables. The models in *Stages 1* and *2* are quite simple as they only include the features of the process that need to be studied. In *Stage 3*, a rigorous model of the process is used to validate the design decisions and if necessary, to improve the design. The results from *Stages 1* and *2* are used as initial estimates, therefore, the robustness and efficiency of the rigorous model-based solver is improved. Typically, steady state as well as dynamic simulation models can be used at this stage, while in *Stages 1* and *2*; mainly steady state models are used.

3. Study Case

The TE Problem (Downs and Vogel, 1993) has been selected in order to highlight some of the new features of the model-based methodology for integrated design and control structure. Details of other examples can be obtained from the authors.

3.1. Process Description

The TE process produces two products (G & H) from four reactants (A, C, D, E), while B and F are an inert and a byproduct, respectively. The reactions, which are all irreversible and exothermic, are modelled by the following kinetic rate expressions,



One of the main characteristics of the TE problem, also studied by others (for example, McAvoy (1994) and Ricker (1995)), is the high non-linearity and open-loop unstable behaviour of the process, due mainly to the reactions occurring in the system.

3.2 Stage 1: Use of models with coupled (design) parameters

A model that includes the reaction kinetic expressions for the reactor but the separation operations are modelled for specified separations (fixed separation factors) has been developed according to the method outlined by Ramírez and Gani (2004). The important behaviour to model is the effect of the recycle flow on the reactor operation, since it is the chief source of non-linear behaviour and assuming that the separation problem can be designed to match the separation factors used. The derived *Stage 1* model has the following assumptions:

1. A constant pressure is assumed in the reaction zone, so $p_{i,r} = y_{i,r}P_{T,r}$
2. Reaction 1 is taken as a reference due to its highest sensitivity to temperature
3. The feed flow rate of component A is considered as the reference flow rate
4. No recovery of products or byproducts is considered

The steady state mass and energy balances for all the unit operations are represented in their compact form by,

$$\mathbf{0} = \mathbf{f}\{\mathbf{x}, \mathbf{d}, \mathbf{p}\} \quad (2)$$

where,

$$\mathbf{x} = [y_i, T_6, T_7, T_{cw,out}]^T, i = A, \dots, H \quad (3)$$

$$\mathbf{d} = [Da, \delta_c, \alpha_i, \sigma]^T, i = A, \dots, E \quad (4)$$

$$\mathbf{p} = [A_{0,k}, c_{1,k}, c_{2,k}, \Delta H_{f,k}^0, \dots]^T, k = 1, 2, 3 \quad (5)$$

In the above equations, vector $\mathbf{x}$ represents the unknown process (state) variables; vector $\mathbf{d}$ represents the design (coupled) variables, such as the Damköhler number (Da), heat elimination capacity variable (δ_c), the recovery (α_i) and purge factors (σ); vector $\mathbf{p}$ represents the reaction parameters such as the heats of formation and kinetic constant. The Da number, which represents the relation between the rate of reaction and flowrate of the feed stream, is defined here as,

$$Da = \frac{A_{0,1} \exp(c_{1,1} - \gamma_1) P_T^{2.265} V_R}{F_{A,1}} \quad (6)$$

3.2.1 Model-based Analysis

The model represented by Eqs. 2-5 represent a set of non-linear algebraic equations in terms of vector $\mathbf{x}$, requiring the specification of the fixed parameters vector $\mathbf{p}$ and the adjustable design variables vector $\mathbf{d}$. Figure 2 shows the results for the G/H selectivity or mass ratio (S_{GH}) and reactor heat duty (Q_r) for different values of recovery factors α_C with respect to Da . It can be noted that the recycle of reactants back to the reactor has a positive effect on its performance, evaluated through S_{GH} . However, as α_C increases, the heat content in the reactor also increases, due to the production of component G which is the most exothermic of the reactions taking place. Therefore, as the amount of reactants in the reactor increases, the heat in the reactor increases until the desired operation can no longer take place.

Another measure of the process performance is the conversion of component A, x_A , which may be considered as a limiting reactant as it is present in all the reactions.

Figure 3 shows the behaviour of x_A vs. Da for different values of α_A . Since high recoveries are usually preferred, a low Da number operation can achieve higher conversions, although this may imply high sensitivity to disturbances and short operating ranges. It is well known that in processes with RSR structures, at low Da , the process usually has the snowball effect on the recycle flow due to disturbances in the feed flowrate (Ramirez and Gani (2004)).

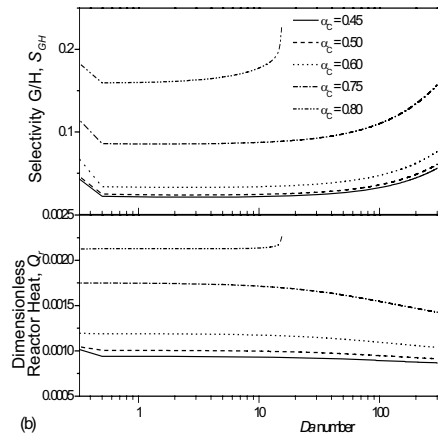


Figure 2. $S_{G/H}$ and Q_r vs. Da for values of α_C .

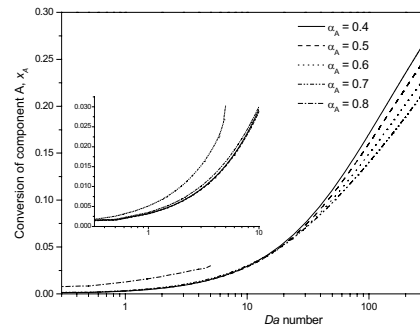


Figure 3. x_A vs. Da for different α_A .

From the above analysis, the target values for the design variables (Da and α_A) can be selected, which in turn, will lead to the desired performance. Also, the model solutions at the selected design variables provide the corresponding process variable values. Selecting upper and lower bounds on the design variables, define therefore, the operational window, within which undesired and/or unstable process behaviour (such as snowball effect) can be avoided. Note that choices of the design variables for the above process variables, also determine the optimal value for the recycle flow and its effect on the process. The objective here is to make these decisions without the need or use of rigorous model based simulation, since at this early stage of the design, enough data or information is usually not known to perform such calculations.

3.3 Stage 2: Use of models with decoupled design variables

The results from *Stage 1* are used as targets that will now be matched with design variables typically encountered in process design and/or control. For example, Eq. 6 is now used to replace Da in the model and the process performance and design targets are matched with the adjustable variables from Eq. 6 (the feed flow rate F_{AI}). Also, all assumptions considered in *Stage 1* are now removed. That is, the separation process is modelled to match the separation factor used in *Stage 1* (this will now give, for example, the temperature and pressure where a single stage vapour-liquid separation will take place). The model used in this work is that proposed Jockenhövel, et. al (2003), where energy balances for the reactor, the product separator, the stripper and the mixing zone have been added to the models given by Downs and Vogel (1993).

3.3.1. Model-based Analysis

The developed model can be used for steady state as well as dynamic simulations and contains 30 ordinary differential equations and 160 algebraic equations. The model has 11 manipulated (design) variables and fixed process parameters. The objective has been to first match the steady state design obtained in *Stage 1* and then to study the dynamic behaviour in open-loop and in closed-loop (by incorporating a control scheme using the set of identified manipulated and control variables from *Stage 1*). While the steady state design can be matched, the process shows highly non-linear process behaviour and the open loop instability, which without any control action reaches shutdown limits within approximately 60 minutes from the start of operation. Detailed simulation results, the model equations and its analysis for *Stages 1* and *2* can be obtained from the authors.

4. Conclusions

The results obtained from the systematic model-based parametric sensitivity analysis has been useful not only to identify operational constraints and/or limiting conditions, but also to identify set of manipulative and control variables that may be useful for control structure design. The analysis also provides the set-point values for the control variables matching the desired target performance of the process. The final step of validation through control schemes is currently being developed. For the TE problem, as far as validation of the design is concerned, stage 3 is not necessary since the stage 2 simulations validate the reported design. Current work is also developing a collection of case studies with their corresponding models and model analysis results.

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