Surrogate subsystem modelling of chemical processes.

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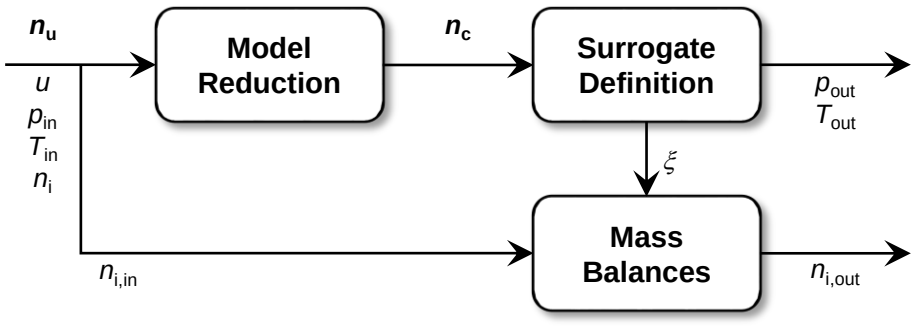
In this work, we present a method to derive simplified steady-state models of complete processes. The objective is to use these models for optimization, which is very difficult with the existing commercial flowsheet simulators like Aspen Plus®, Aspen Hysys®, SimSci PRO/II, or UniSim Design Suite. These simulators mostly solve the equations in a sequential-modular fashion, in which the unit operation are solved sequentially. This is a robust approach but convergence tends to be slow and the approach is not well suited for optimization. For this reason, we (Straus and Skogestad, 2016) have proposed a methodology for separating the process model into submodels, define surrogate models for the submodels, and combine the surrogate models for the optimization. Surrogate models, the core of this approach, can hereby be seen as input-output relationships.

Despite their usefulness, their application is limited by the exponential dependency on the number of independent variables (*u*), n_u , with respect to the number of points *N* per independent variable. Hence, it is crucial for our approach to reduce the number of independent variables. This work applies therefore a three-step procedure. First, the mass balances of the subsystem are defined *via* the introduction of auxiliary variables like the extent of reaction ξ. This may reduce the number of latent variables later, because we do not need to model all the outflows. Second, a partial least square regression (PLS) is performed on the remaining output variables (*pressure p, temperature T (or enthalpy h) and* extent of reaction) with two aims: a) Identifying additional linear input-output relationships, for which the explanation is almost 100%, b) identify a smaller set of inputs (latent variables) to be used in the third step. Through the application of the partial least square regression, it is then possible to reduce the number of independent variables by defining a specified number of components ($n_c < n_u$) which still represent the data adequately. In the third step, nonlinear regression methods are applied which involves fewer independent variables than for the original system, reducing the costs for calculating the submodels. For the nonlinear regression one may use a variety of methods, including splines (Foss et al, 2015), table look-up (interpolation), and neural networks. This procedure is also shown in Figure 1 including the relevant equation structure.

The reaction loop of the ammonia process is applied as case study. Initially, 9 independent variables are identified and varied to map the output space. The mass balance for this submodel in step 1 can be easily derived through the extent of reaction ξ, as shown in Figure 1, whereas the pressure and temperature remain as dependent variables.



$$n_{i,out} = n_{i,in} + \nu_i \xi \quad (1)$$
$$\xi = f_1(n_{c,1}) \quad (2)$$
$$p_{out} = f_2(n_{c,2}) \quad (3)$$
$$T_{out} = f_3(n_{c,3}) \quad (4)$$
$$n_{c,i} = g_i(n_u) \quad (5)$$

Figure 1: Separation of the overall input-output relationships into mass balances and auxiliary variables, in this case the extent of reaction ξ.

Through the application of PLS, it is possible in step 2 to present the outlet pressure p_{out} with 4 and the temperature T_{out} with 5 independent components. The extent of reaction can be defined by 6 independent variables. The resulting simplified model is sampled with respect to the new components in step 3 and B-Splines or neural networks are fitted to the sampled values. These reductions hence allow the introduction of surrogate models with a reduced number of points necessary, which subsequently can be applied for the optimization routine described by Straus and Skogestad (2016).

References

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