

Decision support for the development, simulation and optimization of dynamic process models

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Abstract Simulation is besides experimentation the major method for designing, analyzing and optimizing chemical processes. The ability of simulations to reflect real process behavior strongly depends on model quality. Validation and adaption of process models are usually based on available plant data. Using such a model in various simulation and optimization studies can support the process designer in his task. Beneath steady state models there is also a growing demand for dynamic models either to adapt faster to changing conditions or to reflect batch operation. In this contribution challenges of extending an existing decision support framework for steady state models to dynamic models will be discussed and the resulting opportunities will be demonstrated for distillation and reactor examples.

Keywords decision support, multicriteria optimization, model validation, dynamic model, sensitivity analysis

1 Introduction

Growing population and diverse regional availability of feed stocks require development of new sustainable processes and products [1]. These developments are based on experimental investigations in lab or mini-plants as well as on simulation and optimizations using a process model. The use of a process model is to answer questions about the real process by simulation and optimization [2] thereby reducing the effort for experimental investigations. Usually, process designers like to compare process simulations based on different what-if scenarios [3]. One example is the evaluation of the impact of uncertainties

with sensitivity analysis (SA) where a nominal scenario is compared with uncertainty scenarios [4]. Another example is the investigation of trade-offs of different objectives, e.g., sustainability criteria, in multi-criteria optimization (MCO) problems [5]. Pre-requisite for reliable results in these studies is a validated model. For model validation or in case of larger discrepancies model adjustment plant data are required [1]. Measurement tags and operating data are usually available in plant information management systems like for example ASPEN IP21 or OSI PI. In cases of missing rigorous models for specific process steps, plant data can be used to setup data-driven models. These models can then be used together with rigorous models in so-called hybrid or gray box modeling [6–8]. Model selection and parameter estimation in model adjustment can be supported by model-based design of experiments (DoE) [9]. At the end of the modeling based on plant data a reliable and validated model should be available, which could be used for the investigation of different what-if scenarios. To easily explore the design and decision space tools for a sound decision making are required [1]. A scheme of a decision support framework which supports this workflow is shown in Fig. 1. Similar schemes have been discussed before [3,5] and tools supporting this workflow have been successively implemented within BASF's steady state simulator CHEMASIM as can be seen in various publications [4,6,10–18]. In this contribution we discuss the extensions and modifications which were necessary to adopt these workflow tools for a use within the dynamic counterpart of CHEMASIM which is called CHEMADIS.

Process models for chemical production in general require the use of multi-scale models as we have models for the unit operations like reactors or distillation columns which mainly define mass and energy balances [2]. Additionally, models describing the physical properties

of the treated chemicals and their mixtures or their reaction behavior like equilibrium or kinetics are used. The physical property and reaction models are usually based on interaction properties of molecules. In the past, they often have been parameterized based on dedicated experiments. This is of course still the recommended way to proceed since it avoids the influence of model mismatch on parameter values. However, there is an increasing demand to have also access to these model parameters within the process simulator [19]. There are several reasons for this development: on one hand, for some components molecular models or lab data are not available and a dedicated investigation with required accuracy is too expensive (time, costs), not feasible since substances are not possible to isolate or analytics are sometimes extremely challenging; another reason might be that the experimental setup is complicated and could only be described using a process model with the need to parametrize the physical property or reaction model within the simulation environment; on the other hand, sometimes the question arises how properties of an optimal molecule must look like to improve overall process performance which is known as continuous molecular targeting [20]. Especially the availability of process data of plants or first batch experiments also triggered the idea to use existing data to parametrize models [17,21].

In the present contribution we describe the necessary extensions to enable the previously developed workflow tools for a use of model validation and adjustment (MVA) based on plant data, SA and MCO for dynamic process simulation models. We will give an example of a combined model adjustment of thermodynamic parameters and process variables to measurements of a batch distillation. Then we will demonstrate our decision support for the MCO results of the semi-batch Williams-Otto reactor. Finally, for a bioreactor for lysine production example, we will show how uncertainties might be investigated by SA for simulation results and results of a MCO.

2 Extensions for dynamic process simulation models

The workflow for an iterative use of steady-state process simulation and optimization to support decision making in process development is sketched in Fig. 1. The developed workflow tools for BASF's inhouse simulator CHEMASIM support the use of plant data for model selection, validation and adjustment and the application of the model within simulation and optimization studies to investigate for example what-if scenarios, trade-offs of competing objectives or to optimize the DoE.

There is a dynamic counterpart called CHEMADIS for batch or dynamic processes sharing a huge repository of common code with CHEMASIM. For a brief outline of the differences and the solution method refer to Appendix A (cf. Electronic Supplementary Material, ESM). For this reason, it was an obvious next step to transfer the existing tools and methods from the steady state to the dynamic flowsheet simulator. Although, looking from a software engineering point of view obvious, the dynamic nature of the problems to be addressed increases significantly the complexity. Reading plant data for model validation for example includes measurements at different time points as well as integral or final values and the corresponding simulation properties need to be extracted from simulation. Another example in the context of DoE but also for optimization is the determination of derivatives. Typical event-driven recipes or scheduling increase complexity in the calculation of derivatives since they trigger jumps [22]. Since the number of optimization variables in optimal control can become huge due to the discretization of manipulated variables the use of analytical derivatives seems mandatory to perform optimization tasks. Apart from these algorithmic issues, data management and visualization are essential in order to unveil chances for improvements in the processes. Although the scope facing all these issues was quite ambitious, we were able to setup

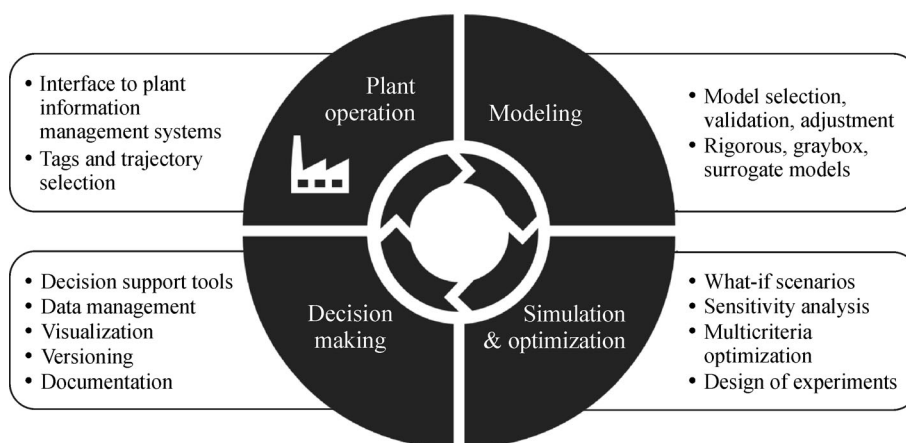


Fig. 1 Modeling, simulation and optimization workflow to support decision making in the development of dynamic chemical processes.

a functioning version of all workflow tools. In this contribution, the new possibilities for dynamic simulation within the flowsheet simulation environment will be demonstrated for batch distillation and reactor examples.

2.1 Plant data selection for MVA

2.1.1 Plant data manager (PDM)

In a previous contribution [12], we showed how the selection of steady state operating points could be supported. This so-called “PDM” includes interfaces to plant information management systems as for example ASPEN IP21 or OSI PI, supports selection of relevant measurement tags and enables a mapping between tags and properties of the simulation model. The PDM has been extended to identify and store time trajectories for dynamic systems. These time trajectories are called operating trajectories (OT) and small intervals on these trajectories are used to define time operating points (TOPs). The OT is divided into several TOPs. We use here small intervals for the TOPs to avoid selection of peaks caused by measurement noise. Using the data in this time interval, the average and the standard deviation of the data will be stored at the arithmetic mean of time interval bounds. Measurements at a certain time only are denoted as single time measurements (STMs). STMs could be for example analytical data for different fractions of a batch distillation. These measurements can be read from a MS Excel file.

2.1.2 MVA preparer

As mentioned already, before the process model is used, it has to be validated with process data. If the agreement is not sufficient, it is also possible to adjust some model parameters to the available process data. A general scheme for this model adjustment (or more precisely parameter

estimation) is shown in Fig. 2. The process data consists in $k = 1, \dots, N_{OT}$ OTs. Each OT comprises $j = 1, \dots, N_{TOP}$ TOPs. In each, $i = 1, \dots, N_x$ control variables \tilde{x}_{ijk} are available, which define the operating point, and measurements \tilde{y}_{ijk} with standard deviations $\sigma_{\tilde{y},ijk}$. Of course, also the control variables are measured with standard deviations $\sigma_{\tilde{x},ijk}$. The simulation of the process includes as input variables x and model parameters p to be estimated and will predict the measurements $y(p, x, t)$ of the TOPs or $y'(p, x, t)$ of the STMs. For solving the parameter estimation problem there exist several options for the objective function to be optimized (cf. for example [17]). If the inputs of the simulation are set equal to the measured values, one obtains a classical least-squares problem. If the inputs of the simulation are also used as variables in the optimization problem, this is usually known as error-in-variables model. To account for the different orders of magnitude of the measurements, the measured standard deviations σ are used to scale them. Additionally, individual weighting factors w could be used to influence the contribution of the residuals in the objective function.

As a part of the decision support framework we implemented the MVA preparer, which uses the available information from the PDM to set up the optimization problem. The information used is the list of available tags, the mapping of tags to simulation properties and the selected operating data. The MVA preparer supports the user in setting up the “sum of squared errors” as objective for the parameter estimation problem as shown in Fig. 2 in the same manner as it is possible for steady-state simulation. The preparer uses the information about the chosen measurement tags. In the preparer all data or a subset thereof could be chosen and defined as “to be set” or “to be validated”. “To be set” will define a continuous step function based on the measurements at the TOPs and include this function in a specification, which will be set inactive. The user has to activate these specifications

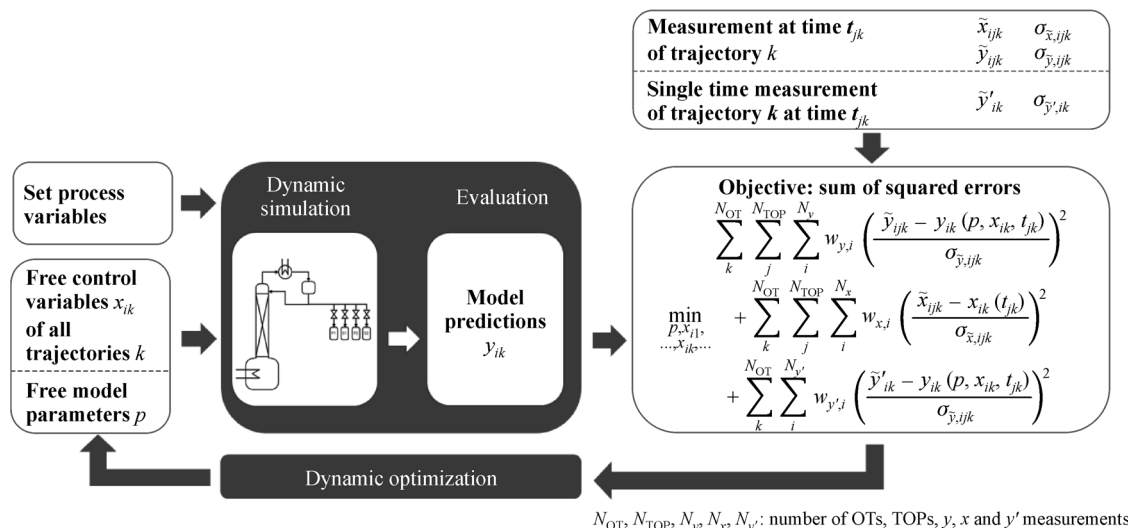


Fig. 2 Principle of combining models with data to set up the least squares problem for parameter estimation.

afterwards manually and has to choose, which degrees of freedom should be used to achieve the specifications. Therefore, it is recommended only to choose tags to be set which can be directly influenced like for example an outlet temperature of a heat exchanger which can be achieved by varying the heat input. Otherwise convergence issues due to infeasible specification might arise. To select tags as “to be set” reduces the problem but assumes that the values are exact (without measurement error). While tags classified as “to be validated” will be part of the objective function of the parameter estimation problem (cf. Fig. 2). If possible, it is recommended to use all tags as “to be validated”.

2.2 Simulation and optimization

2.2.1 SA

For steady state simulation with CHEMASIM it is possible to quantify selected parameters as uncertain and to specify a range of uncertainty [12]. In the sensitivity tool, it is possible to choose between different sampling methods to explore this uncertainty range. For these scenarios, simulations will be run, and the results can be visualized in the SA navigator [12]. This is now also possible for CHEMADIS. For dynamic simulations the time steps depend on the scenario and therefore differ between different scenarios (cf. Appendix A.1). Therefore, it is not possible to calculate sensitivities at each time point. We therefore find it more intuitive to rely on the visualization of the impact of uncertainties in the time trajectories (cf. section 3.3.1).

2.2.2 MCO

Dynamic optimization typically often includes the optimization of control variables. Here, control variables are looked for which optimize the objective of interest. To reduce the problem usually the control trajectory is discretized in several time intervals, in which parametric basic functions (e.g., linear or constant functions) of time are assumed. The parameters of these functions are used as optimization variables. Quite often simply constant values in these time intervals are assumed because these are easily implemented in operation by just simply change the set points of the controls at fixed time points.

Besides these special variables and objectives, there is no difference in the setup of an MCO problem in CHEMADIS compared to CHEMASIM. The MCO navigator was extended to include additional visualizations of trajectories for selected indicators. The amount of data to be handled is much more than in steady state simulation, since each time step includes as much information as an equivalent steady-state simulation. Data base access has therefore been optimized and significantly enhanced by grouping requests (up to factors of 200).

3 Results and discussion

3.1 PDM and MVA

In the following an example from literature with available measurements is used to demonstrate the use of the PDM and the MVA preparer: Nad and Spiegel [23] describe measurements in a batch distillation like sketched in Fig. 3 for the separation of a ternary mixture of cyclohexane, *n*-heptane and toluene.

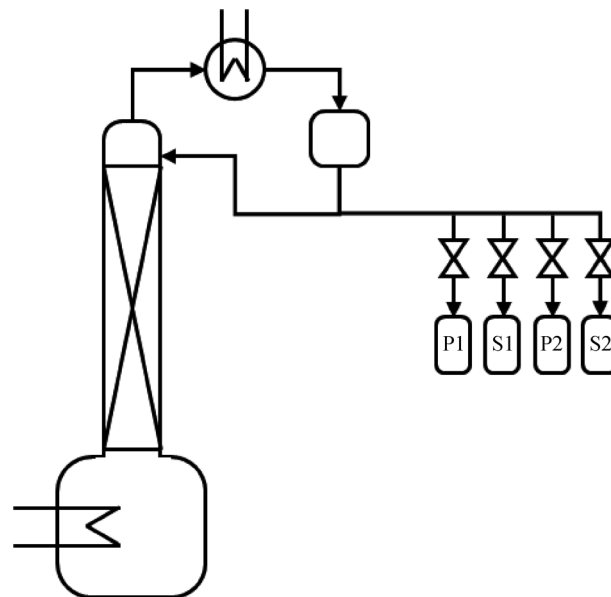


Fig. 3 Scheme of a batch distillation with different sample lines for product (P) and slop cuts (S).

The available measurements include time-dependent data of the vapor mass flow and molar concentration at the top of the column, distillate mass flow, liquid molar concentration in the still, temperatures at the top and the bottom of the column and pressure at the top. In the original source there is even more data given, but only complete sets of measurements are taken to facilitate the setup of the sum of squared errors as objective for the model adjustment. Besides these time-dependent measurements, amounts and concentration measurements for the initial filling, the residue in the still and the fractions (so-called STMs) together with the times when the valves are switched to the next collector are available. The sum of the amounts of the residue in the still and the fractions was less than the initial amount. Reasons for these deviations could be either inaccuracies in the measurements or losses due to sampling. For the simulation the initial amount was set to the lower value of 2.843 kmol. For the column and the condenser holdups were taken into account and set to the values given by Nad and Spiegel: 0.015 m³ for the column and 0.005 m³ for the condenser. In the simulation these

holdups are not part of the initial amount. Due to changes in composition of the holdups some mass is accumulated which reduces a little bit the total amount of all fractions and the residue in the still at the end compared to the initial amount. The number of theoretical stages for the column (inner diameter 162 mm) equipped with Mellapak 250Y (bed height 8 m) was taken from Nad and Spiegel and was set equal to 20. Top pressure was set to 962 mbar as measured and a constant pressure drop of 2 mbar per stage was assumed.

During the batch experiment the reflux ratio was changed. But the measurements of the reflux ratio were not very accurate as discussed by Nad and Spiegel [23] and also the exact switching times were not given. Furthermore, no information about the time-dependent reboiler heat duty was given. As an alternative to the reboiler heat duty either the vapor or distillate mass flow could be specified. Here the distillate mass flow was chosen. So, as the control variables for the process the reflux ratio and the distillate mass flow were used. These controls have been discretized in 7 intervals similar to the ones shown by Nad and Spiegel [23] with constant values as given in Table 1. For the reflux ratios and for the distillate mass flows average values of the measurements were used as initial values.

Table 1 Initial values for the controls

<i>t</i> /h	Reflux ratio	Distillate mass flow/(kg·h ⁻¹)
1	3.92	55.8
1.62	7.57	32.15
2	11.7	22.35
3.5	11.4	22
4.7	4.788	52.5
5.8	10.403	25
6.37	8.37	30

For all concentration measurements a standard deviation of 0.02 mol·mol⁻¹ was taken, while for all other measurements a standard deviation equal to 5% of the measured values has been assumed. Since no numbers were given in Nad and Spiegel [23], these numbers have been assumed to scale the contributions in the sum of squared errors as indicated in Fig. 2. The measured reflux ratios were not taken into account, since they are calculated based on the measured mass flows. For the measurements of the vapor concentration at the top a weighting factor of 100 was chosen, while for all other measurements the default weighting factor of 1 was taken.

As optimization variables for the minimization of the sum of least squares the 14 control variable values were used together with the coefficient *A* for the vapor pressure of *n*-heptane. The initial value for this coefficient converted to bar and *ln* was 9.25354607. The lower and upper bound for the coefficient were 9.15 and 9.35 and for the reflux ratio values were 1 and 13. For the distillate mass

flow values corresponding to 80% and 120% of the initial value were used as bounds. The sum of least squares was multiplied by a scaling factor of 10⁻⁵. Starting from a value of 3.190 the optimization ended after 48 optimization iterations with the sequential quadratic programming method from Schittkowski [24] successfully at an objective of 0.06066. The final optimized variables are given in Table 2 for the control variables, while the optimized value for the coefficient for the vapor pressure of *n*-heptane was 9.1656809.

Table 2 Final, optimal values for the controls

<i>t</i> /h	Reflux ratio	Distillate mass flow/(kg·h ⁻¹)
1	3.92	64.21
1.62	7.57	36.19
2	11.7	23.03
3.5	11.4	23.82
4.7	4.788	55.78
5.8	10.403	25.44
6.37	8.37	29.57

In Fig. 4 as an example the results for dynamic simulation based on the initial and the optimized values for the vapor composition are compared with the measurements. Further results can be found in Appendix B in the Figs. B1–B4 (cf. ESM). As can be seen, the model adjustment results are in nearly perfect agreement with all concentration and temperature measurements. Only, the vapor mass flows have larger deviations, since reflux ratios are similar to Nad and Spiegel significantly deviating from the measured ones between 1 and 3.5 h (compare Tables 1 and 2).

In Fig. B5 of Appendix B (cf. ESM) for the vapor-liquid equilibrium (VLE) data of the systems cyclohexane + *n*-heptane and *n*-heptane + toluene a comparison is shown between the experimental data at 1 bar and the prediction of the original thermodynamic model of Nad and Spiegel as well as of the one using an adjusted vapor pressure for *n*-heptane. As can be seen there the vapor pressure coefficient estimated from the batch distillation experiment significantly improves the agreement with the experimental data. This is just to show the reliability of the optimization. Usually, as mentioned before, the thermodynamic model is recommended to be parametrized based on the VLE data and then just used in simulation. This example is only a showcase for situations where reliable VLE data is not available or obtainable with reasonable effort as discussed in the introduction.

3.2 MCO and evaluation of uncertainties

3.2.1 Semi-batch Williams-Otto reactor

In this example the model of the semi-batch Williams-Otto

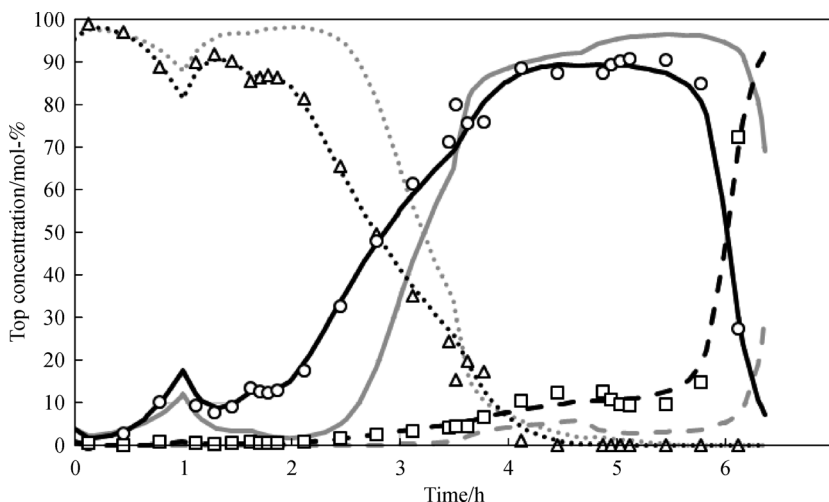
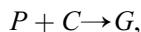
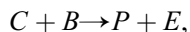
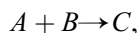


Fig. 4 Comparison of the dynamic simulation based on the initial (gray lines) and the optimized values (black lines) with the measured vapor concentration at the top of the column (symbols): ..., Δ Cyclohexane; —, \circ *n*-Heptane; —, \square Toluene.

reactor [25,26] is used. Figure 5 shows a scheme of the semi-batch reactor. The following reactions occur in the stirred vessel:



C is here an intermediate and P and E are the target products. In the last reaction from product P a degradation product G is formed. The full set of model equations for this semi-batch reactor is given in the Appendix C (cf. ESM).

Initially there is only 2 m³ educt A in the vessel at a temperature of 65 °C. Then B is fed with a temperature of 35 °C. The process can be controlled by adjusting the feed rate F_B of B between 0 and 5.784 L·s⁻¹ and by adjusting the wall temperature T_W between 20 °C and 100 °C. The reaction temperature T_R has to be maintained between 60 °C and 90 °C and the reaction volume V_R is limited to 5 m³. Total batch time is fixed to 1000 s. The wall temperatures are scaled with a factor of 1000.

The objectives of the multicriteria optimization is to find the optimal control strategies to maximize the amount of P and to maximize the amount of E . For this purpose, the control variables F_B and T_W have to be discretized over the time horizon of 1000 s. In this example 40 equidistant time segments were taken each with constant values for the control variables. In this case we have 80 optimization variables: $F_{B,1}, \dots, F_{B,40} \in [0; 5.874]$ and $T_{W,1}, \dots, T_{W,40} \in [20; 100]$ respectively the scaled ones $\in [0.02; 0.1]$. Furthermore, we have 3 path constraints: one lower limit of 60 °C for the reaction temperature T_R , one upper limit (90 °C) and one upper limit for the reaction volume (5 m³).

In Fig. 6 the results of the MCO are given as screenshots of CHEMADIS. We intentionally show screenshots here in

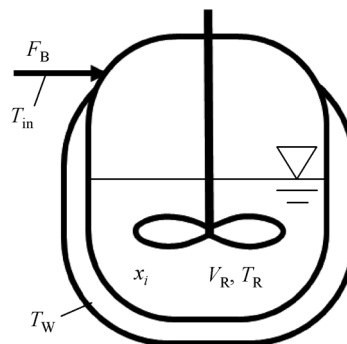


Fig. 5 Scheme of the semi-batch Williams-Otto reactor.

order to give an impression also about the graphical user interfaces that were developed in order to present the results to the user and offer decision support.

Here two objectives were taken into account: one to maximize the mass of product E and one to maximize the mass of P in the reactor. Figure 6(a) shows the Pareto-optimal solutions (best compromises between the competing objectives) in the MCO Navigator which is available in the CHEMADIS results. Furthermore, it is possible to visualize the corresponding trajectories for selected indicators as demonstrated in Figs. 6(b–e). In this example, as can be seen, the path constraint for the reactor temperature T_R and the reactor volume have been fulfilled. In the lower part of the Figs. 6(d) and 6(e), the profiles of the control variables are presented. This view shows only values at time steps where the function has been evaluated or corresponding to the defined printing time. The underlying function is still a step function.

3.2.2 Lysine semi-batch bioreactor

The second example shows results for a semi-batch

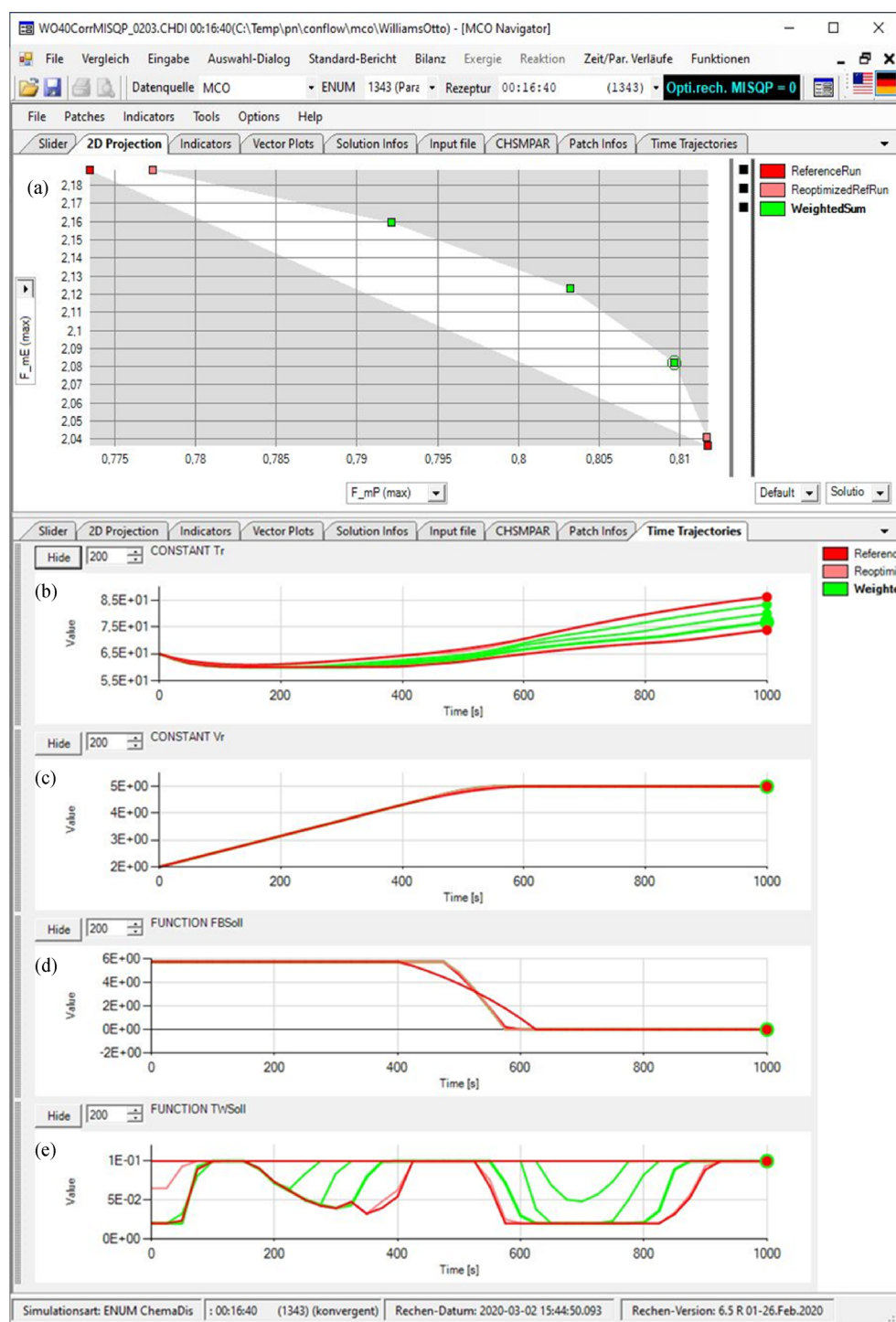


Fig. 6 (a) Pareto-optimal solution of the semi-batch Williams-Otto reactor problem in the MCO Navigator of the CHEMADIS results (Red squares are showing the reference runs, which are results of a single-objective optimization. In pastel-red the reoptimized reference runs are shown these are obtained by optimizing the other objective with the constraint not to become worse in the objective of the reference run. The green symbols show the results of minimizing a weighted sum. The weights are determined by the sandwiching algorithm [10]). Visualization of trajectories of selected indicators of the semi-batch Williams-Otto reactor problem: (b) reactor temperature (CONSTANT Tr); (c) reaction volume (CONSTANT Vr); (d) control for the feed (FUNCTION FBSoll); (e) control for the wall temperature (FUNCTION TwSoll is scaled with factor 1000). The trajectory of the selected point in (a) is shown with a bigger symbol and a bold line.

bioreactor to produce lysine. The model is taken from [27,28] and is summarized in Appendix D (cf. ESM).

In the bioreactor (cf. Fig. 7), we have biomass X , substrate S and lysine, the product P . V is the volume of the mixture in the reactor. $C_{S,F}$ is the concentration of the substrate in the feed and u is the flow rate of the feed, which is the control variable. The model depends on a specific growth parameter μ_p , a substrate consumption parameter σ_p and the production rate parameters $\pi_{p,1}$ and $\pi_{p,2}$. For the optimization there are path constraints for the amount of product P , the volume of the mixture in the vessel V , the amount of substrate consumed $(V - V_0)C_{S,F}$ and the total batch time t_F and a lower and upper bound of the control variable u . The competing objectives are the productivity J_1 and the yield of lysine J_2 .

In Fig. 8 the results for this multicriteria optimization are shown, again as a screenshot from CHEMADIS. In the following for one solution a SA will be presented and the MCO results will be compared to results for different uncertainty scenarios of the parameters μ_p and $\pi_{p,2}$.

3.3 Impact of uncertainties

3.3.1 SA

For the lysine example the impact of uncertainties on a

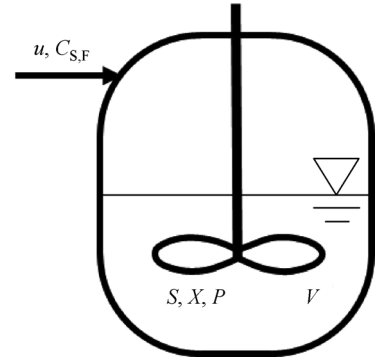


Fig. 7 Principle of the bioreactor for the production of lysine (P) (Reactor holdup (volume V) includes besides the product P , biomass X and substrate S . The feed rate u has a substrate concentration $C_{S,F}$).

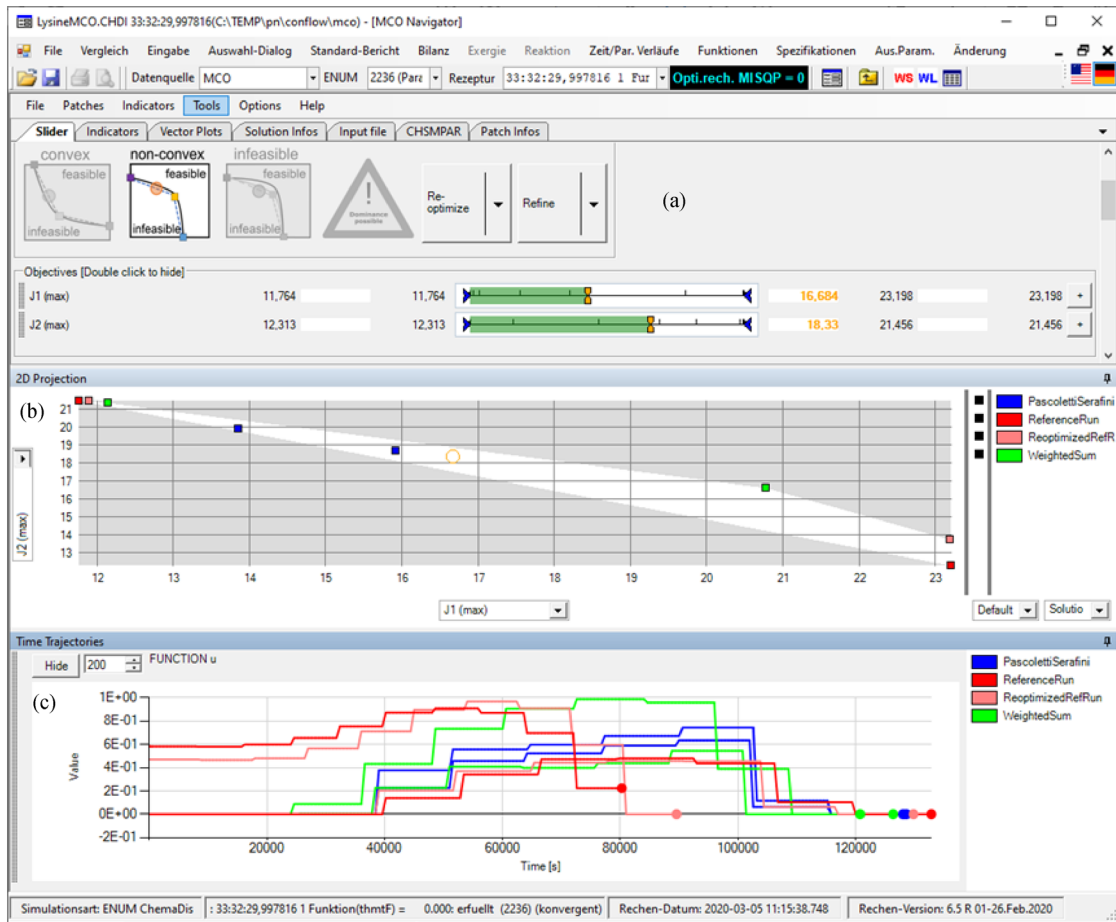


Fig. 8 Results of the multicriteria optimization of the lysine example with non-convex Pareto frontier and non-convex navigation (orange): (a) slider view with navigation; (b) 2D projection of Pareto frontier; (c) trajectories of the Pareto-optimal points (For the symbols and lines the same color code than in Fig. 6 is used. Additionally, there are blue symbols and lines indicating Pascoletti-Serafini runs resulting from the hyperboxing algorithm (for details see ref. [10])).

single solution has been investigated. In this case for fixed control variables (cf. Table 3) the impact of uncertainties in the parameters μ_p and $\pi_{p,2}$ was considered. The uncertainties assumed are $\pm 10\%$ of the nominal parameter value. This is only one example to investigate the impact of uncertainties in these parameters on the results. A factorial design is chosen as the scenario generation method to explore the uncertainty range. The trajectories of the selected indicators (here u , P and J_1) are shown in Fig. 9 as screenshots from CHEMADIS. As can be seen J_1 is negative for some uncertainty scenarios for time below 20000 s. For these scenarios with the fixed control values only a negative product amount P is found. This is of course not realistic, therefore an enumerated MCO as described in the next section is a more appropriate way to investigate the impact of uncertainties.

3.3.2 Enumerated MCO

Besides the optimization variables, parameters which

Table 3 Parameters of the discretized control variable of the solution for a total batch time of $t_F = 24.882$ h investigated with SA

i	t_i/t_F	$u_i/(L \cdot h^{-1})$
1	0	0.46925
2	0.1	0.46498
3	0.2	0.4813
4	0.3	0.56487
5	0.4	0.7108
6	0.5	0.89758
7	0.6	0.96715
8	0.7	0.91066
9	0.8	0.59615
10	0.9	0

should be enumerated could be used to investigate the impact of uncertainties. Here two factors (Fmup and Fpip2) have been multiplied to the original parameters μ_p

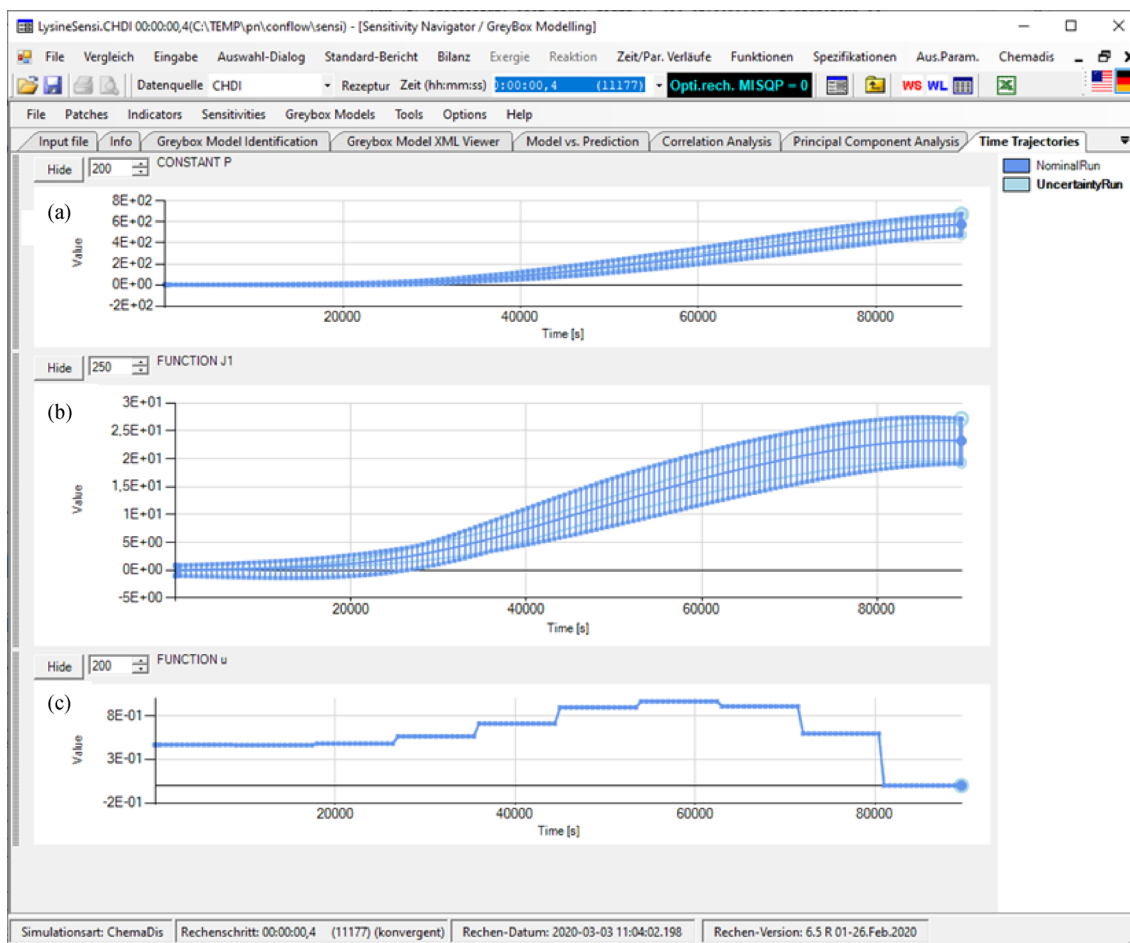


Fig. 9 Results of SA with factorial design for the solution of Table 3: trajectories for (a) mass of product P , (b) the objective reactor productivity J_1 and (c) the feed flow rate as control variable u .

and $\pi_{p,2}$ and specified as enumerated parameters. These two parameters have been varied between 0.9 and 1.1 in a factorial design leading to 4 scenarios: $(0.9\mu_p; 1.1\pi_{p,2})$; $(1.1\mu_p; 1.1\pi_{p,2})$; $(1.1\mu_p; 0.9\pi_{p,2})$; $(0.9\mu_p; 0.9\pi_{p,2})$ besides the nominal scenario $(\mu_p; \pi_{p,2})$. In an enumerated MCO for each of these scenarios a MCO will be performed. The results for these scenarios are compared in the MCO navigator shown in Fig. 10. There a big impact on the objectives can be observed.

The impact on the objectives J_1 and J_2 of the factor on μ_p is lower than the factor on $\pi_{p,2}$. The higher value for the first one increases the maximal reachable J_1 for both high and low values of the factor on $\pi_{p,2}$. On the other hand, it decreases the maximal reachable J_2 in both cases. The higher (lower) factor on $\pi_{p,2}$ increases (decreases) both objectives J_1 and J_2 compared to the nominal value independent of the factor on μ_p . This shows that this factor should be known with higher accuracy to get good predictions and it also shows that caused by the high sensitivity of the results on this factor it is probably also easier to determine it with higher accuracy when measuring J_1 and J_2 .

4 Conclusions

An existing decision support framework within BASF's simulator CHEMASIM for steady state simulation models has been extended for dynamic models based on the established dynamic counterpart CHEMADIS. All tools have been successfully adopted and their usefulness has been shown for MVA for a batch distillation as well as multicriteria optimization and the evaluation of the impact of uncertainties for reactor examples. Furthermore, methods for model-based DoE for batch experiments have been implemented, which can be used to identify optimal experimental settings and time points for measurements to get reliable parameter estimates or to select the most reliable model in case of rival model approaches as an extension of the DoE method for steady-state experiments [18]. This completes the workflow shown in Fig. 1 but is not part of this contribution. With the decision support framework process designers are enabled to develop reliable dynamic models which can be used in various what-if-scenarios leading to rational decision in process design, analysis and optimization of dynamic chemical processes.

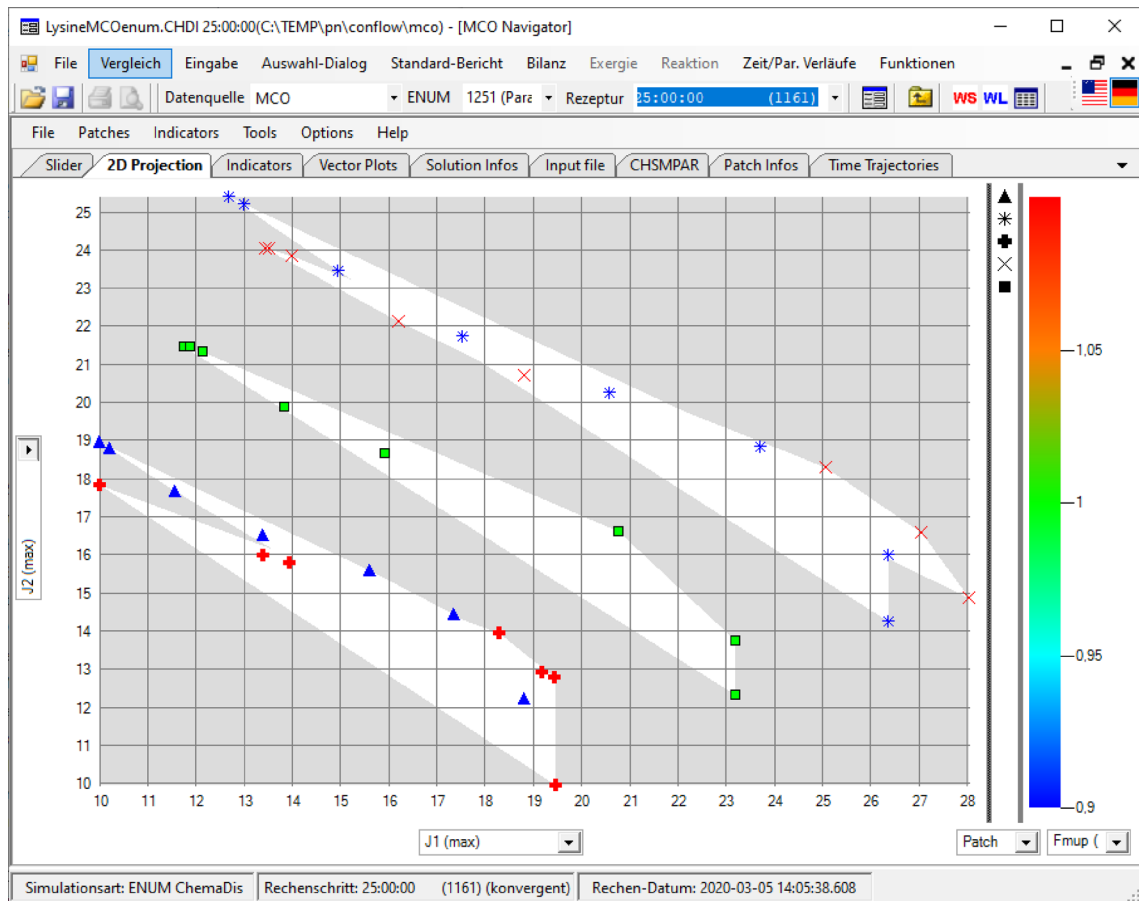


Fig. 10 Results of MCO for enumerated uncertainty scenarios: $\blacksquare \mu_p; \pi_{p,2}$; $\ast 0.9\mu_p; 1.1\pi_{p,2}$; $\times 1.1\mu_p; 1.1\pi_{p,2}$; $+$ $1.1\mu_p; 0.9\pi_{p,2}$; $\blacktriangle 0.9\mu_p; 0.9\pi_{p,2}$.

Electronic Supplementary Material Supplementary material is available in the online version of this article at <https://dx.doi.org/10.1007/s11705-021-2046-x> and is accessible for authorized users.

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