The Potential of Hybrid Mechanistic/Data-Driven Approaches for Reduced Dynamic Modeling: Application to Distillation Columns

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Extensive literature has considered reduced, but still highly accurate, nonlinear dynamic process models, particularly for distillation columns. Nevertheless, there is a need for continuing research in this field. Herein, opportunities from the integration of machine learning into existing reduction approaches are discussed. First, key concepts for dynamic model reduction and their limitations are briefly reviewed. Afterwards, promising model structures for reduced hybrid mechanistic/data-driven models are outlined. Finally, crucial future challenges as well as promising research perspectives are presented.

Keywords: Distillation columns, Dynamic model reduction, Hybrid modeling, Machine learning, Surrogate models

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1 Introduction – Revisiting an Old Topic

Separation sequences are of crucial importance for process economics. Consequently, improving the operation of distillation columns has always been an important research topic in process systems engineering (PSE) [1]. However, distillation columns pose severe challenges for model-based control strategies due to large system sizes and nonlinear thermodynamics. These circumstances led to substantial efforts in the 1980's and early 1990's targeting the development of reduced nonlinear dynamic distillation models for use in model predictive control (MPC) algorithms [2–10].

Early works addressing nonlinear MPC (NMPC) for distillation columns were conducted in times of process operating strategies focusing on maintaining desired stationary operating conditions by rejecting disturbances. Nowadays in contrast, transient operating schemes become increasingly important in order to cope with increasingly volatile market conditions, in particular fluctuating electricity prices resulting from an increasing penetration of renewable energy sources [11, 12]. In this context, energy-intense air separation units (ASUs) gained much attention from the scheduling perspective [13–15]. Strategies for exploiting time-variable electricity prices inherently rely on transient process operation. However, this poses severe challenges for the process control of ASUs due to large liquid holdups in distillation columns and thus large time constants and dead times [16, 17]. Hence, industrially common MPC schemes employing linearized models appear unsuitable for this purpose due to limited predictive capabilities across the entire operating range [18].

This change in operating strategies motivates further research efforts concerning NMPC schemes for distillation processes, which includes the further development of suitable reduced nonlinear dynamic models. For instance, Cao et al. [19] proposed the use of reduced-order collocations-based models (e.g., [3, 4]) for distillation columns in ASUs and investigated their application for process control [20, 21]. Likewise, we recently presented an extended compartment model that uses artificial neural networks (ANNs) as surrogate models replacing complex intra-compartment relations [22] and demonstrated its suitability for applying economic NMPC to ASUs [23]. In that approach, the combination of mechanistic modeling principles and machine learning enables a favorable trade-off between model accuracy and computational efficiency. Thereby, reductions in

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computational times of almost two orders of magnitude compared to a full-order stage-to-stage model were achieved while ensuring similar predictive capabilities.

Herein, we provide a critical discussion of opportunities and limitations of such hybrid mechanistic/data-driven approaches for reduced dynamic modeling with a particular focus on the operation of distillation columns. Note that efforts addressing the development of efficient NMPC algorithms [24–28] are complementary, i.e., real-time capable control solutions will require both reduced dynamic models and efficient numerical algorithms. This discussion is, however, out of the scope of this manuscript.

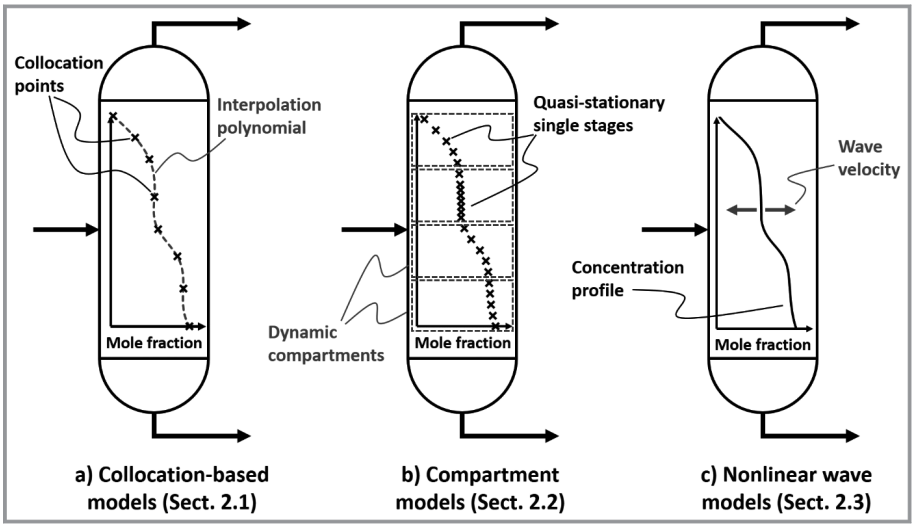

Figure 1. Illustration of the key concepts of classical dynamic model reduction approaches for distillation columns.

In the remainder, first an introductory review of existing dynamic model reduction approaches is provided, and their strengths and weaknesses are discussed. Afterwards, it is outlined how the integration of machine learning can overcome limitations of existing reduction approaches by using data-driven techniques. Although the focus is on ASUs, the conclusions will hold for any distillation system. Moreover, a generalization of the concepts is presented to account for other spatially distributed process systems and potential fields of application. Finally, the most crucial remaining challenges as well as and promising future research activities are addressed.

The main contribution of this work lies in encouraging researches to revisit classical reduced modeling approaches in the light of recent progress in data science and machine learning. We emphasize that we herein do not intent to claim a general superiority of one particular method. Rather, we believe that the method to be applied has to be selected in a very case-sensitive manner. Nevertheless, a thorough comparative assessment of the variety of potential approaches arising from the integration of machine learning into existing model reduction techniques is of a high practical interest and recommended for future research.

2 Limits of Classical Reduced Dynamic Modeling Approaches for Distillation Columns

Existing approaches for reduced dynamic modeling of distillation columns can be classified into three categories (Fig. 1): (i) collocation-based approaches, (ii) compartmentalization / stage aggregation, and (iii) nonlinear wave models. In the following, their concepts and limitations are briefly reviewed.

2.1 Collocation-Based Approaches

Collocation-based model reduction approaches (Fig. 1a) approximate the column profile by interpolating between a finite number of collocation points. By selecting substantially fewer collocation points than theoretical stages, a substantial model reduction is achieved [3, 4]. The column states above and below each collocation point, which are required for the mass and energy balances, are calculated through interpolation. For instance, Cao et al. [19] apply second-degree Lagrange polynomials. The locations of the collocation points can but do not necessarily need to coincide with the locations of actual stages.

Using a collocation-based approach, the number of MESH equations is reduced, leading to a smaller differential algebraic equation (DAE) system for a distillation column. As the structure of the DAE system, however, remains almost unaffected, the reduction of the size of the system will directly translate into savings in computational time for integration. For instance, Cao et al. [19] find a nearly linear scaling of simulation times with respect to the number of collocation points used. This behavior constitutes an important advantage of collocation-based models: the degree of reduction can a priori be chosen by selecting the number of collocation points.

The achievable degree of reduction of collocation-based models is obviously limited by accuracy requirements. In other words, too high degrees of reduction lead to substantial deviations from the predictions of full-order models for both the stationary and the transient behavior. For a detailed study on this trade-off, refer to the work of Carta et al. [29]. Most importantly, the authors find that there is a minimum number of collocation points that is required to accurately reproduce the characteristics of the transient

behavior, which strongly depends on the considered mixture. Consequently, desirable large degrees of reduction might easily introduce unphysical behavior, such as additional steady states.

2.2 Compartmentalization and Stage Aggregation

Compartmentalization (Fig. 1b) has been proposed as an alternative to collocation-based approaches [5]. Its mathematical derivation is given by Lévine and Rouchon [8] and builds on singular perturbation theory. In addition, there is a physically meaningful interpretation (e.g., [30]): A column model is split up into a number of compartments. One compartment is described by the dynamic compartment balances, stationary single-stage balances for all included stages except for one so-called sensitivity stage, and equilibrium calculations for all stages. Thus, the approach applies a separation by time scales assuming single-stage dynamics to be negligible compared to overall compartment dynamics.

Compartment models reproduce exactly the corresponding full-order model's steady state. This finding is independent of the degree of reduction and, thus, represents a major advantage compared to collocation-based reduction approach. In contrast, the transient behavior of compartment models depends on the number of compartments, their sizes, and the locations of the sensitivity stages. Horton et al. [7] present heuristics for these choices and demonstrate that dynamic responses of compartment models can be close to those of the corresponding full-order models, even if relying on substantially fewer differential equations. Likewise, Bian et al. [31] apply the compartmentalization approach to a distillation column of an ASU and find only small influences on the dynamic behavior even if reducing the number of differential equations by one order of magnitude.

Linhart and Skogestad [30] propose a different perspective of compartment models and introduce the concept of stage aggregation. More precisely, the mathematical formulation of a compartmentalized column is equivalent to interconnecting dynamic stages (with aggregated holdups) and stationary columns (without holdups), making the definition of compartments superfluous. Instead, the selection of aggregation stages and the definition of their initial holdups become relevant. The authors also provide a study on the computational efficiency of stage aggregation (and hence also of compartment) models. Summarizing their findings, the reduction approaches manipulate the stiffness of the DAE system instead of reducing its size. Consequently, improvements in the computational efficiency strongly depend on the integration method as well as the time constants of the input signal and are in no case guaranteed. In a second study, the same authors identify the solution of the large-scale nonlinear algebraic equation systems describing the intermediate stationary columns to be the computational bottleneck of compartment and stage aggregation models [32]. To overcome this limitation, they propose the use of explicit functions interpolating between precalculated solutions, which exhibits an unfavorable scaling with both the level of detail of the table and the number of components in the column. However, we recently extended this concept by integrating machine learning techniques [22].

2.3 Nonlinear Wave Models

The last class of reduction approaches interprets column profiles as travelling waves (Fig. 1c) and describes their movement in space and time by partial differential equations [33]. Early work of Gilles and Retzbach [2] proposes a first wave model for binary columns assuming sharp, i.e., discontinuous, temperature and concentration profiles. Later on, the wave model presented by Marquardt [6] overcomes the limitation to sharp profiles. The work by Kienle [10] finally generalizes the concept to multicomponent mixtures. Under certain thermodynamic assumptions (in particular, constant molar overflow and relative volatilities), the wave equations can be solved analytically and embedded into overall column balances. For this purpose, we recently extended the nonlinear wave model by an overall mass and energy balance that account for varying column holdups occurring in case of load changes [34]. More precisely, we thereby embed the wave equations into a compartmentalization approach.

Nonlinear wave models correspond to low-dimensional representations of distillation columns by definition, enabling promising opportunities for savings in computational times. As an important advantage compared to collocation-based or compartment models, the size of the DAE system describing the nonlinear wave model is independent of the size of the original full-order model. Moreover, the approach does not rely on a priori definitions of collocation points, compartment boundaries, aggregated stages, etc., mitigating risks for impaired model performance from suboptimal model set-ups.

As a limitation, nonlinear wave models inherently rely on simplifying assumptions on the thermodynamic properties. Consequently, there is a significant dependence of the model's predicting capabilities on the considered mixture. For instance, when applying the extended multicomponent nonlinear wave model to the high-pressure nitrogen column of an ASU, good prediction capabilities in case of rarely nonideal behavior (a mixture containing mostly nitrogen and oxygen) were shown [34]. At the same time, large deviations from full-order stage-to-stage models in case of strongly nonideal mixtures are likely and restrict the applicability of nonlinear wave models.

2.4 Interim Conclusion

A variety of dynamic model reduction approaches is available for distillation columns with numerous successful applications in literature for all of them. Moreover, one finds no general superiority of one approach. That is, each of the approaches offers certain promising advantages, which make it promising for specific use cases. Nevertheless, these advantages are in all cases accompanied by disadvantages that certainly limit the performances.

a) Collocation-based models represent a convenient way to reduce the number of MESH equations and, hence, the size of the DAE system. However, they bear a severe risk of introducing unphysical behavior for desired large degrees of reduction.
b) Compartmentalization and stage aggregation make use of a separation by time scales that does not depend on the thermodynamic properties. Thereby, they effectively reduce the number of differential equations. In standard variants, their computational performance is, however, not promising.
c) Nonlinear wave models allow for representing an entire distillation column by only one wave equation per component. However, they make strong assumptions on the underlying thermodynamics when deriving the solution, limiting their applicability to near-ideal mixtures.

Desired novel reduction approaches should combine the benefits and avoid the drawbacks by (i) enabling substantial reductions of the size of the DAE system that directly translate into savings in computational times, (ii) reproducing physically meaningful behavior even for high degrees of reduction, and (iii) being independent from the considered thermodynamic system in terms of performance.

3 New Opportunities through Machine Learning

Machine learning techniques have already been applied in PSE several decades ago (e.g., [35, 36]). Currently, research in this field is re-emerging after a period of low activity [37] with numerous successful applications [38, 39]. In particular, hybrid mechanistic/data-driven (also called semi-parametric/empirical or gray box) modeling approaches appear promising as they enable a balance between first-principle mechanistic (white box) and data-driven (black box) models [40].

In the following, some recent relevant applications in chemical engineering are reviewed. Afterwards, a structural classification for using these techniques to enhance existing dynamic model reduction approaches is introduced. Finally, a more detailed discussion of a recently published example of a hybrid mechanistic/data-driven approach to reduced dynamic modeling of distillation columns is provided.

3.1 Hybrid Mechanistic/Data-Driven Modeling in Chemical Engineering

The idea to combine mechanistic equations with efficiently evaluable data-driven model parts has gained substantial attraction in PSE. During the last decades, hybrid model structures have widely been used to replace complex equation systems that would arise from purely first-principle mechanistic models and thereby accelerate process simulations and/or optimizations [40, 41]. In particular, numerous authors used surrogate models to replace thermodynamic property calculations in order to speed up process simulations/optimizations. Here, the surrogate models of choice are typically artificial neural networks (ANNs) and Gaussian processes (GP, also referred to as Kriging).

For instance, Nentwich et al. [42] apply both ANNs and GPs as explicit surrogate models for calculating fugacity coefficients in a hydroformylation process replacing an iterative procedure from the PC-SAFT property model. Likewise, we replace implicit thermodynamic functions from the Helmholtz equation of state for working fluid properties in an organic Rankine cycle by ANNs that allow for calculating any property in an explicit way, thereby speeding up deterministic global optimization of the process [43, 44]. Moreover, there are further approaches that directly replace tedious iterative calculations of phase equilibria by surrogate models, e.g., both McBride et al. [45] and Nentwich et al. [46] use GPs for explicitly calculating liquid-liquid equilibria compositions in a decanter, whereas we replace vapor-liquid equilibrium calculations in a flash by ANNs [47].

3.2 Enhancement of Existing Dynamic Model Reduction Approaches Using Machine Learning

Due to the progress in hybrid mechanistic/data-driven modeling, it is promising to investigate the suitability of this concept for dynamic model reduction. In particular, we target the integration of data-driven sub-models into existing dynamic model reduction approaches to overcome their limitations (see Sect. 2.4). We confine to structures with the data-driven part accounting only for stationary (i.e., algebraic) relations, which is motivated by three key observations:

a) Recent literature (Sect. 3.1) shows that data-driven approaches are highly suited for replacing stationary chemical engineering relations.
b) The reviewed dynamic model reduction approaches for distillation columns (Sect. 2) already lead to reduced-order DAE systems comprising a low number of differential model equations.
c) In general, the differential equations for describing physical systems inherently correspond to linear conservation laws, for which effective model order reduction techniques exist (e.g., [48–50]).

Depending on the arrangement of the mechanistic and the data-driven model parts, we distinguish between two basic structures for reduced hybrid dynamic modeling (cf. [51]) as shown in Fig. 2. Note that we therein further confine to semi-explicit time-continuous DAE systems of differential index one for the sake of simplicity.

In the first structure (Fig. 2a), a data-driven model $\mathbf{d}(\cdot)$ estimates the residual $\varepsilon(t)$ between the predictions of a reduced-order mechanistic model $\tilde{\mathbf{y}}(t)$ and the corresponding full-order model's outputs $\mathbf{y}(t)$. This residual can in general be a function of the system input $\mathbf{u}(t)$ as well as the current state of the reduced-order model, represented by the differential variables $\hat{\mathbf{x}}(t)$ and the algebraic $\hat{\mathbf{z}}(t)$. Note that this hybrid model structure is very general, as it requires no knowledge about the full-order mechanistic model. It rather treats the full-order model as a black box and aims at minimizing output deviations. The approach depicted in Fig. 2a appears highly suited if a reduced-order model that exhibits a promising mathematical form, but still captures the most relevant output dynamics, is readily available. In this case, a data-driven residual estimator could be used to compensate for any non-negligible deviations from the behavior of the original full-order mechanistic model. For instance, considering the application to reduced-order dynamic distillation models, one could enhance a nonlinear wave model by a data-driven residual estimator to account for nonideal thermodynamic behavior.

The alternative approach (Fig. 2b) uses an explicit surrogate model for calculating selected algebraic variables $\tilde{\mathbf{z}}(t)$ used in the mechanistic equation system of the reduced-order model, for which analytic expressions are either unknown or computationally too expensive (e.g., [52, 53]). As above, the complicating algebraic variables $\tilde{\mathbf{z}}(t)$ are given as an explicit function $\mathbf{d}(\cdot)$ of the system input $\mathbf{u}(t)$, the differential states $\hat{\mathbf{x}}(t)$ of the reduced-order model and its remaining algebraic states $\hat{\mathbf{z}}(t)$. In contrast to the approach using a residual estimator, this type of hybrid model requires insights into the full-order model. Consequently, the approach in Fig. 2b aims at cases where the reduced-order model still relies on detailed modeling of some of the involved phenomena and, thus, suffers from an impaired computational performance. Following this discussion, compartment models could be enhanced in that way by using surrogate models to replace the solution of the complex nonlinear algebraic equation systems describing the intra-compartment relations. Likewise, stage aggregation models could be enhanced by using surrogate models to replace the stationary columns between two aggregated stages.

Both presented basic structures for reduced hybrid dynamic models give rise to a large variety of potential concrete models for a specific application, particularly by selecting both the complexity of the mechanistic model part and the structure of the surrogate model. Below, such a concrete reduced hybrid dynamic model is presented for a distillation column. Note that this is one illustrating example among the vast amount of opportunities and it is not claimed to be the best hybrid model for all purposes. Depending on the intended use case, the hybrid model will have to meet specific needs as will be discussed in Sect. 5, so that other model structures might be favored.

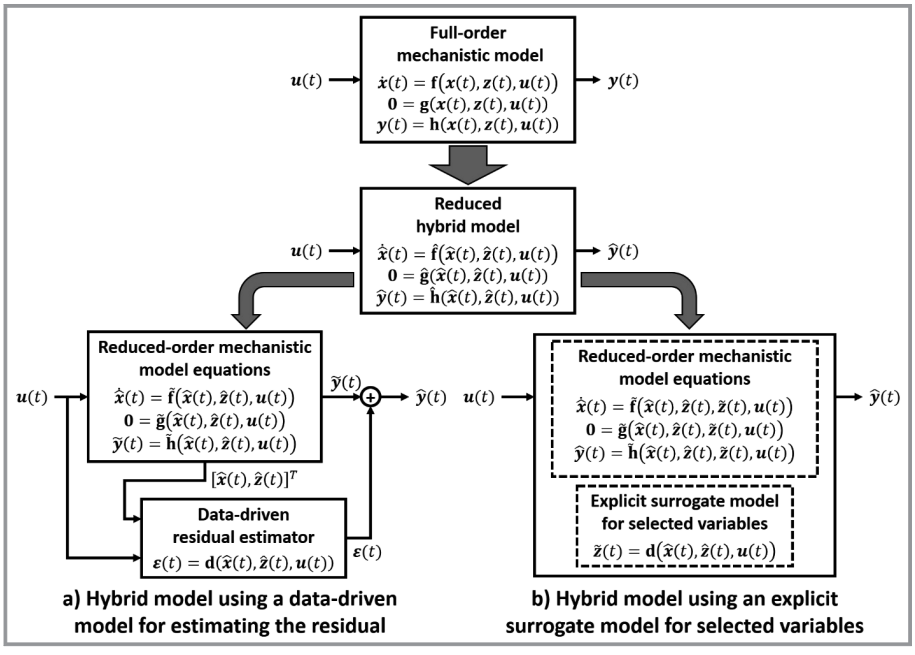

Figure 2. Structural classification of hybrid mechanistic data-driven approaches for reduced dynamic modeling assuming that data-driven model parts only account for stationary relations.

3.3 Example: An ANN-Based Compartment Model

In the following, we discuss our recently presented ANN-based compartment model as a prototype of a reduced hybrid dynamic model. We herein confine to discussing its properties. A detailed derivation as well as a numerical study on its computational performance can be found in [22]. The ANN-based compartment model builds on the classical compartmentalization by dividing a column into a predefined number of compartments comprising several consecutive stages. Instead of relying on the solution of large complex algebraic equation systems within the compartments defined by the stationary MESH equations of inner stages, ANNs are used as explicit surro-

gate models (Fig. 3a). The ANNs compute the compartment outputs (outgoing streams and their compositions) from the compartment inputs (ingoing streams and their compositions) and the differential compartment states (overall compartment mass and compositions). Thereby, a compartment is modeled in a similar way as a simple flash unit, where the outputs are given as explicit functions of the inputs and the differential states, e.g., a *T*-*x*-flash. An ANN-based compartmentalized distillation column model can, thus, still be considered as interconnected MESH equations. However, it comprises substantially fewer differential balance equations compared to full-order stage-to-stage models. Moreover, an ANN-based compartment model satisfies fundamental balance relations, representing a major advantage of any compartmentalized model over collocation-based approaches.

The use of surrogate models represents a second source of errors in addition to potential errors from manipulating the stiffness of the DAE system through compartmentalization (Sect. 2.2). Whereas the latter only affects the transient model behavior, errors from the ANNs are also present in steady state. However, previous results (cf. [22]) show that the complexity of the ANNs does not significantly influence the computational performance in dynamic simulations. Thus, the additional model error from the ANNs can be reduced to almost arbitrary size by using adequately complex networks and well-distributed data sets for training, while only insignificantly impairing computational times. In contrast, the number of compartments used and thus the degree of reduction of differential states represents the bottleneck. More precisely, the desired accuracy of the transient model behavior defines a minimum number of required compartments, which can be identified before the surrogate modeling. The introduction of any additional compartment is accompanied by an inevitable increase in computational times.

As is the case for any hybrid mechanistic/data-driven model, the prediction capabilities of the ANN-based compartment model depend on the training data. However, as the ANNs only replace well-defined stationary (algebraic) equations, training data can be obtained easily by solving these equations offline. Here, a suitable coverage of the relevant input space can be achieved by using advanced sampling methods (e.g., [42, 54, 55]). Assuming maximum internal column flows to be known and considering that compositions are inherently bounded between zero and one, the risk for extrapolation of the ANNs could, thus, in principle be entirely circumvented.

Note that the stage aggregation analogy from Linhart and Skogestad [30] again allows for an alternative perspective on the model (Fig. 3b). Here, the ANNs replace a series of interconnected stationary stages, which corresponds to learning the input-output behavior of stationary distillation columns. This hybrid model set-up, therefore, also appears appealing considering previous progress in replacing single flash units including the analysis of guaranteed worst-case accuracy [47].

4 Generalization to Spatially Distributed Systems and Possible Fields of Application

Many authors recognized analogies between mathematical models for distillation columns and those for other spatially distributed process units. These analogies motivated the adaptation of classical dynamic model reduction approaches developed for columns to other spatially distributed process units, including fixed bed reactors [33, 56] and heat exchangers [19, 56]. Applying the proposed hybrid mechanistic/data-driven model structures (Fig. 2) to other spatially distributed processes is indeed also possible and has a high potential. For instance, intensified processes like reactive distillation are highly promising for reducing both capital invest and energy use [57]. Likewise, the transition towards bio-based process routes causes a need for integrated separation techniques by combining, e.g., distillation and extraction [58]. Finally, flexible energy processes are designed to cope with fluctuating sources, e.g., organic Rankine cycles for waste heat recovery in vehicles [59]. Note that all of these examples are governed by strong nonlinearities and/or transient

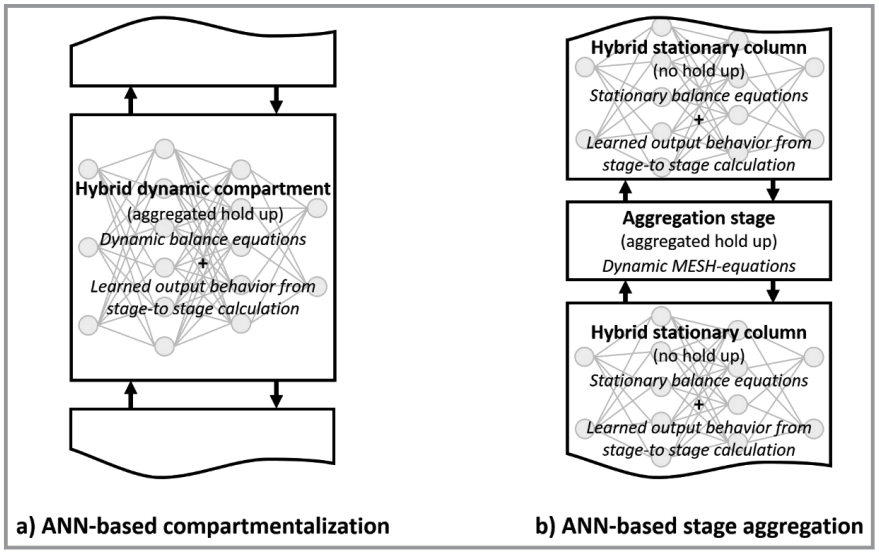

Figure 3. Structure of ANN-based compartment (a) and stage aggregation (b) models as examples for hybrid mechanistic/data-driven approaches to reduced dynamic modeling of distillation columns.

behavior, motivating the development of advanced control methods that in turn require accurate, but not too complex nonlinear models. These models might as well be improved by combining mechanistic knowledge with data-driven approaches as shown above.

Moreover, many relevant applications involve the appearance and disappearance of phases, e.g., during start-up and shutdown of flexibly operated distillation columns [60]. Likewise, operation of evaporators with transient heat sources leads to moving phase boundaries [61]. Consequently, future work should also investigate the applicability of the hybrid reduction approaches with regard to optimization-oriented model formulations accounting for discrete event [62, 63].

5 Future Challenges and Opportunities

Although the described ANN-based compartment model enables a promising trade-off between model reduction and accuracy [22, 23], several issues remain concerning an industrial NMPC implementation and are discussed in the following. We again emphasize that these issues are also relevant for other hybrid mechanistic/data-driven modeling approaches.

5.1 Balance between Mechanistic Knowledge and Machine Learning

As stated earlier, hybrid mechanistic/data-driven models represent a compromise between first-principle mechanistic models and data-driven techniques. Here, the extent of replacing mechanistic equations with data-driven models (i.e., the complexity of the reduced-order mechanistic model in Fig. 2) is an important degree of freedom during modeling and crucial for the model's performance. In particular, a high use of surrogate modeling can improve the computational performance due to beneficial mathematical forms but also increase the reliance on suitable training data. For instance, considering our ANN-based compartment model, one could confine to replacing only the single-stage flash equations instead of replacing the entire algebraic equation systems comprising mass and energy balances as well. This would certainly lower the reliance of the alternative model on data by using available mechanistic knowledge about intra-compartment relations. However, at the same time, the computational performance would likely be impaired, as strongly interconnected single-stage equation systems would remain.

Future research should thoroughly investigate up to what extent mechanistic model parts should best be replaced by data-driven approaches. Note that this decision will need to account for the availability of data. In other words, the decision will likely be different in cases where excessive amounts of data can be generated easily in-silico compared to cases where the generation of data involves either costly experiments or interventions of the operation of a process. Whereas in the first case (data is easily available from in-silico simulations), the selection of the data-driven model parts might solely depend on computational issues, in the latter case (costly data generation from experiments), the structure of the hybrid model needs to match the available data. In particular, it becomes obvious that in the latter case, only those relations can be replaced where both the input and output of the data-driven model can be measured or estimated.

5.2 Model Reduction vs. Model Identification

Revisiting the referenced approaches for hybrid mechanistic/data-driven modeling independently from the question of stationary vs. dynamic, one finds that in almost all cases, authors have been in the comfortable situation of having the "real" model for data generation. Undeniably, in industrial settings, this will not always be the case, as the construction of high-fidelity full-order models is tedious and expensive.

Conditions will, therefore, change in many practical situations, so that the required data will necessarily originate from measurements, involving the previously described implications concerning the selection of the extent of replacing mechanistic equations (Sect. 5.1). This observation makes a further distinction necessary: first, consider the case where the data is obtained in offline lab-scale experiments, e.g., heat/mass transfer coefficient correlations, partition coefficients, or reaction rates. Then, the conceptual procedure is essentially the same as in cases where a high-fidelity model is available, i.e., an adequate sampling of the input space is conducted, and only needs to respect additional constraints on the number of experiments one is willing to perform. In contrast, in cases where the only data source is an existing monitored process, one finds a severe conflict of interest between model identification (that aims at covering the entire operating range) and a safe operation of the process (that preferably stays in regions where the model is accurate). In order to identify the data-driven model parts without consciously disrupting the operation for identification purposes, adaptive approaches represent an alternative, where the data-driven model is successively identified (cf. [64]).

5.3 Industrial Application

The promise of getting reduced hybrid models adaptively from available, i.e., measured, plant operating data (Sect. 5.2) would certainly facilitate the application of the proposed model structures in industrial practice. Such a procedure becomes even more appealing considering that it matches the current industrial workflow for obtaining linear control models through small excitations of the plant very

well. In contrast, deriving a high-fidelity full-order process model possibly from scratch in order to replace some of its parts by surrogate models would represent a much stronger intervention of established workflows and might thus struggle with acceptance problems.

The increasing importance of digitalization and concepts like digital twins, however, indicate an upcoming paradigm change. In particular, the benefits from having sound model-based decision-support throughout the lifetime of a plant are increasingly recognized as a measure to ensure the competitiveness of the chemical industry [1, 65, 66]. Certainly, this trend might at some point help to overcome several of the presented issues.

Finally, hybrid mechanistic/data-driven modeling approaches need to become ready-to-use in state-of-the-art dynamic modeling environments. In particular, there is a strong need to simplify the current cumbersome academic hybrid modeling workflow. That is, generated data irrespective of its source is first transformed manually to the desired input format of the surrogate-modeling environment, e.g., the MATLAB Deep Learning Toolbox (The MathWorks, Inc.) or TensorFlow (Google LLC). Afterwards, the surrogate model needs to be parsed into the desired modeling language, e.g., Modelica (The Modelica Association) or gPROMS (PSE Ltd.), via ad hoc solutions. Obviously, in future, all required steps should preferably be conducted in one tool, which ideally should enable comfortable ways of processing real or in silico generated plant data and provide guidance for non-expert users through all steps.

6 Conclusion

The construction of reduced dynamic models for spatially distributed process units, particularly for distillation columns, has been a well-investigated research field for more than three decades. However, recent advances in data-driven and hybrid mechanistic/data-driven modeling motivate to revisit this research field and open promising opportunities for overcoming the limitations of known approaches.

Herein, possible model structure for such an enhancement of classical reduction approaches through machine learning are outlined and a recently published ANN-based compartment model representing a prototype of these hybrid model structures is discussed. The described model shows a good performance in reproducing the same transient behavior as a full-order model while substantially reducing computational times. Nevertheless, several issues remain to be resolved, before such model structures become ready-to-use in industrial applications. In particular, in absence of high-fidelity full-order process models, there is a crucial dependence on data. Consequently, the set-up of the reduced hybrid dynamic models will require either many costly experiments or significant disruptions of the operation of a process.

In the future, the advancement of digital twins might play a crucial role by providing simulative decision-support through detailed modeling. This means that high-fidelity full-order dynamic models for processes might eventually become readily available, allowing for generating accurate process data in-silico without performing costly experiments or disrupting the plant's operation. Consequently, having digital twins as standard would substantially facilitate hybrid mechanistic/data-driven approaches to reduced dynamic modeling.

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Symbols used

ε	[–]	residuals calculated using data-driven model
t	[s]	time
$\mathbf{u}$	[–]	system inputs
$\mathbf{x}$	[–]	differential states of full-order mechanistic model
$\hat{\mathbf{x}}$	[–]	differential states of reduced hybrid model
$\mathbf{y}$	[–]	outputs of full-order mechanistic model
$\hat{\mathbf{y}}$	[–]	outputs of reduced hybrid model
$\tilde{\mathbf{y}}$	[–]	outputs of reduced-order mechanistic model equations
$\mathbf{z}$	[–]	algebraic states of full-order mechanistic model
$\hat{\mathbf{z}}$	[–]	algebraic states of reduced hybrid model
$\tilde{\mathbf{z}}$	[–]	selected algebraic states in reduced-order mechanistic model equations calculated using data-driven model

Abbreviations

ANN	artificial neural network
ASU	air separation unit
DAE	differential algebraic equation
GP	Gaussian process
MESH	mass balance, equilibrium, summation and heat balance
MPC	model predictive control
NMPC	nonlinear model predictive control
PSE	process systems engineering

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