Dynamic Simulation of Oxyfuel CO2 Processing Plants

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Abstract

This paper illustrates the application of dynamic simulation for the development of CO2 processing plants which are part of oxyfuel power plants. It is shown how dynamic simulation models are used to study transient processes such as load changes and disturbances, to evaluate and improve process design concepts, and to develop control and operational strategies. Furthermore, key success factors for dynamic simulation, such as appropriate model visualization and an early integration into the engineering workflow, are discussed. In order to study the behavior of the entire oxyfuel process, the application of model reduction methods is proposed. This facilitates the integration of dynamic simulation models that were initially implemented using different simulation tools, into a common simulation platform.

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1. Introduction

Dynamic simulation of process plants plays a key role in the engineering workflow at Linde AG, Engineering Division, especially in the area of process innovation. This paper illustrates the contributions and benefits of dynamic simulation for the development of oxyfuel CO2 processing plants.

As a leading international engineering and contracting company, Linde Engineering designs and builds turnkey process plants for a wide variety of industrial users and applications: The chemical industries, air separation, hydrogen and synthesis gas production, natural gas processing and more. Being able to call on its own extensive process engineering know-how in the planning, project development and construction of turnkey plants, Linde Engineering is also pursuing a strategy for Computer Aided Process Engineering (CAPE) which is based on a long tradition of internal know-how: High quality methods and tools available from universities or commercial suppliers are combined with internal developments to achieve optimal solutions [1]. These tools include programs for dynamic simulation of process plants which are especially valuable for new process developments such as carbon capture and storage (CCS) technologies.

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Linde Engineering is working closely with industry partners to develop technical solutions for CCS [2], among them the oxyfuel process where coal is combusted in an atmosphere of oxygen, produced by an air separation unit (ASU), and CO₂. The CO₂–rich flue gas is further concentrated and compressed in a CO₂ processing plant (gas processing unit / GPU) and then transferred to storage (see Figure 1). ASU and CO₂ processing plants are part of Linde Engineering’s product range [3,4].

In order to identify the most appropriate process concepts for these plants out of numerous process variants, dynamic simulation is applied right from the project start. Both technical requirements such as guaranteed product purities at specified load change rates, and business requirements such as lowest investment costs aligned with highest energy efficiency and flexibility have to be satisfied.

An exemplary CO₂ processing plant and key success factors for dynamic simulation are described in Section 2. Sections 3 and 4 show how dynamic simulation is applied for the evaluation and improvement of process design concepts, and for the development of control and operational strategies, respectively. The application of simulation model reduction, which is required for an oxyfuel plant-wide simulation, is discussed in Section 5.

2. Dynamic Modeling and Simulation

In general, dynamic simulation models allow to study the transient responses of an entire process or a particular unit to planned and unplanned disturbances, and thus to improve the design, control, operation, and safety of the process. In order to verify static equipment design and develop control strategies for the Oxyfuel ASU and GPU, dynamic simulation models are derived from steady-state design process models in the Linde-internal process simulation tool OPTISIM® [5], and in the commercial system UniSim®, respectively.

Figure 2 shows an overview graphic for the dynamic simulation model of the GPU. In this particular design [4] CO₂ is separated from the oxyfuel flue gas stream using a cryogenic approach - raw gas compression, CO₂ liquefaction via a main heat exchanger and two separators operating close to the triple point of CO₂, vaporization and consequent product compression. Before being partially used for adsorber regeneration, vent gas is routed through the main exchanger and two expansion turbines, which drive booster compressors in the raw gas and in one of the product streams. The process objectives are to maintain a required CO₂ recovery rate while satisfying the product purity specifications for a given range of feed conditions.
Dynamic simulation can play a key role in a variety of engineering tasks - process design, control and operational strategy design including startup and shutdown procedures, safety and abnormal situation handling, etc. However, its use still faces barriers as dynamic simulation is often considered an "expert tool" and is not easily accessible to engineers of various backgrounds and design responsibilities. In order to remove these barriers and facilitate efficient communication between subject matter experts, Linde Engineering uses even at an early project stage Human Machine Interface (HMI) visualization to develop graphical user interfaces for dynamic models. This approach provides an intuitive and common environment in which process configurations, control and operational strategies can be demonstrated and discussed. It lets the user better focus on the relevant (e.g. operational) information than by using the simulation software interface directly, which typically provides a detailed process design view. For the current process example, such a process visualization consisting of a process overview (see Figure 2) and a series of more detailed process area views has been implemented in UniSim® Operations, resulting in significantly improved acceptance of the dynamic model.

Besides an appropriate visualization technique, an early integration into the workflow is crucial for the success of dynamic simulation:

It is generally accepted that the benefits of dynamic simulation tend to be largest if the findings become available early enough in a project so that design changes can still be incorporated. Yet, a high-fidelity dynamic model can only be developed if detailed design information is available. To reconcile these opposing trends it is imperative to integrate dynamic simulations tightly into the process design workflow. Initially, steady-state design has not advanced sufficiently to specify detailed simulation models for equipment such as turbo machines, heat exchangers, or piping. Hence, the fidelity of the initial dynamic models is low as e.g. constant efficiencies for turbo machines are assumed. At this stage the focus of dynamic simulation is on evaluating general operability and control concepts, and understanding the dominant dynamic modes of the process. As the design advances, more equipment details get specified (e.g. performance maps for turbo machines) which have to be transferred to the dynamic model. Therefore, the simulation software needs to be flexible to allow for different modelling levels within individual process units. Findings from dynamic analysis impact the static process concepts, resulting in an iterative design procedure. Typical applications of high-fidelity dynamic models using the GPU as an example are discussed in the following sections.

3. Design Evaluation and Improvement

It is determined whether the design objectives are met during transitions between steady-state design points, and how robust the design is with respect to disturbances (such as varying feed and utility supply conditions) and
equipment failures (such as turbine trips or loss of cooling water). As an example, the GPU model is subjected to a 30% rate reduction introduced over 7.5 min and a concurrent 2% increase in feed CO₂ concentration. The simulation results in Figure 3 confirm that the product purity specifications (>95% CO₂, <1% O₂) are maintained throughout the transition. However, the specific energy consumption increases due to the lower efficiency of the turbo machines which at around t=7 min start to move into recycle mode.

Knowledge of the dynamic behavior can be used to improve the design of the overall process as well as the individual units. As an example, the temperature peak at the adsorber exit resulting from a switchover between adsorber beds impacts the operation of the main heat exchanger. While the exchanger was initially designed based on steady-state (worst-case) inlet temperature predictions which resulted in a certain level of over design, the dynamic temperature predictions are used to further improve the exchanger design.

![Figure 3. Model predictions during a feed transition](image)

4. Development of Control and Operational Strategies

While the basic control strategies can be developed and evaluated using a low-fidelity model, a thorough evaluation of control and operational strategies requires both accurate process unit models and specification of all control-relevant equipment and logic such as compressor anti-surge and expander speed limiting controllers. For the GPU process, simulations covering a wide range of operating conditions revealed the need for additional temperature control loops in the vent gas path.

With such high-fidelity models strategies can also be developed for managing various disturbance scenarios and equipment outages. As an example, the temporary outage of the low pressure Booster Compressor 2 is considered. A strategy is developed which includes opening the expander bypass valve and adjustments of several pressure setpoints. The simulation results in Figure 4 indicate that the assumed disturbance does not cause violations of product purity specifications. CO₂ recovery requirements are also maintained once the process has settled into a new steady-state. However, the specific energy consumption increases.
5. Model Reduction for Plant-Wide Simulation

For operability analysis and control system design of the complete oxyfuel process, the dynamic simulation models of each of the oxyfuel process units, i.e. ASU, GPU, and others (see Figure 1) need to be combined into a plant-wide model. The fact that each industry partner contributing process units for the oxyfuel process usually applies its own design and dynamic simulation software, calls for a strategy to efficiently combine dynamic models from different simulation programs, e.g. OPTISIM®, UniSim® and others, within a simulation target environment. Since the integrated model shall be available to all contributing partners, know-how protection needs to be ensured. Furthermore, the effort of transferring dynamic models to the simulation target platform, reasonable computing times, and acceptable model fidelity levels of the transferred model, need to be considered. What clearly needs to be avoided is the attempt to re-implement an existing dynamic model in a new software tool.

In order to maintain flexibility for integrating the models into different simulation target platforms, the following two options have been pursued for the ASU and the GPU:

- An operating point linearization is applied to the nonlinear dynamic ASU model in OPTISIM®, an equation based simulation tool, which results in a linear dynamic state space model. The transfer to the target platform then includes a linear model reduction step [6] to gain a reduced dimensional linear state space model [7].

- A system identification method is applied to the nonlinear dynamic UniSim® model of the GPU, where responses of the original system to step inputs or PRBS (pseudo-random binary sequence) signals are generated [8]. This information is input to commonly available system identification software for linear systems or e.g. artificial neural networks. Input signals and system responses can be generated with models in any simulation tool.

Either approach for model transfer results in an encoded model of reduced order. Prior to integration into the target platform, the range of validity of the reduced model must be evaluated via comparison runs with the original models. Working with linear models provides the benefit that powerful control system analysis and design tools can be applied when studying the plant-wide process.

In the following, the transfer of the GPU model from UniSim® to a linear reduced model using system identification tools is discussed. Applying system identification techniques to data sets arising from detailed fundamental models instead of measured plant data has the advantages that (i) there is no measurement noise, (ii) there are no unmeasured disturbances, (iii) there are no operational limits w.r.t. duration and the type of...
identification experiments. For this reason, a simultaneous excitation of all relevant inputs to generate data sets for identification is feasible. In the current example, the following model inputs are considered: Flue gas rate, temperature and composition (characterized by the CO₂ impurities Ar, N₂, O₂, H₂O). Outputs of the model could be any of the internal states or derived quantities in the fundamental model. The following output variables are chosen: Product and vent stream properties (mass flow, temperature, composition), feed header pressure (which affects the operation of the upstream units), and overall compression power. A data set for identification is generated by applying (independent) PRBS signals to all of the inputs listed above. The identification inputs cover a range of +/- 5% in feed rate and +/- 16.5% in concentration of flue gas impurities from their nominal values. A standard system identification routine based on Least-Squares estimation is used to derive a linear discrete-time ARX (Auto-Regressive with eXogenous inputs) model of the form

\[ A(z^{-1})y(k) = B(z^{-1})u(k) + Se(k) \]

where \( u \) and \( y \) are the model input and output vectors, respectively, and \( e \) is a white-noise sequence with variance 1. \( A \) and \( B \) are defined as,

\[
A(z^{-1}) = I + a_1z^{-1} + \ldots + a_rz^{-r}, \quad B(z^{-1}) = b_0 + b_1z^{-1} + \ldots + b_sz^{-s}
\]

where \( a_i \) and \( b_j \) are coefficient matrices, and \( r \) and \( s \) are the model orders. The model quality is usually assessed via validation data sets that are different from the data set used for identification. Exemplary results from such a model validation (for a data set within the same input range as used for identification) indicate that the process behavior is closely approximated by this linear reduced model (Figure 5). However, if a wider operating region needs to be represented by the reduced model, a single linear model will not be sufficient as suggested by the results in Figure 6, which shows model responses to step changes in feed rate in the range 60% to 110%. Clearly, extensions to capture nonlinear effects would be required. This could be accomplished by "scheduling" multiple linear models over a desired operating range, by combining linear dynamic models with static nonlinearities using block-oriented modeling approaches [9], or by applying general nonlinear system identification methods [9].

Figure 5. Comparison of nonlinear model and linear reduced models: Product stream
Figure 6. Nonlinear and linear reduced models for feed rate changes (60%-110%): Product stream

6. Conclusions

It was shown how dynamic simulation can improve the process and control design of a CO₂ processing plant as part of an oxyfuel power plant. Additional benefits were realized by an early workflow integration and HMI visualization. Furthermore, methods and results of model reduction were presented, which provides the basis for integrating models from different simulation tools with the goal of optimizing the overall oxyfuel process.

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