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Pressure-Driven Dynamic Simulation of Distillation Columns in Air Separation Units

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At the moment, the change in power generation from fossil energy sources to renewables poses several challenges to the energy system and major energy consumers such as cryogenic air separation plants. Due to a more volatile power generation and the lack of storage systems, the energy price fluctuates and power intensive processes need to adapt regarding their operational agility and flexibility.
Currently, air separation units are designed for steady state operation at their optimal operating point with a minimum amount of load change procedures during their lifetime.
Within this work, detailed dynamic models of all plant components are developed which are an important tool to get a deeper understanding of flexible plant operations. Based on this, the process design can be adapted to allow for a more flexible mode of operation. In addition, those models can be used to develop and optimise advanced load change control strategies, which are more agile and consume less equipment lifetime compared to the state-of-the-art load change procedures. Hence, air separation plants are able to perform more frequent load changes and participate in a fluctuating energy market. Furthermore, these tasks are particularly challenging for air separation units, since they are mainly characterised by a high degree of process integration, high demands on product purity and non-linear column responses during plant start-up.
The main focus of this work lies on the dynamic modeling of the cryogenic distillation columns. For simulating the whole load range of an air separation unit, a **f**ull-**o**rder **s**tage-wise **m**odel (FOSM) for distillation columns is presented. All flows are pressure-driven, i.e. they result from a quasi-stationary impulse balance. Using this approach, specific scenarios for start-up or load change procedures, such as zero flow condition and reverse flow, can be simulated.
The “warm” start-up procedure is chosen as a representative scenario for any load change procedure, since it is the numerically most challenging simulation. “Warm” start-up means to initialise the model inventory at ambient conditions with zero flow. Based on this scenario, more technically relevant scenarios like the “cold” start-up after a plant shutdown as well as advanced control strategies can be investigated to allow a more flexible and agile operation.

1. Introduction

The Kopernikus-projects were introduced by the Federal Ministry of Education and Research due to the German energy policy. As part of the “Energiewende”, Germany wants to increase the share of renewable energies in its power supply. The goal of the Kopernikus-projects is therefore to develop new energy concepts which can be used in industry on a large technical scale as well as are accepted by society. (BMBF, 2017)
As part of the subproject “FlexASU”, **a**ir **s**eparation **u**nits (ASUs) are investigated further. Air separation plants have a high potential of helping to stabilise the power grid due to their high energy demand, widespread application and high density storage capacity. The main challenge of a flexible ASU is to get a deeper understanding of dynamic plant behaviour to adapt the design and the control strategies. Regarding the increasing volatility in the energy market, the importance of product scheduling rises significantly. The optimal scheduling calculation can be formulated as a dynamic optimisation problem with the goal to minimise the operating costs. Therefore, insight into the dynamics of an ASU is vital. It is important to display the highly

non-linear, transient behaviour of an ASU, which mainly results from the column dynamics. Pattison et al. (2016) suggest an empirical approach based on historical plant data to provide a dynamic ASU model.
On a more detailed level, dynamic simulations are crucial for the development of advanced control strategies. Therefore, complex models of unit operations are developed and submitted to model reduction to match the requirements regarding complexity and computational effort while maintaining accuracy (Romijn et al., 2008). Cao et al. (2016) develop physical models of the ASU components which are used to simulate a whole ASU including the argon rectification. A FOSM for distillation columns is developed and reduced via collocation.
In this work, a FOSM of the so called Double Column system is presented. Furthermore, an innovative simulation framework is being used, which facilitates a strictly modular-hierarchic modeling approach and simplifies the modeling effort (see sec. 2). In addition, a pressure-driven approach is used which allows to simulate the full operational range of an ASU including the most extreme operating condition, the “warm” start-up procedure from ambient conditions to a steady state at cryogenic temperatures (see sec. 3).

2. Simulation Model Infrastructure

To implement the dynamic models of an ASU, the new simulation model infrastructure SMILE (**S**imulation **M**odel **I**nfrastructure at **L**inde **E**ngineering) is applied. SMILE is a universal modeling framework which accumulates the detailed process and equipment knowledge gathered at **L**inde **E**ngineering (LE) into simulation models.On the one hand, the models can be used for standard process engineering tasks such as process and equipment design, process simulation or optimisation. On the other hand, there are emerging trends in process industry like volatile plant operations (dynamic simulation), predictive maintenance or the development of advanced control strategies which have new, more complex requirements for the simulation model. Therefore, these models need to be continuously refined to match the emerging requirements. To do that, the models need to be numerically robust and efficient as well as future-proof with respect to maintainability, re-usability and vendor-independency. (Thomas, 2017)
The SMILE modeling environment only requires an ISO C++ compiler and (optionally) a Python™ interpreter. Hence, it works on a wide variety of platforms. Process models are represented as shared libraries (on Windows machines: “DLLs”, Linux: “shared objects”, Mac OS X: “dynamiclibs”). The typical target platform will be Windows. There are applications intended which may run on Linux-based web servers or on site on single board computers such as the Raspberry Pi. For the more traditional process engineering applications, the models can be used within the process simulators that are in use at LE (i.e. OPTISIM® and UniSim® Design). Alternatively, there is an experimental modeling environment based on Python™, which targets at innovative embedded model-based applications. Figure 1 shows the workflow to create and integrate a SMILE model. (Thomas, 2017)

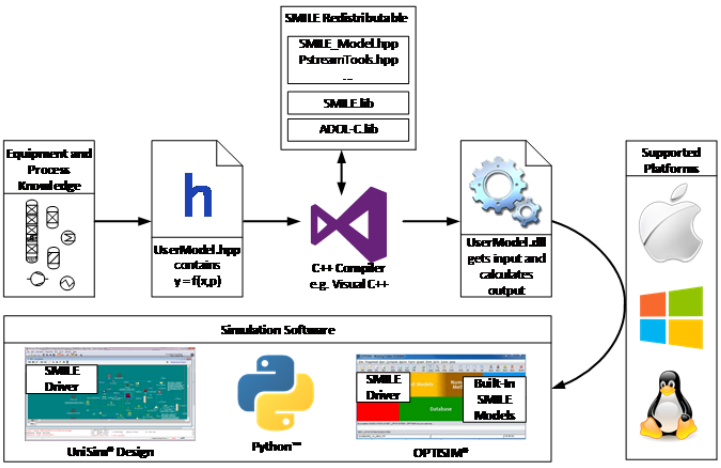


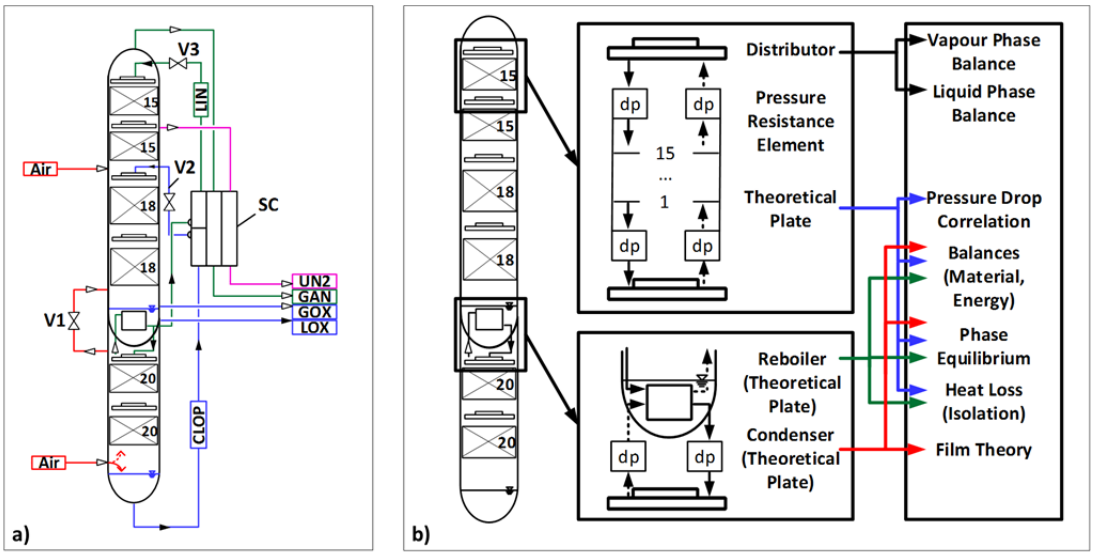
Figure 1: Typical workflow to create and integrate a SMILE model in process simulation software (Thomas, 2017)

From a software engineering point of view, a SMILE model is a C++ or Python™ class which is derived from a generic base class (SMILE_Model.hpp). As can be seen in Figure 1, the model equations that describe the desired unit operation, are implemented in a C++ header file which is the (header only) implementation of this class. SMILE contains standardised interfaces for process streams, parameters and physical properties. The strictly object-oriented set-up of SMILE models facilitates a modular-hierarchic modeling approach. This

approach is further explained in sec. 3. In addition, the C++ class inheritance allows the creation of SMILE model templates which can be further specialised or customised to generate models for specific purposes.
To create the shared library, only a C++ compiler is required. There are no third-party software license or library dependencies, hence, there are no obstacles regarding usability and availability of SMILE models. By relying on a standardised, vendor-independent programming language (ISO C++), SMILE models are easy to maintain and future-proof. Technically, the SMILE modeling environment is a C++/ Python™ library which is referred to as “SMILE Redistributable”. This library encapsulates software engineering details such as the creation of derivatives, discontinuity treatment, low-level (FORTRAN) interfaces for physical properties or memory management. Derivatives are generated either by the ADOL-C library (.lib), for which both forward mode as well as tape mode are supported (Walther and Griewank, 2012), or, preferably, by ADEPT (Hogan, 2014). In addition, the SMILE library contains means to model pressure-driven flow (PstreamTools.hpp) which is further explained in sec. 3. The main advantage of hiding the implementation details in the “SMILE Redistributable” is that the modeler can focus on the actual model and does not need to have a deep understanding of software engineering. From a mathematical point of view, a SMILE model is a mathematical model of a technical or physical system (e.g. unit operation). The mathematical model can either be a function, an **o**rdinary **d**ifferential **e**quation (ODE), a **d**ifferential-**a**lgebraic **e**quation (DAE) or an optimisation problem. A SMILE Model has inputs (which may include model parameters) and outputs. The inputs and outputs are typically communicated to the respective simulation software using software interfaces. (Thomas, 2017)
Within this framework, the pressure-driven dynamic models for a flexible ASU are developed which, as already mentioned, can be run on any machine and be integrated easily in the existing simulation environment of LE.

3. Pressure-Driven Dynamic Column Model

The focus of this work is to simulate a simplified start-up procedure for the cryogenic distillation columns in an ASU, since the column dynamic behaviour strongly affects the transient behaviour of the whole plant. Therefore, the Double Column is simulated to obtain two of the three main components of air, nitrogen and oxygen. Here, the additional Argon Column is not considered. A detailed description of the process of cryogenic air separation can be found in Hausen and Linde (1985). The Double Column consists of the Pressure Column (bottom) and the Low-Pressure Column (top). Figgure 2a shows a schematic representation of the Double Column system used for the dynamic simulation.



Figures 2a and b: a) Double Column system with 40 theoretical plates in the Pressure Column and 66 theoretical plates in the Low-Pressure Column b) strictly hierarchic modeling approach

A FOSM is used to describe the two thermally coupled columns. To simulate a realistic setup, the liquid distributers and the Sub-cooler (SC), a heat exchanger in between the two columns, are simulated as well. In this scenario, the main products are oxygen in gaseous (GOX) and liquid (LOX) form as well as pure gaseous nitrogen (GAN). The stream from the Pressure Column to the Low-Pressure Column is oxygen enriched liquid

air (CLOP). In addition, there is an impure nitrogen enriched side product (UN2) which is used for the regeneration of an upstream adsorber unit in an ASU. A more detailed description of the FOSM can be found in Wunderlich (2018). A characteristic feature of this model is the strictly hierarchic modeling approach. The dynamic column model is composed of several sub-models. Each sub-model is a closed system which can be simulated for itself. The sub-models communicate with each other over defined interfaces. This structure of the column model is predestined for the usage of the SMILE infrastructure. For each sub-model, a separate DLL is created. Those DLLs can easily be integrated into a simulation environment and combined to the complex column model. In addition, a debugging environment for each sub-model can be set up in e.g. Python™. This allows the modeler to systematically troubleshoot in case of error. Possible errors in the overall column model can be narrowed down to the particular sub-system which can be debugged by itself. This concept makes model building more convenient and efficient. Another advantage is that each sub-model can easily be replaced as long as the interface remains equal. This allows to switch e.g. the pressure drop correlations without having any further effort for the modeler. Figure 2b depicts the hierarchic structure of the column model. Due to the usage of pressure-driven flows, pressure resistance elements between any sub-models are necessary to generate flow. With this modeling approach, the actual value and the direction of a material stream $\dot{N}$ are not specified by the user but determined by the pressure difference Δp between the source and the sink of the stream and a resistance coefficient R, which is characteristic for the flow path. The molar flow is calculated according to the following equation:

$$\Delta p = R \cdot \dot{N}. \tag{1}$$

This generalised term allows to describe either linear or non-linear pressure-flow dependencies since R can be mapped to any user-specified function.
Furthermore, the pressure-driven approach allows to simulate reverse flow as well as zero flow condition. Therefore, a cumulative stream vector $\vec{S}_p$ needs to be defined which includes upstream and downstream entries.

$$\vec{S}_p \equiv \left[\dot{N}_{i=1,\,DS},\ldots,\dot{N}_{i=n_c,\,DS}, p_{DS}, \dot{H}_{DS}\,,\, \dot{N}_{i=1,\,US},\ldots,\dot{N}_{i=n_c,\,US}, p_{US}, \dot{H}_{US}\right]$$

The index DS stands for downstream and US for upstream, respectively. n_c is the number of components and $\dot{H}_i$ the enthalpy stream. To simulate zero flow conditions, all possible singularities need to be prevented. Furthermore, the transition between single and two-phase flow is regularised to ensure steady phase transitions. This approach allows to simulate the whole operating range of an ASU. It is now possible to initialise the inventory in the Double Column system at ambient conditions. The process streams are initialised with zero flow and the composition of air. By increasing the pressure of the feed stream sources, a flow into the Double Column system is generated. By reducing the temperature of the feed source additionally, it is possible to simulate a start-up procedure of the cryogenic distillation of air from ambient conditions (“warm” start-up).

4. Start-Up Procedure

A simplified “warm” start-up procedure is simulated. Table 1 shows the characteristic steps of this procedure. The results are explained by the vapour and liquid flow of the Low-Pressure Column.

Table 1: Characteristic steps of the simplified “warm” start-up procedure of the Double Column system

Time in s	Number	Step
0	1	Initialisation at ambient conditions and zero flow
300	2	Pressure build-up finished
400	3	Beginning of the partial feed liquefaction
3,200	4	CLOP flow by opening the valve V2
6,100	5	Reboiler/Condenser activation
7,950	6	Begin closing bypass valve V1
8,200	7	End closing bypass valve V1
8,550	8	LIN flow by opening the valve V3
12,100	9	Reboiler/Condenser maximum duty
12,500	10	LOX product flow due to LIC
13,000	11	Steady flow conditions

Figure 4 shows the vapour and liquid flow of the Low-Pressure Column on four different theoretical trays. The trays are numbered in ascending order, beginning at the bottom of the column. In the first 300 s, the pressure of the feed to the Pressure Column as well as to the Low-Pressure Column is increased to the operating pressure in the respective column (2). This results in an increase of vapour flow. The smallest vapour flow on tray 66 is a result of the UN2 stream which is subtracted at the liquid distributer above tray 51.
After reaching a constant pressure, a small drop in the vapour flow can be detected. Over the first 400 s, the feed streams are also cooled down to slightly above the dew point (3). For the next 100 s, the feed of the Pressure Column is cooled down further until it reaches a liquid fraction of 10 %. This builds up a liquid level in the Pressure Column which reduces the vapour flow a little further until a steady vapour flow is reached. After 3,200 s, the level set-point of the Pressure Column is exceeded (4). Therefore, CLOP is fed to the Low-Pressure Column by opening the valve V2. The CLOP inlet is the liquid distributer above tray 36. With a slight delay, liquid flow can be detected on tray 20 and 1 eventually.
At 6,100 s, the Reboiler/Condenser becomes active which results in a higher vapour flow in the Low-Pressure Column (5). Also, an increase of the liquid flow on trays 20 and 1 can be seen. This results from the liquid reflux in the Pressure Column and the increase of CLOP fed to the Low-Pressure Column. At 7,950 s the closing of the bypass valve V1 is initiated (6). This leads to a vapour flow decrease until a minimal vapour flow is reached at 8,200 s when V1 is fully closed (7). After that, an increase in vapour flow of the Low-Pressure Column can be seen, since the Reboiler/Condenser is evaporating the liquid in the bottom of the Low-Pressure Column.
At 8,550 s, the valve V3 is opened (8). Therefore, LIN is fed to the top of the Low-Pressure Column and liquid flow can be detected on tray 66 and with delay on tray 40. At 12,100 s, the duty of the Reboiler/Condenser reaches its maximum at a liquid level of 1 m in the Low-Pressure Column (9). Subsequently, a reduction of the duty can be seen, since the pressure increases due to hydrostatics of an increasing liquid level. This leads to a decrease of the vapour flows and a further increase of the liquid flows. The liquid flow on tray 66 is an exception. It is only determined by the flow of LIN which is constantly fed from the Pressure Column. Finally, at 12,500 s, the set-point of the Low-Pressure Columns level controller is exceeded and LOX is produced (10). With the production of LOX, the desired concentrations can be reached throughout the Double Column system. With a constant duty of the Reboiler/Condenser after levelling off the level controller, steady flow conditions are reached at around 13,000 s (11).

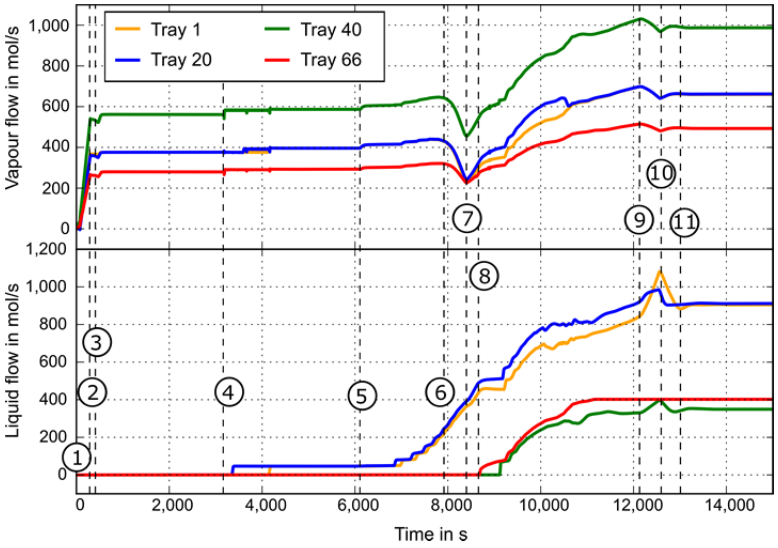


Figure 4: Vapour (upper diagram) and liquid (lower diagram) flow in the Low-Pressure Column on different trays

After reaching the steady flow conditions, it takes approximately another 18,000 s simulation time until steady state is reached with the final concentrations of argon throughout the Low-Pressure Column. At that time, the characteristic concentration profile of the gaseous phase of the Low-Pressure Column of an ASU can be seen in Figure 5. As expected, pure nitrogen can be found at the top of the Low-Pressure Column whereas pure oxygen is located at the bottom of the column. In addition, the accumulation of argon with its maximum around tray 30 can be simulated as well. At the maximum of the argon accumulation, the side stream for an additional argon rectification can be drawn.

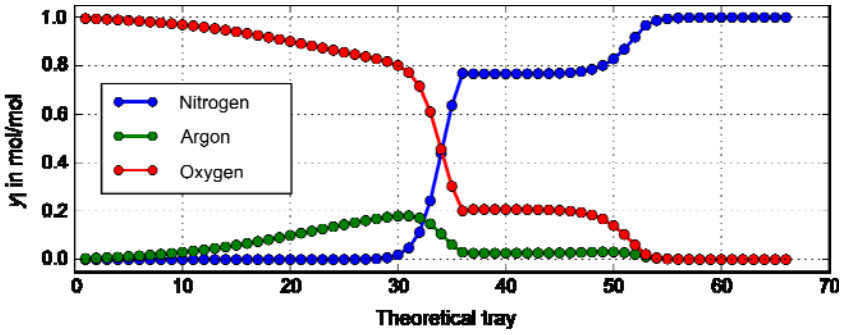


Figure 5: Steady state gas phase concentration profile of the Low-Pressure Column

5. Conclusions

This work emphasises the need for detailed simulation models to get a better understanding of the dynamic behaviour of an ASU. Given the complexity of the FOSM, it is important to provide a modeling environment which allows to focus on the different aspects of a distillation column (e.g. pressure drop calculation) by itself to simplify model development, maintenance and troubleshooting. Therefore, the SMILE framework is used which strongly supports the strictly modular-hierarchic model structure of the Double Column system.
In addition, robust dynamic models are crucial to be able to simulate load change procedures. For this reason, all process streams are pressure-driven which allows the simulation of both reverse flow as well as zero flow condition. A simplified “warm” start-up procedure is simulated which represents the most extreme operating condition of an ASU. This is the basis for further studies because it can be seen as the numerically most challenging scenario.
In the upcoming work it is planned to develop pressure-driven models of the remaining ASU components. Having a robust dynamic model of the complete ASU allows to develop advanced control strategies to ensure a more flexible and agile operation of an air separation plant.

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