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Safety Assessment on Distillation Columns: from Shortcut Methods and Heuristics to Dynamic Simulation

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A new method for the design of safety devices for distillation columns based on dynamic simulation is presented. A simulation model for the description of the column behavior after an operational failure was developed and successfully validated. The model includes the description of weeping, entrainment, and pressure relief (one-phase or two-phase flow). Based on the simulation results, a more efficient design of safety measures is possible. © 2010 American Institute of Chemical Engineers *AIChE J,* 57: 458–472, 2011
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Introduction

Because of their large contents, consisting often of flammable and/or toxic liquids, distillation columns possess a high-safety risk potential. The breakdown of different plant components can cause the process to leave the field of normal operation and finally lead to an emergency situation in which the intervention of safety measures becomes necessary. The most common safety method is the installation of pressure relief valves (PRV) for an efficient and fast pressure reduction. Safety relief valves have the advantage that they are independent from any external intervention and are still reliable in any emergency situation even after a power breakdown. They open automatically when their set pressure, which is correlated with the maximum allowable working pressure of the column, is reached.[1] Recently computer process control systems (PCSs) are more and more used to prevent undue overpressure.[2] However, the installation of pressure relief devices is still industry standard and will persist in the future.

Often the sizing an layout of relief devices for distillation columns is done by using shortcut methods, heuristics or rules of thumb. Common shortcut methods are to adjust the relief capacity to the reboiler or the overhead vapor rate. Also very common heuristic is to adjust the relief area of the safety relief valve to the area of the overhead vapor line (often used: 40%). These methods are quick but they comprise a high level of uncertainties that lead to an over sizing and an unnecessary large relief flow or an under sizing, which can cause a bursting of the column (worst case). Furthermore, important aspects of the plant dynamics and interaction of different plant components are completely neglected. A frequently used method based on dynamic simulation is a reduction of the distillation column to a simple pressure tank with no internals and no peripheral devices and assuming an external heat input. The more common reactor simulation models for emergency pressure relief can then be applied. However, this method implies critical disadvantages. The fluid dynamics and the thermophysical interaction happening inside the column are not considered

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adequately and therefore the quality and the reliability of the simulation results are limited. The reason for this simplification is that still today appropriate dynamic simulation models for the description of distillation columns during an emergency situation including a pressure relief do not exist.

Within the scope of this research work, a systematic approach is presented to fill the mentioned gap. A validated dynamic simulation model was developed and is described below covering the relevant phenomena like pressure relief, weeping, and entrainment.

Frequently Used Methods for the Calculation of the Relief Capacity

An overview of the different methods for designing the relief requirements of distillation columns is given by Bradford and Durrett.[3] The standard general procedure for the design of safety relief valves can be divided into six steps[4]:

1. Determination of the most credible worst-case failure scenario: The worst-case failure scenario is causing the fastest and most critical pressure or temperature increase.
2. Determination of the fluid phase condition at the PRV inlet: The inlet condition whether one-phase (vapor) or two-phase (vapor/liquid) has a big influence on the possible mass and volume flow and therefore on the pressure trend.
3. Calculation of the minimum required discharge mass flow ($\dot{M}$): Knowing the inlet condition and the worst-case failure scenario, the necessary mass flow, to keep the pressure below the desired limit, can be calculated.
4. Calculation of the mass flow density ($\dot{M}_{\mathrm{ideal}}$): The mass flow density in the PRV can be calculated knowing the inlet condition and the pressure ratio.
5. Calculation of the necessary cross-sectional area of the PRV: Knowing the mass flow density and the necessary mass flow, the necessary geometric cross-sectional area can be calculated ($A = \dot{M}/\dot{m}_{\mathrm{ideal}}\alpha$).
6. Consideration of the upstream and downstream pressure losses: The pressure drop in the valve inlet line should be lower than 3% and in the blow down line lower than 15% to prevent valve malfunctioning (according to manufacturer's recommendations).

The Steps 4–6 are only dependent on the properties of the PRV and therefore identical for a pressure tank, a reactor or a distillation column and can be done according to general approved safety valve flow models (e.g., Schmidt and Westphal[5] or Diener and Schmidt[6]). The application and the implementation of Steps 1 and 3 for distillation columns according to the most common design methods are described below. In Step 2, a vapor flow is assumed prematurely for distillation columns by all methods. However, it was shown by Can et al.[7] that depending on the operating conditions also a two-phase relief flow can occur. The option of a two-phase relief flow must be recognized early because it has a major impact on the relief dynamics and capacity. Using the standard methods discussed below, the prediction of a two-phase relief flow is not possible.

Adjustment to the reboiler vapor rate

This method assumes as the worst-case failure scenario (Step 1) a condenser breakdown. A one-phase relief flow is prematurely expected (Step 2). Therefore, the safety valve must be able to discharge the whole vapor produced by the reboiler (Step 3). The method can be refined by taking into account that if the pressure increases, less vapor is produced. This is due not only to the thermodynamics but also to a reboiler temperature pinch. A higher working pressure results in a higher boiling temperature and therefore in a reduced heat duty from a steam heated reboiler. A proper prediction of the heat input and the vapor generation rate during the scenario is difficult (especially after the opening of the safety valve), because the pressure is changing continuously. However, the major disadvantage of this method is the assumption that the reboiler hold-up consists of heavy components. However, it is not true that the heavy components from the bottom are discharged through the PRV. Mostly, the light components from the top are discharged. Depending on the molar heat of vaporization, it is likely that more vapor consisting mainly of light components can be produced by the given heat input. The actual needed relief capacity is therefore higher than the one calculated if considering only the vapor production in the reboiler.

Adjustment to the overhead vapor rate

Also a condenser failure (Step 1) and a one-phase vapor relief flow are assumed (Step 2). The necessary relief capacity is calculated according to the overhead vapor rate under steady-state operating conditions. The complete vapor flow going into the condenser has to fit through the PRV under relieving conditions. The assumption that the steady-state overhead vapor rate is the highest possible vapor rate which has to be discharged is not always true. Depending on the column state, higher vapor rates are possible, which is described below.

Sizing according to the overhead vapor line

An even more simplified method is to adjust the cross-sectional area of the relief device to the cross-sectional area of the overhead vapor line. Often a ratio of 40% is used. This is a pure heuristic method. All aspects of the column operation and dynamics are neglected.

Pressure vessel dynamic simulation

Common tools for the dynamic simulation of pressure relief events for reactors and pressure vessels are SAFIRE (Diers User Group), REAKTOR (BASF In-house-Tool), and RELIEF (CEC Joint Research Center). The basic assumption is that an integral volume is existing, which is not separated by internals. The failure scenario is simply simulated as an external heat input. Because of the very simplified model assumptions, the calculation method inherits some distinct insufficiencies: the composition of the discharged mass flow cannot be calculated, a possible two-phase relief flow is not detected due to the negligence of the liquid distribution over the column and crucial pressure drops over the trays cannot be predicted.

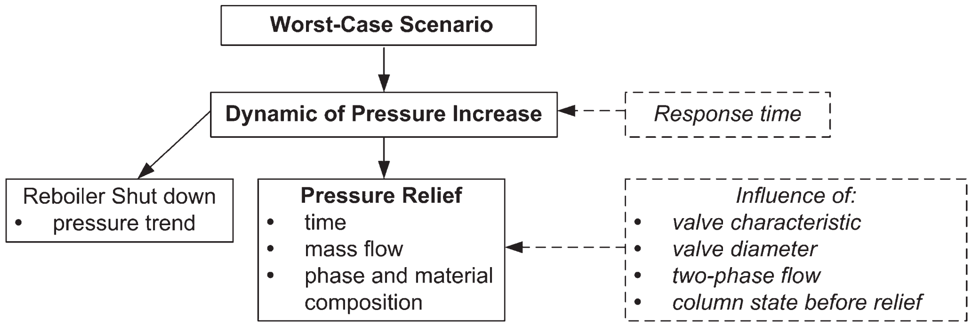

Figure 1. Experimental investigation concept.

Alternative Method: Reboiler Shutdown

In recent times, it becomes more and more common to prevent a pressure relief event completely and instead use the PCS to bring the process to a safe state. The requirements concerning the reliability (e.g., Safety Integrity Level) of PCS measures is described in the international Norms EN 61508 and EN 61511 and in the German national norm VDI/VDE 2180.[2] The standard procedure is to shut the reboiler down. A further energy input is prevented. However, a further pressure increase is still possible in spite of the reboiler shutdown. Because of the decreasing vapor flow, the liquid is not kept any more on the trays and begins to flow downward through the opening holes of the trays (not for valve trays). The light components from the top of the column begin to flow backward toward the bottom very quickly. If the low temperature liquid light components reach the bottom (higher temperature), they begin to evaporate until the equilibrium temperature of the new composed mixture is reached. A further pressure increase, even much higher than the pressure at the moment of the reboiler shutdown, is possible. The maximum and the trend of this further pressure increase are difficult to estimate due to the complex dynamics of the incident. A description and an evaluation of this safety measure with the previous mentioned methods are not possible. However, an increase of the column pressure is not safely prohibited by cutting off the heat input.

Experimental Investigation

Because of the lack of published experimental data on column dynamics in the field of not normal operation especially during an emergency pressure relief, experimental investigations under varying plant conditions were carried out. The most relevant investigation goals are shown in Figure 1. Each aspect is discussed in detail below.

Experimental setup

To achieve the required assignment, a specially designed plant configuration was chosen. The flow sheet of the pilot scale plant placed at the Department of Process Control and Operation of the Berlin Institute of Technology is shown in Figure 2. The experiments were carried out with a mixture of methanol/water or pure water. The pilot plant is fully automated with the Process Control System Freelance 2000 from ABB. Pressure and temperature sensors are distributed over the whole column. It has a height of 4 m and a diameter of 100 mm. The column is equipped with 16 sieve trays. The maximum allowable working pressure is 2000 hPa. Further column details are given in Table 1. The column head is a special construction designed for the described purpose. A short section beneath the column head is made of glass to give an insight view of the fluid dynamics during a pressure relief inside the column. The column head with the PRV consists of a screwable cap, which allows a quick and easy exchange. The mounting and the use of different safety valves is possible. The discharge system downstream of the safety valve consists of a blow down line with a short glass segment. The flow pattern of the discharged fluid can be qualitatively investigated. The relief flow is then conducted into a closed collector tank half filled with ice water for an instantaneous condensation of the discharged vapor. To ensure that the whole vapor is condensed and additionally as a pressure stabilizer, a flexible plastic bag is installed downstream of the collector tank. The condensed discharged mass flow is measured over time with a scale. Samples of the fluid are drawn during the pressure relief event from the blow down line and the composition is analyzed by gas chromatography. Using this setup, a time dependent analysis of the relief flow concerning mass, flow pattern, material- and phase composition is possible.

Preliminary experiments

According to the experimental investigation scheme shown in Figure 2, the preliminary experiments were carried out to develop a deeper process understanding and to explore the influence of relevant process parameters. Based on these results, first recommendations concerning the layout of safety measures can be given. In a second step, an adequate model is formulated.

Worst-Case Scenario. Most authors consider a condenser failure at maximum reboiler duty as the most credible worst-case scenario. This assumption was proved by analyzing different operation failures leading to a pressure increase. However, the time between the operating failure and the moment reaching the set pressure of the PRV (response time) is shorter than calculated using standard simulation models. This is due to the decreasing vapor flow after a condenser failure and the weeping from the trays. The light components from the column head are flowing toward the heavy components and evaporate. The pressure increase is

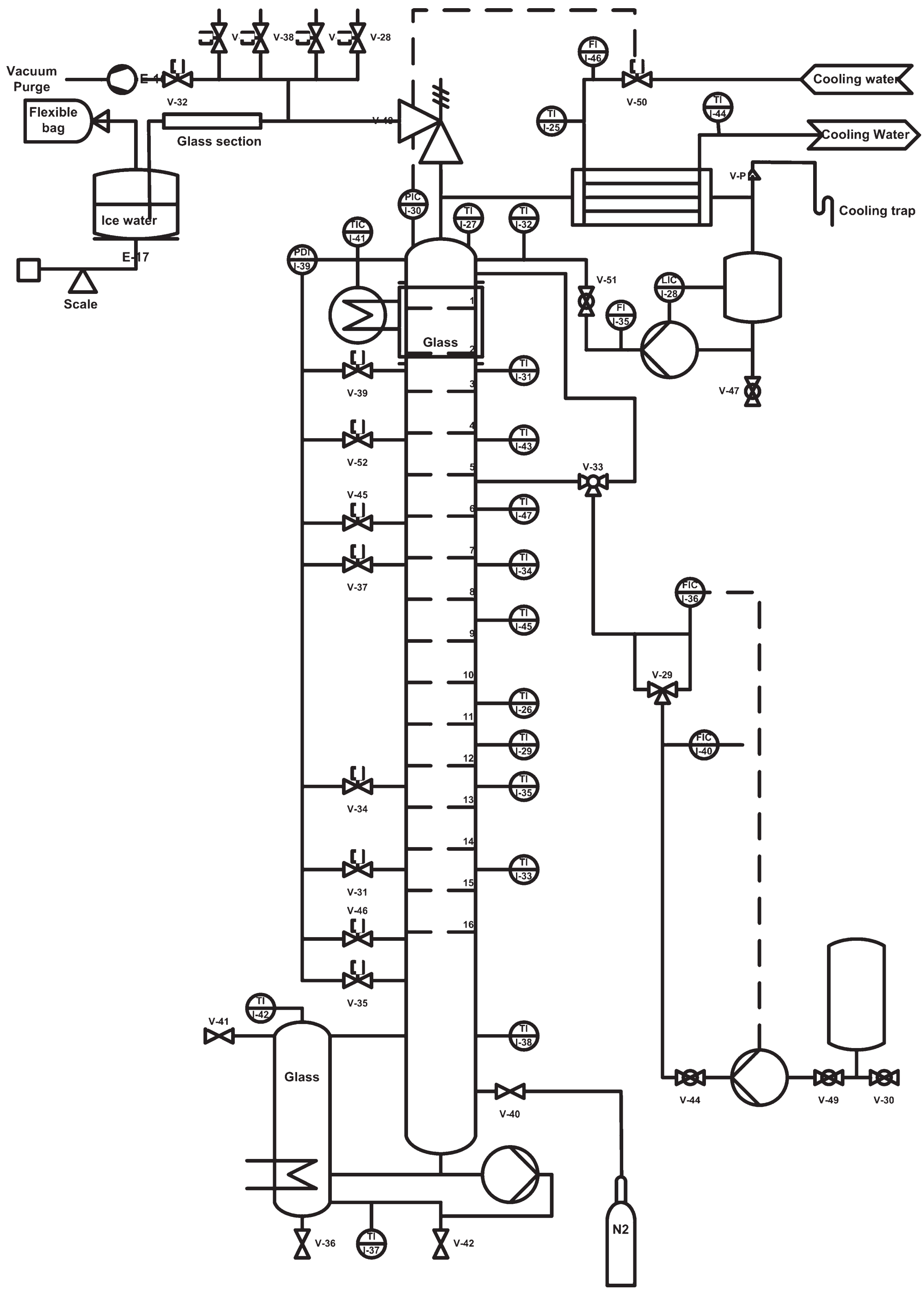

Figure 2. Pilot plant flow sheet.

accelerated. Most simulation tools neglect the influence of weeping. The dynamics of this event is discussed further in detail in the following section.

Influence of the Valve Diameter and the Opening Characteristic. The valve diameter has a significant impact on the column dynamics during a pressure relief event. An

Table 1. Column Parameters

Column height	4 m
Column diameter	100 mm
Internals	16 sieve trays ($\phi = 0.07$)
Reboiler duty and total hold up	30 kW and 28.5 l
Condenser heat exchange area and vapor hold up	4.22 m^2 and 12 l
Max. allowable working pressure	200 kPa
Medium	Methanol/water or water

oversized diameter implicates a number of negative consequences. The discharged relief flow is unnecessarily large. This has also an influence on the necessary design capacity of the blow-down system. The enhanced mass flow is causing high-pressure gradients over the height of the column, which can lead to a destruction of column internals.[8] Additionally, the violent vapor flow is causing a level swell of the liquid on the trays and can even cause a two-phase relief flow, which should be prevented because of the increased mass flow and the limited pressure reduction. Also, it is difficult to handle in the discharge system. On the other hand, an under sizing must be prohibited. An undersized diameter can cause a bursting of the column. If the diameter is too small and the critical pressure ratio is reached, even a further increase of the column pressure causes no larger relief flow, which means that the valve diameter is the only adaptable parameter. Therefore, the challenge is an adequate sizing of the relief diameter.

The opening characteristic of the safety valve is also powerful handle to influence the relief dynamics. Safety valves can be classified according to their opening and closing characteristics into three major types: full lift, proportional, and normal safety valves. The corresponding opening and closing cycles are displayed in Figure 3. The safety valve is normally chosen according to the desired application.

In Table 2, 10 experiments are shown. The Experiments 1–6 were conducted under the same base conditions with a mixture of methanol/water (20/80 vol %) under total reflux. The simulated operating failure in each case was a condenser breakdown given by stopping the cooling water flow. The only varying parameters were the reboiler duty (between 7.5 and 13.5 kW) and the valve characteristics. Two valves with different opening cycles were tested: A normal safety valve with a diameter of 10 mm (Leser series 437) and a full lift valve with a diameter of 9 mm by (Leser series 462). The trend of the column head pressure for both valves for a reboiler duty of 10.5 kW is given in Figure 4.

From Table 2, it can be seen that using a full lift valve under these conditions, an increase of the reboiler duty results in an increase of the relief flow. In this case, the safety valve remains in the proportional range of the opening cycle and therefore opens only as far as necessary to allow the discharge of the necessary vapor flow. This is implicated by the almost constant head pressure after the valve opening in Figure 4. In contrary, the safety valve with a normal opening characteristic is not able to remain in the proportional range due to the fact, that the lift and therefore the free cross-sectional area in the proportional range is much smaller (Figure 3). The valve pops open and the whole cross-sectional area is free for the relief flow at once. This causes the sudden decrease of the column head pressure shown in Figure 4. Because of the instant opening and the relieving under critical conditions, the maximum possible relief flow is always discharged even if not necessary. The mass flow cannot be increased any further (Experiments 1–3 in Table 2). The valve closes again after the closing pressure is reached. The reboiler duty has no influence in that case. It is obvious from these experiments that a significant reduction of the relief flow was achieved by choosing a safety valve with a proportional opening cycle. The shortcut method for the layout of the relief device based on the reboiler vapor rate would not be suitable for this case.

One-Phase Flow vs. Two-Phase Flow. The phase condition (vapor or vapor/liquid) of a relief flow has a large impact on the dynamics of the pressure relief event. Our own investigations[9] have proven that a two-phase relief flow is possible. Table 2 indicates that under critical relieving conditions the maximum one-phase relief flow is ~10 g/s. Experiment 7 shows that under two-phase conditions, the relief flow can be further increased (18 g/s). However, the pressure reduction potential is limited because the volumetric flow is reduced.[10]

Two experiments were carried out and are shown in Figure 5. As safety valve, a manually operated 9-mm ball valve was used. The difference between the Experiments 8 and 9 was the liquid layer on the top tray before relieving. In the first case, the high-liquid layer on the top tray and the entrainment after the opening of the valve were causing a

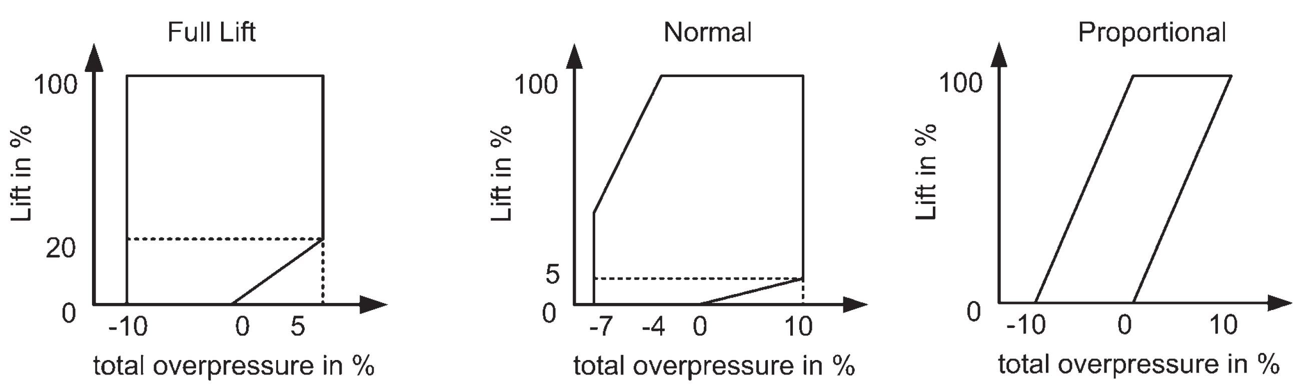

Figure 3. Safety valve opening and closing characteristics.

Table 2. Influence of Opening Characteristic (Methanol/Water, Condenser Failure)

No.	Safety Valve	d_0 (mm)	Reboiler Duty (kW)	Relief Flow (g/s)	Medium	Relieving Condition
1	Normal (Leser 437)	10	7.5	10.0	MeOH/H_20	One phase
2	Normal (Leser 437)	10	10.5	10.2	MeOH/H_20	One phase
3	Normal (Leser 437)	10	13.5	10.1	MeOH/H_20	One phase
4	Full lift (Leser 462)	9	7.5	1.3	MeOH/H_20	One phase
5	Full lift (Leser 462)	9	10.5	2.9	MeOH/H_20	One phase
6	Full lift (Leser 462)	9	13.5	3.4	MeOH/H_20	One phase
7	Normal (Leser 437)	10	24	18.0	H_20	Two phase
8	Ball valve (manual)	9	10	–	H_20	One phase
9	Ball valve (manual)	9	15	–	H_20	Two phase
10	Alternative safety measure: Reboiler shutdown				MeOH/H_20	–

two-phase relief flow. In the second case, the relief flow remains a single-phase vapor flow. The differences are summarized in Table 3. The pressure reduction for the one-phase flow is much more efficient and the pressure reduction per time is 2.5 times higher. Therefore, a one-phase vapor relief flow should be preferred. The prediction of the occurrence of a two-phase relief flow is nowadays still not possible and will be discussed further below.

Column Operating Condition. Shortcut methods and heuristics and also simplified dynamic tank simulations neglect the influence of the column state before the pressure relief event occurs. All methods assume a net power input. However, not only the net power input, i.e., the difference between reboiler and condenser duty, but also the ratio has an important influence on the relief dynamics. If a high condenser rate correlates with an even higher reboiler rate the pressure is increasing and also flooding can occur, which causes a higher liquid level in the column head before the opening of the valve. A two-phase relief flow is likely to occur (Experiments 7 and 8 from Table 2). At a very low-condenser rate, the pressure increases and weeping occurs. The time until reaching the set pressure is reduced and the composition of the relief flow is shifting. Although both events may be caused by the same net power input, the relieving conditions are completely different. A consideration based on a pressure vessel simulation or shortcut methods does not reflect the different scenarios.

Reboiler Shutdown. In recent times, the use of the PCS becomes more and more common to protect a distillation column against overpressure. The standard procedure is to disable a further heat input by shutting the reboiler down. The basic assumption is that no energy is conducted to the column and therefore a further pressure increase is prevented. However that is not always the case. Because of the decreasing upward vapor flow, the liquid light components from the column top start to flow backward through the trays toward the bottom (weeping). Reaching the hot bottom, the light components evaporate. In that case, the pressure increase in the column can be even higher than at the moment of the reboiler shutdown. This is demonstrated in Figure 6 for a mixture of methanol/water.

After shutting the reboiler down, the pressure is first decreasing. This is caused by the heat loss. Afterward, the pressure is increasing again and the methanol (65°C) from the column head is evaporated after contacting the water (100°C) in the column sump. The potential of the further pressure increase is strongly dependent on the difference of the boiling temperatures, the different heats of vaporization and the liquid heat capacities of the light and heavy components and should be checked thoroughly. A worst-case calculation should be carried out before applying this method. Most dynamic simulation models neglect the influence of weeping and cannot describe the dynamics of this event. The developed simulation model presented in this research work considers these effects.

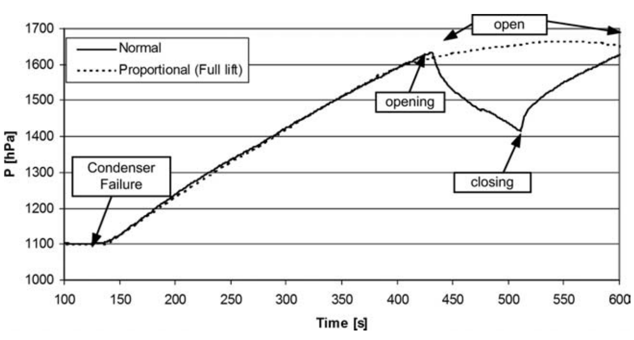

Figure 4. Experiments 2 and 5 from Table 2: influence of the opening characteristic (methanol/water; 10.5 kW reboiler duty).

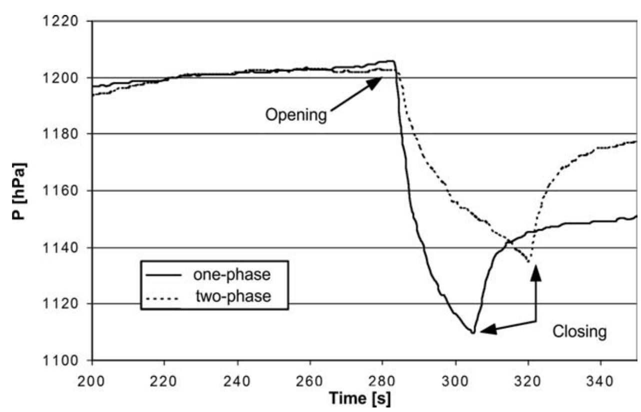

Figure 5. Experiments 8 and 9 from Table 2: comparison of one- phase and two-phase flow.

Table 3. Comparison One-Phase/Two-Phase Flow

No.	Phase	ΔP (mbar)	t (s)	$\Delta P/t$ (mbar/s)	Liquid Layer Tray (1)
8	One-phase flow	96	21	4.5	normal
9	Two-phase flow	66	36	1.8	high (flooding)

Dynamic Simulation Model

The developed dynamic simulation model was implemented in gProms®. It allows the description of the column dynamics at abnormal operating conditions for example after a reboiler or a condenser failure. The model also describes phenomena like weeping and entrainment. The following section illustrates the modeling of the different column elements. Equations for the calculation of the activity coefficients, the enthalpies, vapor pressures (Antoine equation), and physical properties (density, viscosity, surface tension, etc.) are not given.

Composite model

The different units described in the following sections are connected within a composite model by incoming or outgoing predefined streams. The streams contain the mass flow, composition, temperature, pressure, and enthalpy transferred between the elements. Regarding the desired model application for safety analysis in any distillation column the design of the composite model is kept flexible. Not only the column parameters like diameter, weir height, number of stages, etc., but also the number and connection points of the feed flows and the number and connection points of relief devices can be changed. The degree of freedom is $j(nc + 3) + 4$, where nc is number of components. The feed specification (number of feeds and feeding conditions) has to be chosen. A common configuration is to choose additionally the reflux ratio RR, the cooling water flow L_{CW}, the condensate temperature T_C, and the reboiler duty Q_S. Different specifications are possible. A feasible column design is shown in Figure 7. In this case, one feed stream and one relief device on top of the column is applied.

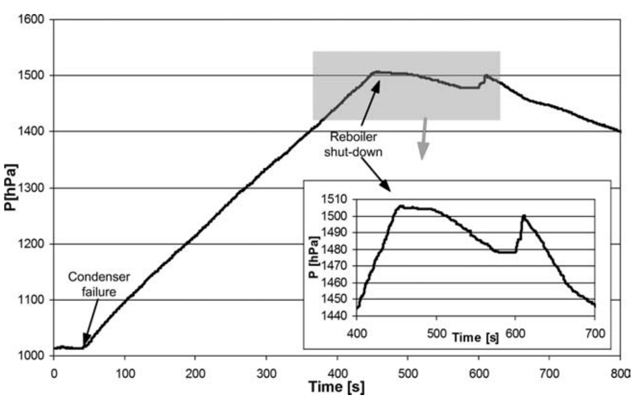

Figure 6. Reboiler shutdown.

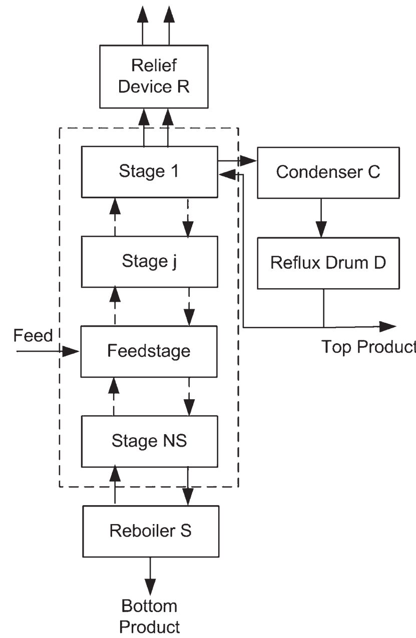

Figure 7. Composite model.

Column stage

Modeling the column stages, a reasonable trade-off between accuracy on the one-hand and computing time and convergence behavior on the other hand had to be achieved. The following assumptions were made:

- Equilibrium stage model with Murphee efficiency.
- The liquid can flow over the weir and also through the opening holes of the tray (weeping).
- Liquid entrainment caused by the vapor flow is possible.
- The liquid and vapor hold-up are considered.

The published flow models for safety relief valves implement uncertainties up to 10% and for two-phase flow even 25%. Therefore, the error regarding thermodynamic equilibrium is not dominant within the range of the planned application. The model validation in the following section shows the appropriateness of this assumption within the scope of the desired purpose. The schematic of a column stage is shown in Figure 8.

Balance Equations. Each column stage is modeled completely dynamic including mass-, energy and component balances and the summation relation. The vapor and liquid hold-up are considered. The energy hold-up of the column shell and the column internals are also included in the energy balance. The Eqs. 1–7 hold for $i = 1$ to nc − 1.

Mass Balance:

$$\frac{d\left(\mathrm{HU}_j^L + \mathrm{HU}_j^V\right)}{dt} = L_{j-1} - L_j + V_{j+1} - V_j + F_j - R_j^{\mathrm{L}} - R_j^{\mathrm{V}} \tag{1}$$

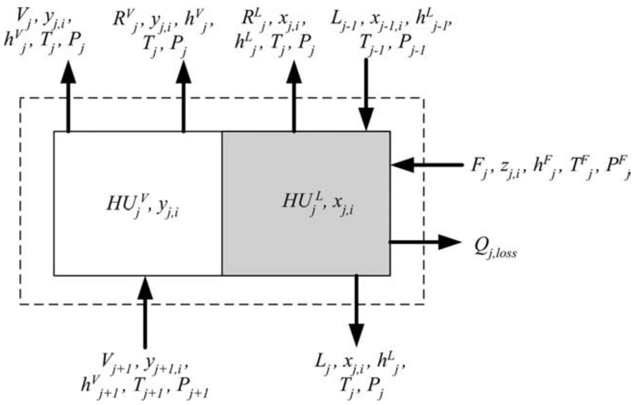

Figure 8. Column stage model.

Energy Balance:

$$\frac{d\left(\mathrm{HU}_j^L u_j^{\mathrm{L}} + \mathrm{HU}_j^V u_j^{\mathrm{V}} + M_{\mathrm{St}} C_{p,\mathrm{St}}(T_j - T_A)\right)}{dt} = L_{j-1}h_{j-1}^{\mathrm{L}} - L_j h_j^{\mathrm{L}} + V_{j+1}h_{j+1}^{\mathrm{V}} - V_j h_j^{\mathrm{V}} + F_j h_j^{\mathrm{F}} - R_j^{\mathrm{L}} h_j^{\mathrm{L}} - R_j^{\mathrm{V}} h_j^{\mathrm{V}} - Q_{j,\mathrm{loss}} \quad (2)$$

Component Balance:

$$\frac{d\left(\mathrm{HU}_j^{\mathrm{L}} x_{j,i}^L + \mathrm{HU}_j^{\mathrm{V}} y_{j,i}^{\mathrm{V}}\right)}{dt} = L_{j-1}x_{j-1,i} - L_j x_{j,i} + V_{j+1}y_{j+1,i} - V_j y_{j,i} + F_j z_{j,i} - R_j^L x_{j,i} - R_j^V y_{j,i} \quad \text{for } i = 1 \text{ to nc} - 1 \quad (3)$$

Summation Equation:

$$\sum_{1=1}^{\mathrm{nc}} x_{j,i} = 1 \quad (4)$$

$$\sum_{1=1}^{\mathrm{nc}} y_{j,i} = 1 \quad (5)$$

Phase Equilibrium. The nonideal behavior of the liquid phase is considered by including the activity coefficient ($\gamma_{j,\ i}$). The nonideality of the vapor phase is represented by the fugacity coefficient ($\varphi_{j,\ i}$). The pointing correction ($\pi_{j,\ i}$) can be neglected at operating pressures below 10 bars.

$$\gamma_{j,i} x_{j,i} p_{j,i}^{\mathrm{LV}} \pi_{j,i} = \varphi_{j,i} y'_{j,i} p_j \quad (6)$$

The deviation from the real $y_{j,i}$ composition compared with the equilibrium composition $y'_{j,i}$ is described by using the Murphee efficiency ($\eta_{j,\ i}$).

$$y_{j,i} = \eta_{j,i,\mathrm{Murphee}}\left(y'_{j,i} - y_{j+1,i}\right) + y_{j+1,i} \quad (7)$$

Incoming Vapor Flow. The actual vapor flow is given then by the vapor velocity (8), which results from the pressure, governing under the considered tray j. It can be calculated from pressure drop, caused by the vapor flow and hydrostatic pressure of the liquid layer (9).

$$V_j = w_{j+1}^{\mathrm{V}} A_j \frac{1}{v_{j+1}^{\mathrm{V}}} \quad (8)$$

$$\Delta p_j = \Delta p_{j,\mathrm{dry}} + \Delta p_{j,\mathrm{hydro}} = \zeta_j \frac{\rho_{j+1}^{\mathrm{V}}}{2}\left(w_{j+1}^{\mathrm{V}}\right)^2 + H_j^L \rho_j^L g \quad (9)$$

Outgoing Liquid Flow. Liquid can leave the stage over the weir or through the opening holes of the tray. The flow over the weir $L_{j,\mathrm{weir}}$ is calculated by the Francis weir formula.

$$L_{j,\mathrm{weir}} = l_{j,\mathrm{weir}} C_{j,fw} (H_j^{\mathrm{L}} - H_{j,\mathrm{weir}})^{1,5} \frac{1}{v_j^{\mathrm{L}}} \quad (10)$$

The liquid flowing through the opening holes of the tray is described by adapting the Torricelli equation. Ω_j is described according to Wijn[11] as a weeping factor which is between 0 and 1.

$$L_{j,\mathrm{weep}} = \Omega_j A_{\mathrm{hole}} \sqrt{2gH_j^{\mathrm{L}}} \quad (11)$$

For the description of the weeping factor, a correlation was developed and validated experimentally in a test apparatus describing the weeping factor as a function of the tray free area and the F-factor. Using this correlation, a description of column states were weeping occurs becomes possible. The parameters k_1^{ent}, k_2^{ent}, and k_3^{ent} were investigated by regression analysis and are given in the Notation section (Parameter).

$$\Omega_j = \mathrm{Min}\left[1; k_3^{\mathrm{weep}} \exp\left(-k_2^{\mathrm{weep}} \frac{F_j}{\varphi_{\mathrm{free},j}} + k_1^{\mathrm{weep}}\right)\right] \quad (12)$$

The complete outgoing liquid flow is calculated by adding the weir overflow and the weep flow.

$$L_j = L_{j,\mathrm{weir}} + L_{j,\mathrm{weep}} \quad (13)$$

Additional Equations. The hold-up of the vapor phase (HU^{V}) is calculated via the stage hold-up (Vol) and the liquid hold-up (HU^{L})

$$\mathrm{Vol}_j = \mathrm{HU}_j^V \frac{\tilde{M}_j^V}{\rho_j^V} + \mathrm{HU}_j^L \frac{\tilde{M}_j^L}{\rho_j^L} \quad (14)$$

The heat loss in the energy balance is calculated by a simple heat transfer equation between the stage temperature and the ambient temperature.

$$Q_{j,\mathrm{loss}} = k_j A_{j,\mathrm{shell}}\left(T_j - T_A\right) \quad (15)$$

Partial reboiler

The partial reboiler obeys also equations, derived above. The following changes are made due to the different conditions in the reboiler:

- External heat input Q_S, additional term in energy balance.
- No vapor inlet flow.
- Liquid outlet only over the weir, no weeping.

Condenser and reflux drum

A total condensation and no vapor hold-up are assumed in the condenser. The hold-up is assigned to the reflux drum. Therefore, the balance equations simplify to:

$$V_1 = L_C \tag{16}$$

$$y_{1,i} = x_{C,i} \tag{17}$$

$$0 = V_1 h_1^V - L_C h_C^L - Q_{CW} \tag{18}$$

The description of the phase equilibrium is only needed for the calculation of the condensation temperature T_C^{LV}, which is included in the vapor pressure calculation.

$$\gamma_{c,i} x_{c,i} p_{C,i}^{LV} = \varphi_{c,i} y_{C,i} p_c \tag{19}$$

$$\sum_{1=1}^{nc} y_{C,i} = 1 \tag{20}$$

The temperature of the condensate leaving the condenser is defined by presetting a degree of subcooling.

$$T_C = T_C^{LV} - \Delta T_{sub} \tag{21}$$

The pressure drop is again calculated by using a simple pressure drop correlation. This equation also specifies the pressure on the first stage.

$$p_1 - p_C = \zeta_C \frac{\rho_1^V}{2} \left(w_C^V\right)^2 \tag{22}$$

The heat transferred from the hot side of the condenser to the cold side and thus the condensation rate is calculated by a heat transfer Eq. 23 and a heat balance (24).

$$Q_{CW} = k_C A_{ex} \frac{(T_C^{LV} - T_{CW,in}) + (T_C - T_{CW,out})}{2} \tag{23}$$

$$0 = L_{CW} h_{CW,in} - L_{CW} h_{CW,out} + Q_{CW} \tag{24}$$

The liquid leaving the condenser (L_C) flows into the reflux drum. It is assumed that the reflux drum possesses only a liquid hold-up and is completely adiabatic. Therefore, the energy balance can be neglected. The mass and component balances are shown below:

$$\frac{(HU_D)}{dt} = L_C - L_D - L_{RR} \tag{25}$$

$$\frac{\left(HU_D x_{D,i}\right)}{dt} = L_C x_{C,i} - L_D x_D - L_R x_D \quad \text{for } i = 1 \text{ to } nc - 1 \tag{26}$$

$$\sum_{i=1}^{nc} x_{D,i} = 1 \tag{27}$$

$$T_C = T_D = T_{RR} \tag{28}$$

$$p_C = p_D = p_{RR} \tag{29}$$

The hold-up is controlled by a weir equation

$$L_D + L_{RR} = l_{D,weir} C_{fw} \left(H_D^L - H_{D,weir}\right)^{1.5} \frac{1}{v_D^L} \tag{30}$$

The ratio of reflux flow and distillate flow is given by the reflux ratio RR.

$$RR = \frac{L_{RR}}{L_D} \tag{31}$$

Relief device

In the previous section, the influence of the relief device on the column pressure was demonstrated. Therefore, a precise modeling is necessary. In contrary to the models of the other column units, it is not only necessary to describe the thermodynamics and the flow model but also the dynamic behavior of the valve itself. The state of the valve is changing over the time and therefore cannot be neglected. Thus, the model is divided into two submodels: the flow model and the opening characteristic model.

Flow Model. The flow model describes the thermodynamic change of state when the fluid is flowing through the safety valve. The schematic is shown in Figure 9. To be able to describe a two-phase relief flow also a two-phase flow model was implemented. It is generally assumed, that the safety valve does not possess a hold-up therefore the mass balance becomes:

$$0 = R_{in}^V + R_{in}^L - R_{out}^V - R_{out}^L \tag{32}$$

The description of a one-phase vapor relief flow is generally approved. An isentropic expansion of the fluid in the safety valve is assumed.

$$R_{in}^V = \frac{\dot{M}}{\tilde{M}_R^V} = \alpha_V A_R \Psi_{OP} \frac{1}{\tilde{M}_R^V} \sqrt{\frac{2 p_{R,in}}{v_{R,in}^V}} \tag{33}$$

Ψ_{OP} is a function of the pressure ratio and the isentropic exponent and is calculated according to Diener and Schmidt.[6] However, the description of a two-phase relief flow is much more uncertain. Because the pressure decreases while the fluid flows through the valve nozzle, the liquid evaporates (flashes). Under certain conditions, even a condensation of the vapor can occur. The flow models describing this phenomenon vary in the assumption how fast a thermodynamic equilibrium state is reached. The "frozen flow" assumes a maximum nonequilibrium. No mass and heat transfer between the phases takes place. An upper mass flow limit can be estimated using this flow model. The lower mass flow limit can be estimated by assuming a homogenous equilibrium (HEM) between the phases at all times. Recently most authors recommend the use of the omega-method

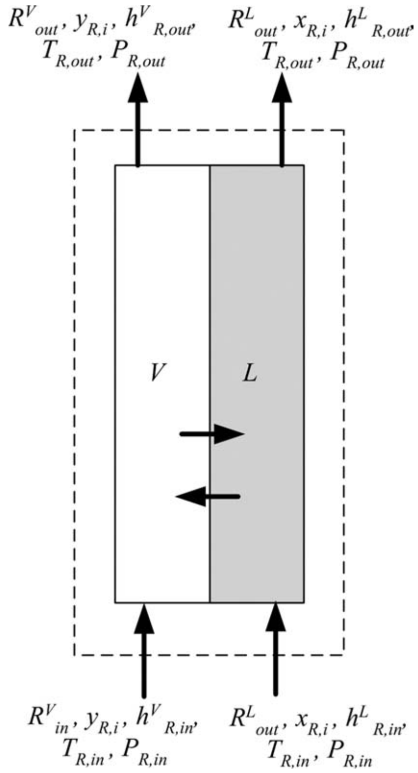

Figure 9. Relief device model.

originally published by Leung[10] and adapted by Schmidt and Westphal[5] and Diener and Schmidt.[6] The set of equations used in the flow model were implemented according to Diener and Schmidt.[6]

To be able to calculate a two-phase mass flow, the stagnation quality at the inlet of the relief device thus the volumetric vapor fraction ε and the vapor mass fraction $\dot{x}$ must be known. This is determined by an entrainment correlation based on experimental analysis in a test stand. The given correlation is valid for the spray regime.

$$E_{\text{spray}} = \frac{\dot{V}^L_{\text{in}}}{\dot{V}^V_{\text{in}}} = k_1^{\text{ent}}(F/F_{\text{max}})^2 + k_2^{\text{ent}}(F/F_{\text{max}}) + k_3^{\text{ent}} \quad (34)$$

$$\varepsilon = \frac{1}{E_{\text{spray}} + 1} \quad (35)$$

$$\dot{x} = \frac{\varepsilon v^L_{R,\text{in}}}{(1-\varepsilon)v^V_{R,\text{in}} + \varepsilon v^L_{R,\text{in}}} \quad (36)$$

Opening Characteristic. The opening and closing characteristic displays the influence of the operational behavior of the relief device, for example, the properties of the spring and the shape of the disc of a spring loaded safety valve. The free area A_R of the valve is defined as a function of the pressure drop over the relief device.

$$\frac{A_R}{A_{\text{tot}}} = f\left(p_{\text{R,out}}, p_{\text{R,in}}\right) \quad (37)$$

Four distinguished pressures are defined (Figure 10: set pressure, full lift pressure, closing pressure, and reseating pressure). By setting theses pressures, the opening and closing characteristic of the relief device is determined. The valve is moving along this cycle. The dynamic behavior of different types of safety valves (normal, proportional, and full lift) and also bursting disks can be covered with the shown implementation. The coupling of the two submodels is done via the valve free area A_R.

Equation switching

Because of the desired application of the simulation model, which is the description of the dynamic behavior of a distillation column after an operating failure, different sets of equations have to be used. Each switching means an equation discontinuity and requires a new initialization of the equation system. Therefore, the switching conditions and the different sets of equation have to be chosen thoroughly to maintain a good convergence. The most important switches are shown below.

Weir Overflow (Column Stage). Liquid flows only over the weir if the liquid level is above the weir height and if the stage pressure drop is lower than the hydrostatic pressure in the downcomer (no flooding).

$$\text{If } H_j^L > H_{j,\text{weir}} \wedge \Delta p_{j,\text{shaft}} > \Delta p_j \Rightarrow \text{Eq. (11) else } L_{j,\text{weir}} = 0 \quad (38)$$

Weeping (Column Stage). Weeping only occurs if liquid is on the tray and the F-factor is lower than the minimum F-factor at the beginning of the weeping range.

$$\text{If } F_{j,\text{hole}} > F_{\text{min,hole}} \wedge H_j^L > 0 \Rightarrow \text{Eq. (12) else } L_{j,\text{weepr}} = 0 \quad (39)$$

Incoming Vapor (Column Stage). Vapor only flows from tray (j + 1) to tray (j) if the pressure on the lower tray is higher, thus a positive pressure drop is existing.

$$\text{If } p_{j+1} > p_j \Rightarrow \text{Eq. (10) else } V_j = 0 \quad (40)$$

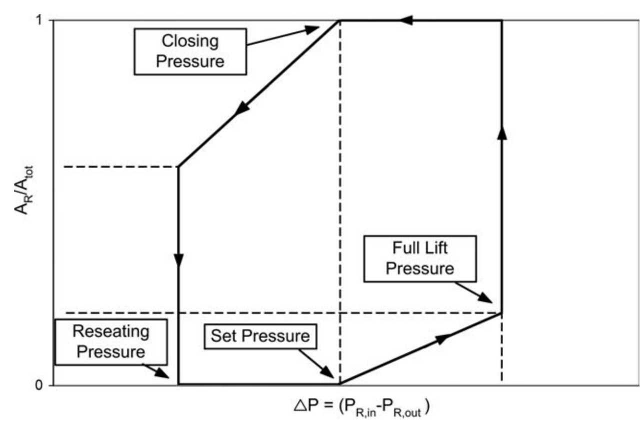

Figure 10. Opening and closing cycle.

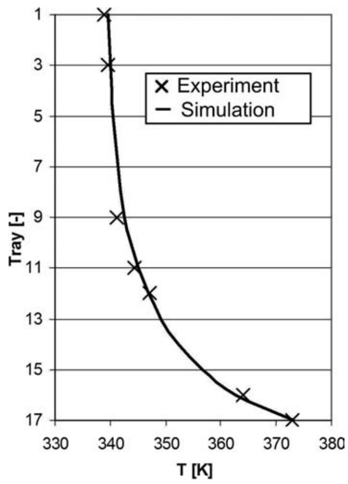

Figure 11. Steady-state temperature profile.

Two-Phase Relief Flow (Relief Device). A two-phase relief flow occurs if the entrainment calculated by Eq. 34 is above a minimum entrainment. The necessary minimum entrainment is set at the stage were the calculated two-phase mass flow is 10% higher than the calculated corresponding one-phase flow.

$$\text{If } E_{j,\text{spray}} > E_{\min} \;\Rightarrow\; R_L > 0 \text{ else } R_L = 0 \tag{41}$$

The two-phase mass flow is calculated using the stagnation quality $\dot{x}$ according to Diener and Schmidt.[6]

Opening and Closing Cycle (Relief Device). The description of an opening and closing cycle and thus the calculation of the valve free area, like shown in Figure 10 is done by a assuming a linear course between the fixed corner points.

Case Study

To prove the suitability of the developed model presented in the previous section experimental case studies were carried out. For a sustainable validation of the model assumptions, a complete failure scenario is presented below. A mixture of methanol/water (20/80 vol %) was chosen due to the large difference of the boiling points (65°C/100°C) and therefore the critical behavior after a reboiler shutdown (see above). The tray efficiency was determined under steady state conditions and assumed constant. The heat transfer coefficients for the heat losses were determined by operating the column under total reflux, with no feed and comparing the difference of the reboiler and the condenser duty in previous experiments. The heat transfer coefficient for the condenser was calculated by measuring the inlet and the outlet temperature and the mass flow of the cooling water flow. A steady-state reboiler duty of 10.5 kW was applied and the column was operated in batch mode (no feed flow, no product drawing, and mixture in sump before start-up). The steady-state temperature profile is shown in Figure 11.

The trend of the column head pressure for the complete event beginning from the steady-state operating pressure is shown in Figure 12. A condenser breakdown is simulated by a sudden reduction of the stationary cooling water flow (t = 150 s). As a consequence, the column head pressure is increasing. As soon as the column head pressure is as high as the set pressure of the safety valve the valve begins to open (420 s). Because of the opening characteristics of the safety valve, the valve is torn completely open and a large relief flow is discharged. The column head pressure decreases, as soon as it falls below the reseating pressure of the safety valve, the valve closes (500 s). The consequence is a newly pressure increase and another opening and closing cycle of the safety valve. After 700 s, the intervention of an operator or the PCS is simulated by shutting the reboiler down. No heat is anymore transferred to the system. However, the pressure is further increasing. This event is caused by the weeping from the column stages and the flowing of liquid light components from the column head into the hot bottom and the evaporation (see above). Each aspect in the course of the shown event is discussed in detail below.

Pressure increase

Starting from steady-state operation the cooling water flow is reduced from L_{CW} =135 l/h to 3 l/h and therefore the condenser duty from Q_{CW} = 6.9 kW to 0.14 kW while the reboiler duty is kept constant at Q_{S} = 10.5 kW. This results in a fast pressure increase. Caused by the very low-condensation rate almost no vapor flow exists anymore. The liquid from the trays is flowing downward (weeping). When reaching the higher temperature stages of the column, the liquid is partially vaporized. This results in an enhanced pressure increase. In the simulation weeping is considered using the developed correlation given in Eqs. 11 and 12. In Table 4, the experimentally measured time to PRV response, as well as the simulation results with and without weeping are shown. It becomes obvious that a simulation which neglects weeping overestimates the response time until the maximum allowable working pressure of the column is reached and therefore is not reliable. To estimate a realistic time interval weeping must be considered.

Relief dynamics

The safety valve used for this experiment is a Leser 437 safety valve. Further details are listed in Table 5. The valve is according to Figure 3 a "normal safety valve." For set pressures p_{set} below 1000 hPa (gauge) the full lift pressure

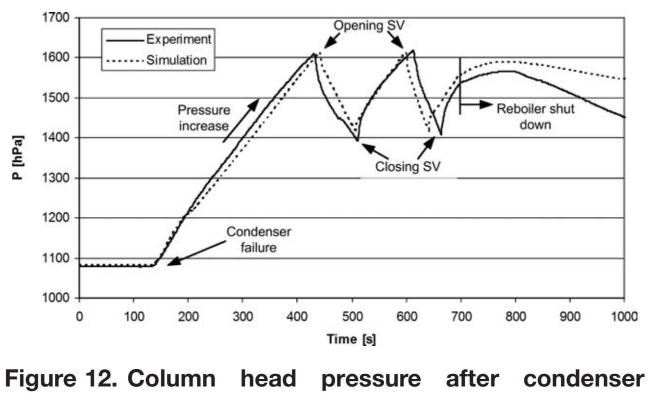

Figure 12. Column head pressure after condenser failure.

Table 4. Response Time

	Time to p_{max}	Δt	Deviation
Experiment (Figure 12)	295 s	–	–
Simulation with weeping (Figure 12)	300 s	5 s	1.7%
Simulation without weeping (not shown)	341 s	49 s	16.7%

Table 5. Characteristic Leser 437 and Leser 462

α_V; α_L	0.41; 0.35	0.71; 0.61
p_{set} (gauge)	500 hPa	500 hPa
Opening Char.	Normal	Full lift
d_0	10 mm	9 mm

p_{fl} is 100 hPa above the set pressure. The flow model by Diener and Schmidt[6] was applied. The entrainment and thus a possible two-phase flow relief are considered.

Pressure Trend. As soon as the column head pressure reaches the set pressure, the safety valve opens. The state of the safety valve follows the opening and closing cycle. First, a little opening is registered and a small relief flow is discharged. However, the relief flow in the proportional range of the valve is not large enough to keep the pressure constant. The pressure is increasing further and after the full lift pressure is exceeded the valve opens completely. This results in a fast pressure reduction and the closing of the valve after reaching the reseating pressure. After the closing the pressure is increasing again and a second relief event is conducted. The shape of the simulated pressure agrees very well with the experimental data. The reseating pressure of the experiment is a little bit lower than the simulated reseating pressure for both opening and closing cycles. Therefore, the safety valve from the experiment remains open for a short-time period after the simulated safety valve is already closed. The details of both relief events, for simulation and experiment, are given in Table 6.

Relief Flow. The relief flow was analyzed using the discharge system presented above. According to the simulation, the entrainment is very low under these relieving conditions ($E_{spray} = 3 \times 10^{-7}$). A one-phase relief flow is therefore expected. This was confirmed by visual analyzing the flow pattern in the glass section of the blow-down line. Further evidence that the simulation predicts the phase condition of the relief flow correctly gives the excellent correspondence between the experimental and the simulated mass flows. If a relevant two phase flow would have occurred in the experiment, the mass flow would be increased. The time-dependent discharged total mass is shown in Figure 13. The two relief events are clearly recognizable. The inclination of the curves reflects the average mass flow. Two major differences between experiment and simulation can be detected. The increase of the experimental graph has a steeper slope in the beginning. This is caused by the vapor hold-up collected in the blow-down line, which was pushed to the collector tank not till then when the valve popped open. The hold-up of the blow-down line was neglected in the simulation. The second difference is that the valve in the experiment closes at a lower pressure and therefore remains open longer than the simulated valve in both cases. This results in a larger total relief amount.

The analysis of the composition of the relief flow shows that during the complete relief event almost pure methanol was discharged ($0.985 < x < 0.99$). This behavior was well reproduced by the simulations. The water vapor from the lower stages obviously does not reach the top of the column during the relief event. This is in accordance with the experimental results.

Reboiler shutdown

After ~700 s, the intervention of an operator or the PCS is simulated by shutting the reboiler down. This is a standard procedure often used to assure the safe state of a distillation column. The prevention of energy input should also prevent a further pressure increase (see above); however, this is not the case. Because of the instant weeping from the methanol toward the hot bottom and the vaporization, the pressure increases further. Because the simulation model includes a weeping term a description of this phenomenon is possible. The experimental and simulated pressure trends after the reboiler shutdown are shown in Figure 12. Because of the earlier closing in the simulation, the simulated pressure increases further within the larger time span and therefore is higher at the moment when the reboiler is shutdown. Afterward, both curves show the same shape and the same progress. The additional pressure increase for both cases is about 35 mbar. After a condenser failure, weeping, two pressure relief events and a reboiler shutdown a good correspondence between experiment and simulation is still given. After the pressure maximum is reached, the pressure decreases again due to heat losses. The experimental pressure descends faster. A possible explanation is that there is a small difference in the heat losses between the experiment and the simulation. While the reboiler was running this was concealed by

Table 6. Pressure Relief Details From Figure 12

	1st Relief		2nd Relief	
	Experiment	Simulation	Experiment	Simulation
Full lift at	436 s	441 s	613 s	600 s
Closing at	511 s	508 s	664 s	642 s
Opening time	75 s	67 s	51 s	42 s
Total mass	953 g	690 g	486 g	417 g
Mass flow	9.84 g/s	9.76 g/s	9.16 g/s	8.28 g/s
Full lift pressure	1608 mbar	1608 mbar	1616 mbar	1608 mbar
Reseating pressure	1392 mbar	1413 mbar	1408 mbar	1414 mbar

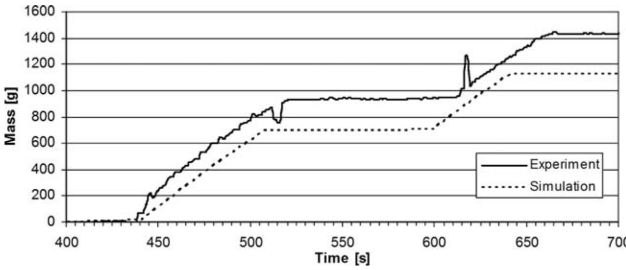

Figure 13. Discharged mass.

the large absolute value of the heat input. After the shutting down of the reboiler, these small differences become much more dominant.

Temperature profile

The most critical model simplification is the assumption of a thermodynamic equilibrium at any time and on every stage during the process. As a consequence of the reflux of light components, much more liquid flows from stage to stage than during normal operation and the composition varies. The model assumes an instant equilibrium. In reality, the achieving of the equilibrium state on a tray is not instantaneous. The more weeping, the more changes the composition and the more time it takes to reach the equilibrium. A comparison of the temperature profiles therefore allows important conclusions. If the temperature profiles show a good correspondence it proves that the weeping is described correctly because the shifting of the concentration caused by the weeping is reflected by the shifting of the equilibrium temperature. Additionally, it proves that the assumption of a thermodynamic equilibrium is reasonable.

The temperature trend for significant trays of the column is shown in Figure 14. The temperatures in the column head and sump as well as the temperatures on Trays 9 and 13 are shown. Until the condenser failure occurs, the steady-state temperature profile can be observed. Caused by the condenser failure, the head temperature (still pure methanol) and the sump temperature (still water) are increasing due to the higher boiling temperature at higher pressures. The trend on Trays 9 and 13 is very characteristic. The temperature on Tray 9 does not increase as fast as the top temperature. This leads to the conclusion that the concentration is shifting toward methanol. This can only be caused by weeping from the higher trays with a higher methanol concentration. The phenomenon is even more distinct on Tray 13. Here, the temperature even decreases (experiment: $\Delta T \approx 9$ K; simulation: $\Delta T \approx 6$ K) due to the weeping liquid flow from the top of the column consisting mostly of methanol. The simulation reflects these incidents very well. Afterward, all temperatures are increasing due to the increasing pressure and the higher equilibrium temperature. After the opening of the safety valve, the temperature profile is changing swiftly. While the bottom and the column head are cooling down, due to the decrease of the equilibrium temperature on Trays 9 and 13, the change of the concentration dominates again. Because of the opening of the safety valve more vapor evaporates in the column, especially in the bottom. This alters the composition on these two trays again to a higher water concentration, which results in a rapid temperature increase. A small deviation during the relief can be observed in the column head. The simulated temperature increases faster. Obviously, the hold-up of methanol was slightly underestimated by the simulation and therefore the water fraction on Tray 1 increases faster in the simulation. The statements made are also valid for the second relief event. After shutting down the reboiler the temperatures in the sump and in the head show a good match, except that the simulated temperatures are slightly higher. However, the simulated pressure at the moment of the reboiler shutdown and therefore the equilibrium temperature is also higher. The comparison of the temperatures on Trays 9 and 13 shows a larger deviation. The experimental temperature decreases faster than the simulated temperature. This also supports the assumption previously made that the real heat losses are higher than estimated by the simulation. This deviation dominates after stopping the heat input from the reboiler. A second reason is that the remaining liquid methanol on the upper trays, which is weeping down after

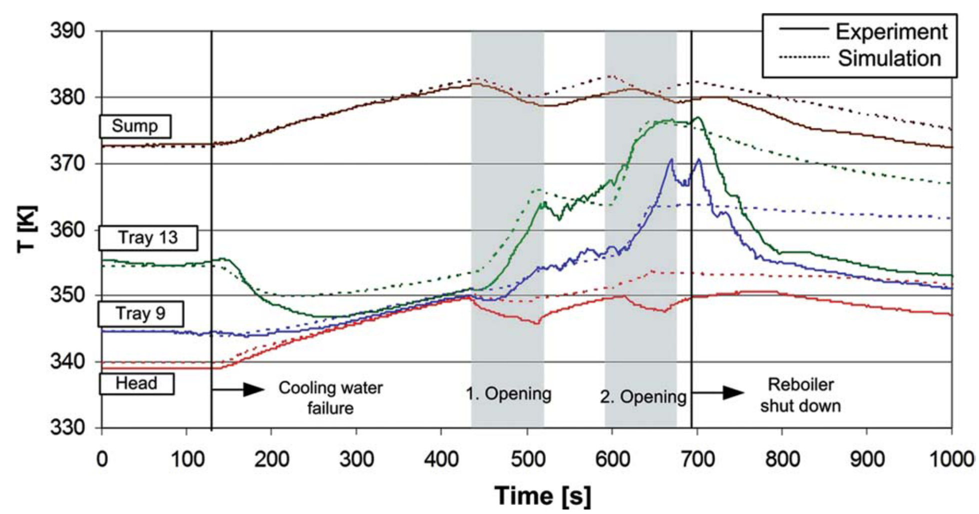

Figure 14. Temperature trend.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

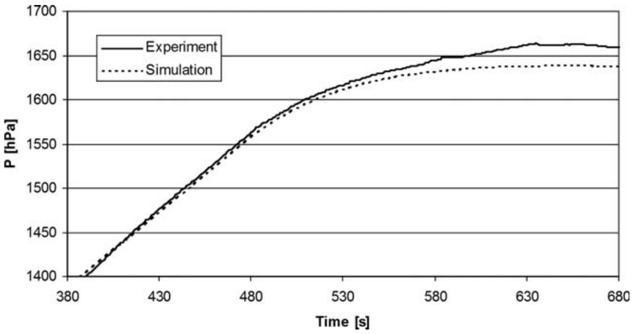

Figure 15. Pressure relief Leser 462, proportional range.

the shutdown of the reboiler and is causing the temperature decrease, is underestimated by the simulation. This is supported by the trend of the column head temperature. The simulated trend is on a higher temperature, which means the concentration is shifting toward water more quickly.

The comparison of the trends of the simulated and experimentally measured temperature profiles shows a good correspondence, especially regarding the immense changes of the column state during the failure scenario. The dynamic behavior is therefore well described by the model.

Proportional valve

For a further validation, especially the implemented opening and closing systematic, a safety valve with a different opening characteristic was used.

The same experiment (methanol/water) was conducted with the full lift valve Leser 462. This valve has a larger lift and thus a larger free area in the proportional opening range and therefore behaves under the given operating conditions like a proportional valve. The opening characteristic of this valve is shown in Figure 3. However, due to the larger proportional range of the full lift valve, it behaves under the given conditions like a proportional valve. Again for set pressures p_{set} below 1000 hPa (gauge), the full lift pressure p_{fl} is always 100 hPa above the set pressure. Details of the valve are given in Table 5. The experimental and the simulated trend of the column head pressure for this case is shown in Figure 15. The pressure increase before the opening of the safety valve is identical with the previous case study due to the same experimental conditions and is not displayed here. A comparison of both experiments is already shown in Figure 4. As soon as the set pressure p_{set} is reached, the valve begins to open. However due to the smooth transition a defining of the exact moment is not possible. However, it can be recognized that the gradient of the pressure is decreasing and the graph finally ends in a horizontal line. The pressure is kept constant. Because of a balance of forces between the force applied by the vessel pressure and the force applied by the valve spring, the valve opens only as far as necessary to discharge the vapor flow, to prevent a further increase of the internal pressure. The valve is only operating in the proportional range. If the internal pressure increases above the full lift pressure, the equilibrium condition is not any more satisfied and the valve opens completely, which is not the case under the given operating conditions. The necessary mass flow to achieve a constant pressure is according to the simulation 2.3 g/s and according to the experiment 2.7 g/s. The relief flow remains also a one-phase flow over the whole time period. The maximum relief flow using a safety valve with a proportional opening characteristic and only discharging the necessary relief flow is $\sim$70% lower than using a slightly oversized valve with a normal opening characteristic, which opens under these conditions and discharges an unnecessary large relief flow. Regarding the comparable two phase relief event above (see Table 2), the relief flow is even 85% lower and the column head pressure is still kept below the desired limit.

Conclusion

A new method for the investigation of the behavior of distillation columns after an operating failure including the option of a possible pressure relief event has been proposed. In contrary to the methods actually used, mostly based on shortcut calculations or heuristic, the presented method based on dynamic simulation allows a detailed investigation of the important process parameters like pressures and temperatures and their dynamic behavior. For an adequate simulation of a real plant, the implemented model was extended for the description of weeping and entrainment, which are relevant phenomena in the field of the desired application. The modeling approach describing the relief device allows the implementation of different opening and closing characteristics, diameters and flow models. The flow models implemented describe a one- or two-phase relief flow.

The model validation shows a good agreement between experimental and simulated data. The simulated relief device corresponds well with the experimental results concerning mass flow, opening and closing characteristic and phase composition. The assumption of a thermodynamic equilibrium between liquid and vapor phase on the column stages is critical due to the fast change of material composition caused by weeping. However, the present investigation shows that this assumption is adequate regarding the desired application of the simulation model.

Based on the experimental study and the simulation results, general valid conclusions can be drawn. A two-phase flow is disadvantageous. The mass flow increases even though the pressure reduction diminishes compared with a one-phase flow. The developed simulation model allows an early detection of a possible two-phase flow. Adequate measures can be taken. The use of a proportional valve is beneficial. The valve diameter should be designed according to the credible worst-case, which is a condenser failure at full reboiler duty. During all other operation failures, only the actual necessary relief flow is discharged. It was shown that by an efficient design based on simulation predictions, a reduction of the relief flow of 85% was possible.

The time to reach the maximum allowable working pressure and thus the set pressure of the relief valve is shorter than estimated via column simulation, without considering weeping. Weeping enhances the pressure increase and therefore should be considered to estimate a reliable response time. The reboiler shutdown and thus the avoidance of further heat input is a frequently used safety measure. However, it does not always prevent a further pressure increase. The weeping of the liquid light components toward the sump and their vaporization is causing a further pressure increase. The dynamic is dependent on the differences of the boiling temperatures, the heats of vaporization and the heat capacities. This should be checked thoroughly and the increase potential should be estimated before applying this method.

The new developed simulation model allows the investigation of the aforementioned phenomena. The gained knowledge can be used for the development of appropriate and efficient protection concepts for the defined failure scenarios.

Notation

Latin symbols

A = cross-sectional area (m^2)
C_{fw} = Francis weir parameter
C_p = heat capacity (kJ/kg K)
E_{spray} = entrainment in spray regime (m^3/m^3)
F = F-factor ($Pa^{0.5}$)
g = acceleration of gravity (m/s^2)
H = height (m)
h = specific enthalpy (J/mol)
HU = molar holdup (mol)
k = heat transfer coefficient (W/m^2K)
l_{weir} = weir length (m)
L = liquid flow (mol/s)
M = mass (g)
$\tilde{M}$ = molar weight (g/mol)
$\dot{m}$ = mass flow density (g/sm^2)
$\dot{M}$ = mass flow (g/s)
P = pressure (Pa)
Q = heat flow (J/s)
R = relief flow (mol/s)
RR = reflux ratio
T = temperature (K)
u = specific inner energy (J/mol)
v = specific volume (m^3/mol)
V = vapor flow (mol/s)
Vol = volume (m^3)
$\dot{V}$ = volumetric flow (m^3/s)
w = velocity (m/s)
$\dot{x}$ = vapor mass fraction (stagnation quality)
x = liquid mole fraction
y = vapor mole fraction
z = feed flow mole fraction

Greek letters

φ = fugacity coefficient
π = pointing correction
η = pressure ratio
$\eta_{Murphee}$ = Murphee efficiency
Ω = weeping factor
γ = activity coefficient
α = discharge coefficient
ζ = pressure drop coefficient
ρ = density (kg/m^3)
Ψ = outflow function (safety valve)
ε = volumetric vapor fraction (void fraction)

Indices

A = ambient
C = condenser
crit = critical pressure ratio
CW = cooling water
D = drum
dry = dry pressure drop
F = feed
hole = tray holes
hydro = hydrodynamic pressure drop
i = components
j = stage
L = liquid phase
loss = heat loss
LV = liquid vapor equilibrium
OP = one-phase flow
R = relief
RR = reflux
S = reboiler
shaft = downcomer hydrostatic pressure
shell = column shell
St = steel
stage = stage height
sub = subcooling
tot = total
TP = two-phase flow
V = vapor phase
weep = weeping
ent = entrainment
set = set pressure
fl = full lift pressure
cl = closing pressure
rs = reseating pressure

Parameter

$k_1^{weep} = 2.2$
$k_2^{weep} = 0.69$
$k_3^{weep} = 0.85$
$k_1^{ent} = 9.47 \times 10^{-3} \exp(-7.4 \cdot H_{stage})$
$k_2^{ent} = -3.24 \times 10^{-3} \exp(-6.8 \cdot H_{stage})$
$k_3^{ent} = 0.27 \times 10^{-3} \exp(-5.8 \cdot H_{stage})$

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