Hamburg University of Applied Sciences

Faculty Life Sciences

Assessing tools for sizing pressure relief devices: Dynamic conditions

Master Thesis

Master Course Process Engineering

Presented by:

Mr. Arian Issel

[redacted]

[redacted]

Bergedorf / Basel

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Reviewer: Prof. Dr.	Margret Bauer (HAW Hamburg)
Reviewer: Dr.	Annik Nanchen (TÜV SÜD Process Safety)

This master thesis was created and supervised in cooperation with TÜV SÜD Schweiz AG, Department Process Safety

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1 Abstract

This thesis deals with the comparison of various commercial software tools with the task to evaluate their suitability for TÜV SÜD to replace the state-of-the-art emergency relief system sizing procedure. As proper relief system sizing is of great importance regarding safety, TÜV SÜD is interested in an improvement of this procedure with the help of specialized software. After an introduction and a theoretical background, the thesis presents requirements for the different software tools. Afterwards, every software is introduced and revised regarding the fulfillment of the requirements. After revision of the requirements, standard emergency relief systems design scenarios are applied to each software (both steady state and dynamic) and compared to the current calculation technique. The software tools evaluated in this thesis are SuperChems, FlowNex, ChemCad SafetyNet and ProSar. If applicable, dynamic simulations are applied and the results are presented and discussed. To provide a better understanding on how the software works, detailed exampled are worked out in the appendix in addition to the standard design scenarios in previous chapters. The thesis closes with a discussion about every software and an outlook.

2 Introduction

Past as well as recent accidents in the chemical industry, like the Bhopal incident in India in 1984, have shown the importance of reliable protection systems against all kinds of process deviations. But accidents did not only happen in the past, where safety was not number one priority. Incidents can always happen, even if the knowledge about past incidents is considered. Incidents like the fertilizer explosion at West in Texas with twelve fatalities in 2016 show, that process deviations are not a myth of the past but a present danger (Chemical Safety Board, 2021). This has shown the importance of understanding what exactly is happening during processes. Numerous books and reports are focused on the explanations of accidents with the aim to avoid them in the future. (Mannan, 2012).

In the chemical process industry advanced care must be taken when handling overpressure in chemical reactors for exothermic reactions. Loss of control of the reaction can lead to a rapid pressure increase. The consequences of a pressure increase can be reduced by a properly sized emergency relief system (ERS). However, there is a wide range of examples where emergency relief systems have malfunctioned highlighting the necessity of proper ERS sizing.

But not only the safety valve itself must function properly – also the effluent treatment systems processing the released (possibly toxic) materials. In the case of the chemical accident at Höchst in Griesheim, an increase of pressure occurred in a reactor due to human error and a safety valve opened correctly, releasing toxic effluent into the atmosphere. Since no effluent treatment was present, all the toxic material was released without further processing. Investigations later showed, that the carcinogenic chemical nitroanisole was released directly into the atmosphere leading to significant human and environmental damages. (Frankfurter Allgemeine Zeitung, 2021)

Nowadays, ERS sizing is done applying certain simplifications to the system, for instance static conditions in the safety valve during pressure relief. Applying those simplifications can lead to valve oversizing, possibly causing chattering or hammering of the safety valve. After a theoretical background on hazard identification, emergency relief systems and its design, this thesis will present different software for improved emergency relief system sizing under dynamic conditions, meaning that actual conditions during relief through a safety device and the relief piping path are considered. Solving pre-defined tasks, the software is being evaluated for its suitability for TÜV SÜD Process Safety. Basis for the evaluation will be a user requirement specification list. Due to the more complex nature of safety valves, this thesis will concentrate on valve sizing.

2.1 TÜV SÜD Process Safety

The process safety department of TÜV SÜD provides impartial and reliable safety concepts and services for a variety of industries including machine safety, risk analysis, quantitative risk assessment, explosion prevention and protection (ATEX, explosion modelling, electrostatic charging modelling), incident investigation, thermal process safety and pressure relief system design. TÜV SÜD uses state-of-the-art techniques, taking applicable laws and regulations into account. Furthermore, TÜV SÜD cooperates with other research sites and international associations to ensure best quality.

TÜV SÜD Process Safety sizes and rates pressure relief devices using international regulations as mentioned in Section 3.2.1. To do so TÜV SÜD uses a highly sophisticated excel tool taking all requirements developed in this thesis into account. These regulations enable TÜV SÜD to do hand-calculations of the desired processes. Underlying certain simplifications, these calculations are always conservative. The software evaluated in this thesis shall improve the calculation techniques used nowadays and avoid oversizing of emergency relief devices and simplify the complex calculations of pressure drop in emergency relief lines.

2.2 Risk assessment

An important role in the life cycle of any industrial process are risk assessments. To acknowledge and address all possible risks and dangers, proper risk assessment is of high importance to avoid incidents but also to provide enough safety measures, if incidents occur. Different levels and types of risk assessments are performed and updated throughout the life cycle. All risk assessments aim at identifying hazards. The main terminology of risk assessment is being defined in this section.

2.2.1 Hazard

Hazard is a situation that has the potential to cause harm to human, environment, and property. (Jones, 2003)

Considering the chemical industry, hazard results from either the properties of processed substances, reactions and the resulting energy release or deviations such as technical failures and human error during operation or process design phase. External causes like fire can also cause uncontrolled situations. Also, hazardous situations can result from failure of identifying specific hazards or insufficient countermeasures during the risk assessment or process changes. (Stoessel, 2020)

2.2.2 Risk

An often-used definition of risk is severity times probability. In this case, “times” should not be seen as the mathematical product but more as a linked coherence of the two expressions. (Jones, 2003)

The risk is linked to a pre-defined scenario that needs to be described with a specific accuracy for evaluation in terms of severity and probability. Severity stands for the impact of a possible event to human, environment, or property but also other social properties like company image. Probability stands for the frequency of occurrence of a scenario. (Stoessel, 2020)

2.2.3 Safety

Safety describes the absence of any hazard. Absolute safety is impossible to achieve, since there is a chance that all safety elements fail at the same time. (Stoessel, 2020)

2.3 Risk analysis

The major steps for analyzing risk are hazard identification, risk evaluation and the definition of risk-reducing measures.

One important preliminary step is the collection of safety data as well as the definition of safe conditions and the identification of process deviations and their consequences. After these preliminary implementation steps, risk-reducing measures must be taken if the risk is not acceptable. As mentioned in section 2.2.3, complete safety cannot be achieved. Therefore, there will always be a residual risk occurring from either consciously accepted risk, misjudged risk, or unidentified risk. All these risks need to be reduced to an accepted level and processes must keep these hazards under control. (Stoessel, 2020)

3 Theoretical background

This chapter gives the theoretical background on hazard identification, pressure relief systems and emergency relief system design and introduces the most commonly known standards.

3.1 Hazard identification techniques and risk assessment tools

Hazard identification techniques have been developed to systematically address and analyze hazards. This section introduces common techniques and studies regarding the assessment of risk and hazard.

3.1.1 Failure mode and effects analysis (FMEA)

Within the FMEA analysis the executing team reviews systems with the intention to discover the mode of failure which may occur and their specific effects. The FMEA technique is more related to equipment rather than process parameters. (Mannann, 2012, p. 254)

3.1.2 Hazard and operability study (HAZOP)

The HAZOP study comes to terms once the complete piping and instrument diagram (P&ID) of the plant is available and is the most used hazard identification technique. Its intention is to discover potential process hazards and operability problems using certain guidewords (No/Not, More, Less, As well as Part of, Reverse, Other than). These Guidewords are systematically applied to every part of the process to discover what kind of deviations from the original design intent might occur, the causes of these deviations and to evaluate their consequences considering hazards and operability problems. The overall design is examined including material, activities, and equipment. (Mannann, 2012, p. 236)

3.1.3 Layers of protection analysis (LOPA)

The LOPA is one of the most popular semi-quantitative technique for the assessment of process risks. Strictly speaking, LOPA is a risk assessment tool but not a hazard identification technique. It is being applies after all hazards are identified. provides an objective, risk-based approach to identify and specify protection layers which are used to mitigate and prevent process risks (see section 2.2.2). (Mannan, 2012, p. 2422)

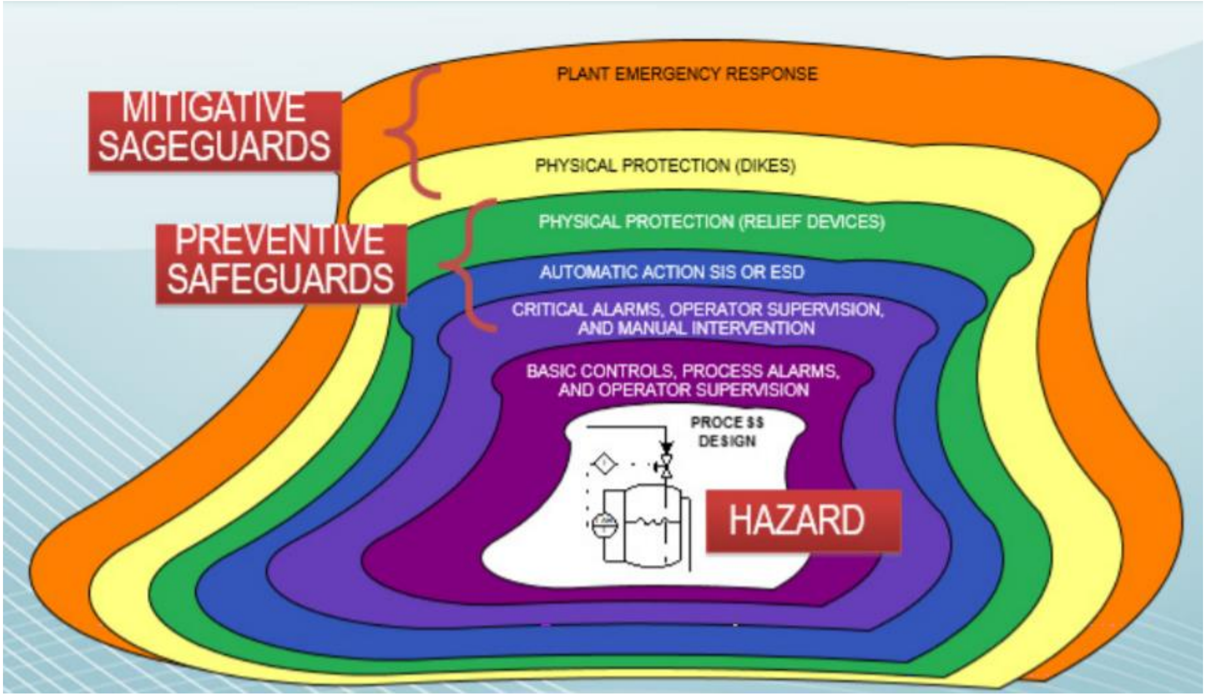


Figure 1: Layers of protection (Willey, 2014)

As Figure 1 shows, the first and most important step to be in control of hazards is the process design (inherently safe process) followed by process control and alarm systems. These steps form the basic protection layers. On top of that, preventive safeguards are installed including critical alarms and automatic action from safety systems but also the first physical protection in form of pressure relief devices. As the change in color in Figure 1 implies, the following safety layers are mitigative measures, reducing the consequences of process incidents. These last measures include emergency response systems for the surroundings of the plant.

3.2 Emergency relief systems

As previously mentioned, emergency relief systems play an important role to control unwanted pressure increases during chemical processes. Therefore, there are regulations and norms concerning pressure relief from different countries (laws, regulations) and institutions (norms) all over the world. There are two different systems for pressure relief – bursting discs and safety valves – in various design executions. Emergency relief systems also include the emergency vent line and the effluent treatment system. Emergency relief systems are the last defense against overpressure and eventually explosions of chemical reactors. (Center for Chemical Process Safety of the American Institute of Chemical Engineers, 2017)

3.2.1 Regulations for pressure relief equipment

There are certain international regulations to ensure a standardized procedure in manufacturing and handling of pressurized process equipment. In this section the main standards relating to pressure relief devices are briefly introduced.

3.2.1.1 Druckgeräterichtlinie (pressure equipment directive)

The german pressure equipment directive was created to regulate all pressure devices with a working pressure of p_{work} > 0.5 bar. The sub-directive “Merkblatt AD-2000” specifies main safety requirements which are listed in the “Druckgeräterichtlinie” (pressure equipment directive). As a European counterpart to the “Druckgeräterichtline”, the EN 13445 standard was created. It also ensures compliance with safety requirements listed in the pressure equipment directive. (TÜV SÜD , 2021)

3.2.1.2 API-STD 520 P1 (American Petroleum Institute)

The API-STD 520 P1 norm recommends practices on the sizing and selection for pressure relief devices used in refineries. More specifically, the practice intends to protect unfired pressure vessels and related equipment with a maximum allowable working pressure of 15 psig (≈ 1.034 bar) against overpressure from operating and fire eventualities. (American Petroleum Institute, 2000)

3.2.1.3 CGA S-1.1 (Compressed Gas Association)

The CGA S-1.1 pressure relief device standards part 1 – cylinders for compressed gases introduces different types of pressure relief devices, gives application as well as design and construction requirements for the introduced devices and their combinations. Furthermore, another section deals with device testing and maintenance requirements of pressure relief devices. (Compressed Gas Association, 2005)

3.2.1.4 ASME VIII (American Society of Mechanical Engineers)

The ASME VIII regulation code provides requirements applicable to the design, fabrication, inspection, testing, and certification of fired or unfired pressure vessels operating at either internal or external pressures exceeding 15 psig (≈1.034 bar). Furthermore, the code includes methods for welding, forging and mandatory and non-mandatory appendices detailing design criteria, non-destructive examination, and inspection standards. (The American Society of Mechanical Engineers, 2017)

3.2.1.5 ISO 4126-10

The ISO 4126-10 is a standard (norm) about safety devices for protection against excessive pressure – part 10: sizing of safety valves and connected inlet and outlet lines for gas/liquid two-phase flow. It specifies the sizing of safety valves for reactors, columns, and piping system based on the omega method, which is extended by a thermodynamic non-equilibrium parameter. Other sizing methods available are referring to ISO 4126. (DIN Deutsches Institut für Normung e.V., 2019)

3.2.2 Bursting disc

A bursting disc is a thin foil made of (stainless) steel or graphite. It is an intentional weak point of the system which breaks below or at the design pressure of an equipment. After the irreversible bursting of the disc, the discharge area is available for pressure relief immediately. After bursting, pressure inside equalizes with the downstream (mostly ambient) pressure. Figure 2 shows a bursting disc with its respective disc holders. A bursting disc can work for overpressure as well as vacuum application. The relief conditions need to be calculated carefully to avoid under-sizing. The opening pressure is temperature dependent and can be affected by cycling pressures. Bursting disc are being used widely in the industry to protect equipment against overpressure in the process and vessel explosion.

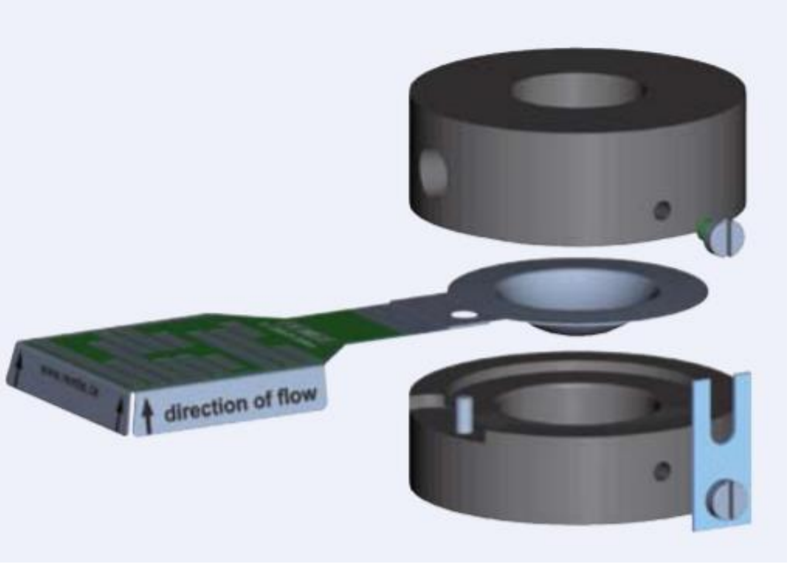


Figure 2: 3-D drawing of a bursting (rupture) disc with the respective disc holder (LESER GmbH & Co. KG, 2009, p. 11)

3.2.3 Safety valves

Other than bursting discs, safety valves are more complex in their build-up and function. A safety valve opens at the set pressure. Most of the time it is a spring-loaded device which is fully opened at 110% of the set pressure and can reseat. Safety valves can have different opening layouts like “normal opening”, “full stroke”, and “proportional” and have different additional design functions like “balanced” safety valves that can handle larger backpressures. Figure 3 shows pressure zones of a conventional and a balanced safety valve as manufactured by LESER. Figure 4 shows the technical build-up of safety valves. (LESER GmbH & Co. KG, 2018)

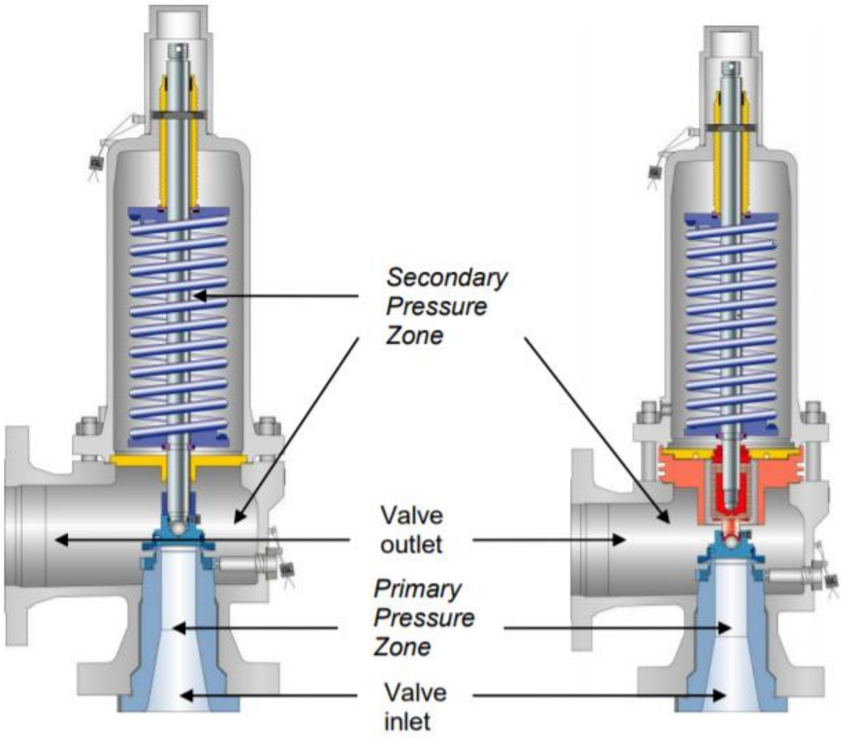


Figure 3: Pressure zones conventional (left) and balanced (right) safety valve (LESER GmbH & Co. KG, 2018, pp. 2.3-1)

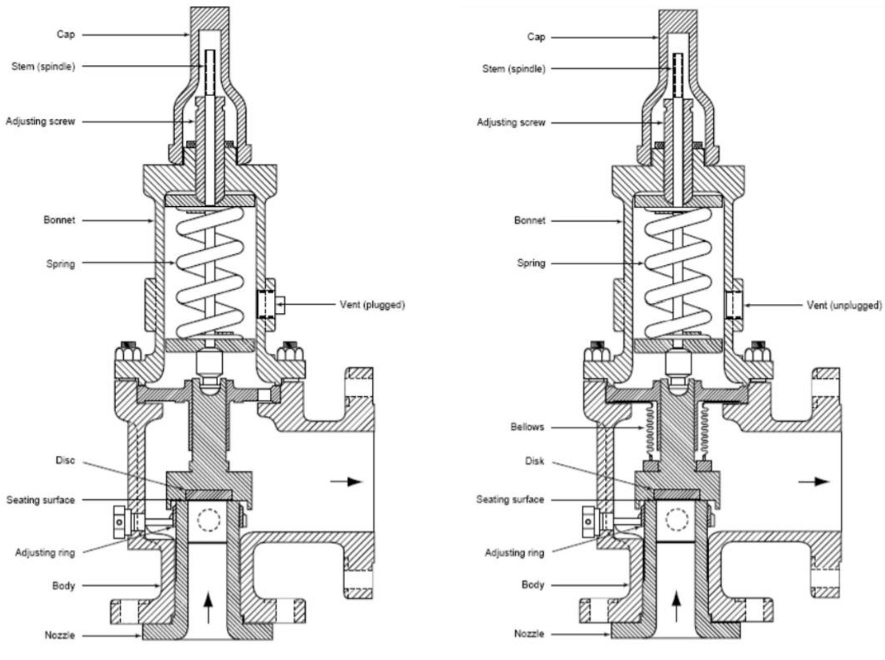


Figure 4: Typical design of conventional (left) and balanced (right) safety valve (LESER GmbH & Co. KG, 2018, pp. 2.5-1 - 2.5-2)

The advantage of safety valves is their ability to close after pressure relief, not unloading the full content of the equipment. The unsafe process condition can be returned to safe condition. On the downside, the safety valve might not be tight after reseating, resulting in leakages, which could be problematic (toxicity). If the problem for the pressure increase is not solved, the system will stay close until the set pressure is reached again. This can lead to a frequent opening and closing of the valve. If this frequency is at resonance frequency of the valve, the safety valve can chatter.

Another potential disadvantage of safety valve is the opening curve meaning that the relief area is a function of time, and the full orifice is not available immediately. Furthermore, safety valves are usually large in size and weight. If a safety valve is contaminated with certain chemicals or abrasive materials, loss of sealing can be the consequence.

3.2.4 Combination of bursting disk and safety valve

Bursting disks (section 3.2.2) and safety valves (section 3.2.3) are often installed in combination as Figure 5 shows. This combination is used to protect the safety valve against splashes. In this combination case, the set pressures of both the disc and the safety valve are equal or at least very close to each other. A combination can also be installed in parallel with the set pressure of the safety valve being lower than the one for the bursting disc. The safety valve protects the vessel against minor relief scenarios like volume displacement. If design scenarios with a higher discharge occur, the bursting disc protects the equipment. Sometimes also two safety valves are placed in parallel to increase the capacity, increase the reliability and be able to do maintenance work during a running process.

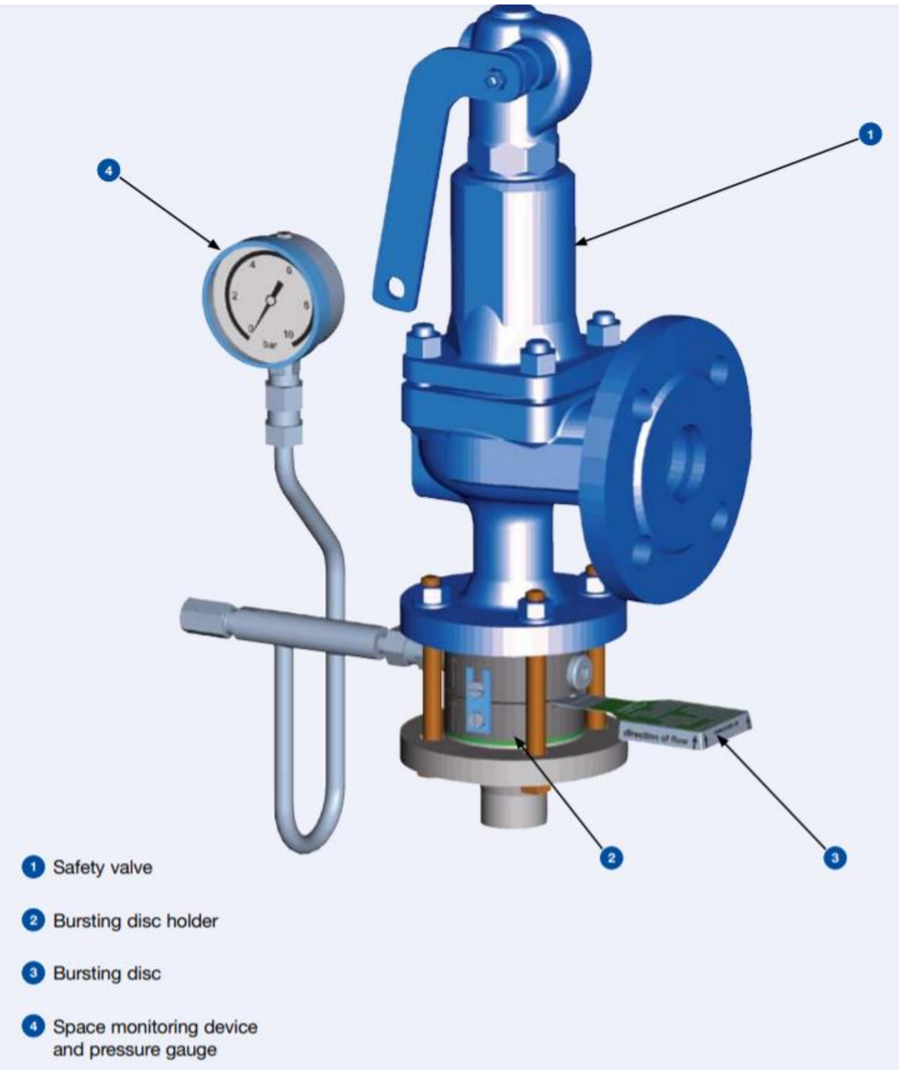


Figure 5: Combination of bursting disc and safety valve (LESER GmbH & Co. KG, 2009, p. 6)

3.2.5 Effluent treatment

Depending on the process, the mass relieved during an overpressure scenario can contain toxic, flammable and/or reactive chemicals or mixtures. A relief of this mass directly into atmosphere can therefore be extremely dangerous. Toxic, flammable or reactive mass must be treated before releasing into atmosphere. This can be done in various ways, depending on the relief mass (vapor/gas, liquid, two-phase), the process and the plant itself. For effluent treatment design all mass flows of both phases must be determined beforehand. Possible treatments are total containment, passive condensing, gravity separation, a cyclone, or a quench tank. As stated in the introduction, incidents like the accident at Icmesa in Seveso in 1976 or the accident at Höchst in Griesheim in 1993 show the importance of proper effluent treatment. (Stoessel, 2020)

3.3 Input data requirements

Considering emergency relief systems sizing, a major part of risk assessment is the proper acquisition of chemical and physical data. The following chapters give an overview of required physical, chemical and plant specific data for ERS sizing.

In this section, tables listing the required input data for ERS sizing calculations are given. Often, not all the listed data is available for sizing and some values need to be calculated or estimated.

3.3.1 Description of the process installation

Process description data is essential for emergency relief system sizing. All the equipment involved and its physical position as well as its size and volume must be known. Furthermore, the purpose of the plant and the materials and chemicals involved are essential for sizing calculations. For more detailed information regarding the plant, a plant P&ID is of great help.

3.3.2 Detailed equipment specifications

The following section gives an overview on the required equipment information needed for ERS sizing. The vessel / reactor is the main equipment to be protected against overpressure. A pressure relief valve is usually located directly on top of the vessel or is connected via small piping paths.

3.3.2.1 Vessel information

Table 1 lists the required information regarding the vessel / reactor.

Table 1: required vessel information

Parameter	Unit
Diameter	[m]
Height	[m]
Maximum working volume	[m^3]
Heat exchange area (heating only)	[m^2]
Heat transfer coefficient (heating only)	[W/m^2*K]
Maximum allowed working pressure	[bar]
Maximum allowed working temperature	[°C]
Design pressure	[bar]
design temperature	[°C]

3.3.2.2 Emergency relief system information

In addition to the manufacturer information like type, article number, and the relief systems identification in the PID, more information is needed as listed in Table 2.

Table 2: required safety device information

Parameter	Unit
Set pressure	[bar]
Set temperature	[°C]
Maximum accumulated pressure	[bar]
Nominal diameter	[m]
Flow area / discharge area	[m^2]
Discharge coefficients (safety valves)	[-]

3.3.2.3 Relief piping geometry

For proper calculation of pressure losses in the relief piping system, the relief line geometry must be known. Required information is the piping material and nominal pipe diameter. Furthermore, the total number of bends, tees, and elbows as well as the total pipe system elevation is required for the calculation of the systems piping friction losses. Pressure drops directly affect the capacity of bursting discs and are therefore an input data. For safety valves, pressure drops are used to determine whether the valve is stable during the relief.

3.3.3 Physical and chemical properties

A variety of physical properties of the chemicals used must be known for ERS sizing.

3.3.3.1 Liquid phase

Table 3 lists the required physical and chemical properties for the liquid phase.

Table 3: required physical properties (liquid phase)

Parameter	Unit
Molar weight	[g/mol]
molar or mass fraction	[-]
Boiling point	[°C]
Specific heat capacity	[J/kg*K]
Surface tension at relief conditions	[N/m]
Density at relief conditions	[kg/m^3]
Volume expansion coefficient	[-]

3.3.3.2 Vapor phase

For the vapor phase, the information listed in Table 4 is required.

Table 4: required physical properties (vapor phase)

Parameter	Unit
Vapor pressure as a function of temperature	[bar]
Latent heat of vaporization at relief temperature	[kJ/mol]
Isentropic coefficient	[-]
Real gas compressibility	[-]
Density of vapor (calculated)	[kg/m^3]

3.3.3.3 Gas phase

If a gas is present, the information of Table 5 is required.

Table 5: required physical properties (gas phase)

Parameter	Unit
Gas composition	[-]
Molar mass	[g/mol]
Maximum gas flow rate	[kg/s]
Isentropic coefficient	[-]
Pressure increase rate	[bar/s]

If a reaction is happening, the heat release rate and the gas release rate under relief conditions must be known.

3.3.4 Relief conditions

Finally, the relief conditions must be known as listed in Table 6.

Table 6: relief conditions

Parameter	Unit
Set pressure	[bar]
Set temperature	[°C]
Mass flow to be discharged	[kg/s]
Mass in the system	[kg]
Back pressure	[bar]
Thermal power at relief temperature	[W/kg]
Maximum accumulated pressure	[bar]
Expected flow regime	[-]

The mass flow to be discharged and the thermal power at relief conditions are calculated in the relief scenario calculations. The maximum accumulated pressure is usually 110% of the design pressure.

3.4 Design scenarios

Prior to all emergency relief sizing calculations, the process conditions of a proposed emergency event need to be defined. At this stage, the most severe venting conditions need to be determined in terms of hazards and consequences (worst-case scenario). Listings of overpressure sources are available in open literature and several standards. These design scenarios include but are not limited to the external fire case, incorrect valve operation, blocked outlets, loss of utility, cooling, and instrument failure. (Stoessel, 2020)

To quantify a scenario the knowledge of either the thermal power input or a volume flow rate is required, depending on the scenario. (Center for Chemical Process Safety of the American Institute of Chemical Engineers, 2017) The most common design scenarios used by TÜV SÜD are explained below.

3.4.1 External fire case

The external fire case represents one of the standard design scenarios in pressure relief device sizing. In this design scenario, an external fire occurs and heats up the vessel and its content resulting in a temperature and pressure increase. The system therefore needs protection against overpressure. Depending on the chemicals inside the vessel and the vessel properties (insulation, geometry) and the reactiveness of firefighting, the pressure relief device needs to be sized in regard to the API 520/ISO 4126-10. (Stoessel, 2020)

3.4.2 Maximum heating

The maximum heating case describes the failure of the temperature control system of a heated vessel. If a volatile compound is present the temperature and pressure will increase. (Stoessel, 2020)

3.4.3 Volume displacement – closed outlets

Volume displacement describes a physical design scenario where a fluid is fed into a closed vessel. This design scenario can occur if the vent is not opened properly before the feeding process starts. In this case, the maximum feed rate into the vessel must be known for calculation of the pressure drop in the system. (Stoessel, 2020)

3.4.4 Loss of cooling – abnormal heat input

In the design scenario of an exothermal batch reaction, the products are fed into the reactor and heated until the desired reaction temperature is reached. This temperature shall remain at the desired level. This is also true for semi-batch and continuous reactors. If a cooling failure occurs, the chemical reaction will lead to a temperature and pressure increase. To avoid an explosion of the reactor must be equipped with a properly sized pressure relief device. (Stoessel, 2020)

3.4.5 Thermal expansion of a liquid

Liquid thermal expansion can occur, if a heat exchanger is blocked or if liquid is present in a pipe below ambient temperature or if blocked liquid in a pipe is heated (e.g., heating through sunlight). The cold liquid will heat up and eventually cause a temperature and pressure increase. The system must be protected against overpressure. (Stoessel, 2020)

3.5 State-of-the-art emergency relief system design

Emergency relief system sizing starts with the design case identification using hazard identification techniques as explained in section 3.1. The causes for pressure increase must be assessed properly.

3.5.1 Quantifying relief scenario

After the assessment of pressure increase causes, worst case scenarios need to be determined for further design steps. Design scenarios can be of physical nature like additional mass or heat input. Also, relief scenarios can be of chemical nature as gas production by a chemical reaction or secondary runaway reactions with temperature and pressure increases. For proper quantification, the source for the pressure increase must be known. The system can be either vapor (pressure increase due to vapor pressure of the system), gassy (pressure increase due to gas production or release) or hybrid (vapor pressure and gas production).

For chemical reactions, ideally, reaction kinetics should be considered. TÜV SÜD does not determine reaction kinetics but uses its own laboratories for the determination of the pressure increase rate and the temperature increase rate in a VSP Experiment.

3.5.2 Screening design scenarios for worst case

Based on the quantification in section 3.5.1, the design scenarios need to be screened for the worst case. Usually, this is done by taking consequences into account. For every design scenario, the consequences need to be measured or calculated and compared to ensure the best choice for the worst case.

3.5.3 Determination of the flow regime

After choice of the worst-case scenarios, the flow regime for each design scenario must be determined. By checking the rate of bubble formation and the time needed for them to escape (bubble flow velocity). This leads to volume swell. If the volume swell is such that the reactor is full of liquid, two-phase flow will occur. If the volume swelling remains below the flange going to the pressure relief device, one-phase flow occurs. The level swell depends on the fill level in the reactor and on the type of bubble flow in the reaction mass (e.g., bubbly flow or churn turbulent).

3.5.4 Mass flow rate to be discharged

State-of-the-art calculation for the mass flow that must be discharged during relief use simplifications as stated in section 3.5.6. Depending on the flow regime, different equations must be applied for the correct calculation of the mass flow that needs to be discharged during the relief scenario. These calculations are done steady state according to standard like the ISO 4126-10. (Stoessel, 2020, p. 439f)

3.5.5 Dischargeable mass flux through nozzle

After the calculation of the mass flow rate that must be discharged during the relief scenario, the necessary mass flux through the nozzle needs to be calculated. For a one-phase flow system the calculation is hands-on and can be found in literature. For two-phase flow, the omega method from Leung is applied using the assumption that thermal and thermodynamic equilibrium are reached in the nozzle. With an extension to the omega method by Diener and Schmidt a correction factor for this simplification can be applied for safety valves. Finally, the mass flux can be calculated as stated in Francis Stoessels Thermal Safety of Chemical Processes. (Stoessel, 2020, p. 441f)

3.5.6 ERS sizing challenges

For state-of-the-art sizing methods, a variety of simplifications (steady state) are assumed. For the determination of the mass flow rate for vapor relief with two-phase flow some conservative assumptions are made using only data relative to stagnation conditions in a static approach. These assumptions are a constant mass flow rate between set pressure (P_{set}) and the maximum pressure (P_{max}), constant heat input (q') during relief, constant physical properties during relief (c_v, ΔH_v, v_{fv}), vapor and liquid flow at the same velocity and that the flow remains two-phase over the relief process. To optimize the sizing procedure, the calculations shall be done dynamically with the help of software tools. (Stoessel, 2020, p. 440)

3.6 Dynamic modelling

In general, dynamic simulations simulate a system and its changes over time. Dynamic systems are usually described with differential equations. Mass and energy balances around defined process requirements of unit operations and complete systems are solved with the use of computer aided design tools with differential equation solvers consisting of suitable solution algorithms. Connections between the different process units are understood as logical connectors for mass and energy flow through the system. Solving such a system can be described as the process of finding the optimal unit operations settings and conditions. To find such solutions, realistic initial values must be specified. In the case of emergency relief system sizing simulations, these values are, amongst others, temperature, and pressure.

The formulas (1), (2) and (3) describe the fundamental laws of nature and are universally applicable in all systems. These differential equations must be solved for each process unit and the whole. (Institute of Chemical Technology and Engineering, Poznan University of Technology, 2020)

3.6.1 Dynamic valve size calculation - governing equations

(1) Continuity

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho * V * A)}{A * \partial x} = 0$$

Formula (1) describes the general equation for the conservation of mass by partial differential equations for a one-dimensional coordinate system. Integrating this general equation yields a discretized continuity equation.

(2) Momentum

$$\frac{\partial(\rho * V)}{\partial t} + \frac{\partial(\rho * V^2 * A)}{A\partial x} + \frac{\partial p}{\partial x} + \rho * g * cos\theta + \frac{f * \rho * V|V|}{2 * D} = 0$$

Formula (2) describes the general equation for the conservation of momentum for one-dimensional compressible flow in a system. Integrating this equation yields a discretized momentum equation.

(3) Energy

$$\frac{\partial(\rho h_0 - \text{ü})}{\partial t} + \frac{\partial(\rho V A h_0)}{A\partial x} - \dot{q} = 0$$

Formula (3) describes the general equation for the conservation of energy (simplified) for one-dimensional flow in terms of stagnation enthalpy. Integrating this equation yields a discretized energy equation. (FlowNex Simulation Environment, 2020)

Table 7: Legend for formulas (1), (2) and (3)

ρ	Density [kg/m³]	*g*	Gravitational const. [m/s²]
V	Volume [m³]	θ	Angle [rad]
A	Area [m²]	*D*	Diameter [m]
t	Time [s]	*h*	enthalpy [kJ/kg]
p	Pressure [Pa]	*u*	internal energy [kJ/kg]

4 ERS sizing software requirements

There are various software tools on the market for the sizing of emergency relief devices. Most manufacturers in the safety valve industry have their own sizing software available with their specific valves to choose from. Nevertheless, some software tools are very basic and allow the user to only do steady state calculations of emergency relief systems. There are special requirements for the software to be of value for TÜV SÜD Process Safety. These requirements have been developed during the thesis after working through various TÜV SÜD relief system sizing projects, after internal discussions, critical analysis, and literature research (Stoessel, 2020), extracting these requirements as the most important. These user requirements are basis for the qualitative evaluation of the software tools (Table 8). Since TÜV SÜD does ERS sizing calculations for a variety of customers and therefore also processes with all kinds of different chemicals involved, the need for an extensive chemical database is given (criteria 1). The software must be able to calculate state points and physical properties of mixtures/chemicals at relief conditions and during the relief (criteria 2). The software should be able to do both one- and two-phase flow simulations as well as calculations in forced two-phase flow (criteria 4&5) since even if one-phase flow is expected it is possible that, for example due to foaming of a system, a two-phase flow occurs. The software should be able to account for that. ERS sizing is done describing worst-case design scenarios of physical and/or chemical nature (criteria 5&6) like the external fire case, the maximum heating case, and the loss of cooling case as described in section 3.4. A software sizing report should highlight the respective scenarios for easier understanding (criteria 20). In addition to a chemicals database, the software should be able to also simulate chemical reactions with both a user input of relevant reaction data (criteria 9) and reaction kinetics (criteria 10). The input of alternative reaction data as received from a VSP experiment is important since reaction kinetics are only rarely available. The applied software should have a relief device manufacturer database as well as the possibility to enter user defined device geometries (criteria 12 to 15). Relief piping pressure loss calculation for functional stability (criteria 16), calculation of minimum relief area (criteria 17), sizing according to the European standard (criteria 18) and backpressure calculations of the safety device are also requirements to the software.

Table 8: Software user requirements

	Software requirements
1	Extensive chemicals database
2	Dynamic calculation of physical properties at relief/critical conditions
3	One- and two-phase flow calculations
4	Forced two-phase flow calculations
5	Easy scenario creation
6	Standard scenario database (physical / chemical)
7	vapor / gassy / hybrid systems
8	Chemical reaction database
9	Chemical reaction data user input
10	Chemical reaction kinetics
11	Flow behavior determination
12	PRV user definition
13	PRV manufacturer database
14	BD user definition
15	BD manufacturer database
16	Piping pressure loss calculation
17	(Minimum data) calculation of relief area
18	Sizing regarding ISO / API - Norm
19	Function stability check (backpressure)

For an easier evaluation of the software regarding norms and the TÜV SÜD's state-of-the-art sizing methods, the following Table 9 gives an overview on additional software requirements regarding the evaluation of results. The main task of ERS sizing is the calculation of the mass flow to be discharge through the relief device (criteria 21) and the dischargeable mass flux through an existing device (criteria 22). These results should be visualized clearly and easily to understand in a sizing report highlighting the calculation method, the heat input and the flow regime occurring and other important sizing values (criteria 20). Best would be if the used calculation methods are highlighted (criteria 23).

Table 9: Software evaluation requirements

	software evaluation requirements
20	understandable visualization of results
21	calculation of mass flow to be discharged
22	calculation of dischargeable mass flux
23	calculation methods from literature

For an easier handling of the software and more effective troubleshooting, the points listed in Table 10 would be appreciated in a software. These points include a clearly structured help section (criteria 24) in addition to meaningful example design scenarios (criteria 25), a helpful support team for questions (criteria 26) and understandable error codes (criteria 27).

Table 10: other software requirements

	other requirements
24	clearly arranged help section
25	well organized example scenarios
26	helpful support
27	user-friendly warnings (phase-change, under sizing, etc.)

The criteria assessed in Table 8 can be considered as hard criteria extracted from previous sizing tasks. They describe the main requirements for a software tool. These requirements serve as the basic suitability test. Table 9 lists requirements regarding the visualization and highlighting of the overall results but also of specific important sizing values (as the mass flow to be discharged and the mass flux through a nozzle). Table 10 can be considered soft criteria. Problems occurring from non-fulfillment of these criteria can be solved with deeper software knowledge. For this thesis though, they were quite important, since all knowledge about the software tools had to be appropriated in a certain time.

5 ERS Software

Chapter 5 introduces and evaluates the software tools researched in this thesis. Before the evaluation process, research regarding proper software tools had to be carried out. Most valve manufacturer have their own (very basic) sizing software. This sizing software is often only taking one-phase flow and steady state conditions into account, making it not suitable for further evaluation (e.g., FAUSKE's PrEVent, FluidFlow, HEROSE Valvio, ValveStar, Fisher's Valve specification manager). Dynamic software tools like Aspen HYSYS or EcoSim Pro are too expensive and too complex for ERS sizing tasks. After a brief introduction of each software tool, the evaluation criteria are being checked for every software using checkboxes. For reasons of comparability, the columns are filled bit by bit for each software.

5.1 SuperChems for DIERS

SuperChems for DIERS is the most known software regarding emergency relief sizing and was written in 1996 after the Design Institute for Emergency Relief Systems (DIERS) awarded Mr. Arthur D. Little to provide the (for that time) next generation computer program for dynamic emergency relief system design. The program's intention was to provide a tool for calculation of thermodynamic and transport properties of non-ideal behavior in both liquid and vapor phase. Furthermore, the program should provide temperature and pressure dependent derivatives and should be equation-of-state based. Other requirements to the program were a major thermophysical database, a differential equation solver, various flow models including two-phase flow. For this thesis, a free six-month academic license was available. (G.A. Melham, 1997)

5.1.1 SuperChems – requirements evaluation

Table 11: SuperChems requirements evaluation – 1 of 3

	software user requirements	SuperChems	FlowNex	ChemCad	ProSar
1	extensive chemicals database	☒	☐	☐	☐
2	dynamic calculation of physical properties at relief/critical conditions	☒	☐	☐	☐
3	one- and two-phase flow calculations	☒	☐	☐	☐
4	forced two phase flow calculations	☐	☐	☐	☐
5	easy scenario creation	☒	☐	☐	☐
6	standard scenario database (physical / chemical)	☐	☐	☐	☐
7	Tempered / gassy / hybrid systems	☒	☐	☐	☐
8	chemical reaction database	☐	☐	☐	☐
9	chemical reaction data user input (VSP)	☐	☐	☐	☐
10	chemical reaction kinetics	☒	☐	☐	☐
11	flow behavior determination	☒	☐	☐	☐
12	PRV user definition	☒	☐	☐	☐
13	PRV manufacturer database	☒	☐	☐	☐
14	BD user definition	☒	☐	☐	☐
15	BD manufacturer database	☒	☐	☐	☐
16	piping pressure loss calculation	☒	☐	☐	☐
17	(Minimum data) calculation of relief area	☒	☐	☐	☐
18	Sizing regarding ISO / API - Norm	☒	☐	☐	☐
19	function stability check	☒	☐	☐	☐

SuperChems provides a tool for static and dynamic calculations of emergency relief scenarios (criteria 1 & 2 fulfilled) for one and two-phase flow (criteria 3 fulfilled). The software user interface is quite overwhelming for beginners, but after a training period, scenarios can be built easily (criteria 5 fulfilled). Every scenario must be created and defined individually (criteria 6 not fulfilled). Relief devices can be user defined or chosen from a (American only) manufacturer database (criteria 13 & 15 partly fulfilled). Static sizing calculations are done regarding the API 520 norm. ISO 4126-10 calculations cannot be done by SuperChems (criteria 18 only partly fulfilled). Furthermore, chemical reaction simulations can only be done with the knowledge of reaction kinetics and not using VSP data (criteria 9 not fulfilled, criteria 10 partly fulfilled). Also, the chemicals involved in a reaction must be present in the SuperChems chemical database. Adding chemicals to that database requires excessive programming skills and cannot be done by the user intuitively. Piping pressure losses are being calculated in SuperChems (criteria 16 fulfilled).

Table 12: SuperChems requirement evaluation – 2 of 3

	requirements for software evaluation	SuperChems	FlowNex	ChemCad	ProSar
20	understandable visualization of results	☒	☐	☐	☐
21	calculation of mass flow to be discharged	☒	☐	☐	☐
22	calculation of dischargeable mass flux (ideal nozzle)	☐	☐	☐	☐
23	calculation methods literature	☐	☐	☐	☐

The simulation results are compiled in a report with all input and output data listed (criteria 20 & 21 fulfilled). Additionally, a pressure curve is being created. Once the user knows where to find the required information, all other charts can be created easily. Literature for calculations cannot be found intuitively and do not seem to be present in the user guide of SuperChems (criteria not fulfilled).

Table 13: SuperChems requirements evaluations - 3 of 3

	other requirements	SuperChems	FlowNex	ChemCad	ProSar
24	clearly arranged help section	☐	☐	☐	☐
25	well organized example scenarios	☐	☐	☐	☐
26	helpful support	☐	☐	☐	☐
27	user-friendly warnings (phase-change, under sizing, etc.)	☒	☐	☐	☐

Unfortunately, SuperChems does only partly provide a useful "help" section. The "help" SuperChems was updated to a more user-friendly interface, but the help section has not been updated to fit the new layout and is therefore not usable for the provided version of the program (criteria 24 not fulfilled). This fact leads to significant confusion using the software. Also, example scenarios are very basic only and not of great help (criteria 25 not fulfilled). During the research the support team was not frequently available, and problems were not solved (criteria 26 not fulfilled).

5.2 FlowNex

The original program called FlowNex was released in 1986 to solve air and water distribution networks on mines. The code was intended to meet requirements from Rolls-Royce for the simulation of aircraft combustion engines and was refined in 1997 with the extension of code to handle dynamic simulations of networks with time dependent flows. In the early 2000's simulation of gas mixtures, chemical reactions and two-phase flow modelling was implemented. Nowadays, its being used for the calculation of pressure losses and heat transfers for a variety of plant applications. For FlowNex, also a free six-month academic trial was available. (FlowNex Simulation Environment, 2021)

5.2.1 FlowNex – requirements evaluation

Table 14: FlowNex requirements evaluation – 1 of 3

	software user requirements	SuperChems	FlowNex	ChemCad	ProSar
1	extensive chemicals database	☒	☒	☐	☐
2	dynamic calculation of physical properties at relief/critical conditions	☒	☒	☐	☐
3	one- and two-phase flow calculations	☒	☒	☐	☐
4	forced two phase flow calculations	☐	☐	☐	☐
5	easy scenario creation	☒	☐	☐	☐
6	standard scenario database (physical / chemical)	☐	☐	☐	☐
7	Tempered / gassy / hybrid systems	☒	☐	☐	☐
8	chemical reaction database	☐	☐	☐	☐
9	chemical reaction data user input (VSP)	☐	☐	☐	☐
10	chemical reaction kinetics	☒	☒	☐	☐
11	flow behavior determination	☒	☐	☐	☐
12	PRV user definition	☒	☒	☐	☐
13	PRV manufacturer database	☒	☐	☐	☐
14	BD user definition	☒	☒	☐	☐
15	BD manufacturer database	☒	☐	☐	☐
16	piping pressure loss calculation	☒	☒	☐	☐
17	(Minimum data) calculation of relief area	☒	☐	☐	☐
18	Sizing regarding ISO / API - Norm	☒	☐	☐	☐
19	function stability check	☒	☐	☐	☐

FlowNex provides a dynamic simulation tool that was invented to simulate aircraft combustion engines (criteria 2 fulfilled) – not safety valves or bursting discs. In general, the simulation of a safety valve is possible, but the actual sizing and rating is not possible in a suitable way for TÜV SÜD. FlowNex provides a small chemical database (criteria 1 partly fulfilled). Chemicals and chemical reactions can be added to the FlowNex database with deeper software and programming knowledge. Since it was not created as an emergency relief sizing tool, there is no manufacturer database for safety valves or bursting discs and sizing cannot be done according to the ISO 4126-10 or API 520 (criteria 4, 5, 6, 7, 8, 9, 11, 13, 15, 17, 18 & 19 not fulfilled).

Table 15: FlowNex requirements evaluation – 2 of 3

	requirements for software evaluation	SuperChems	FlowNex	ChemCad	ProSar
20	understandable visualization of results	☒	☒	☐	☐
21	calculation of mass flow to be discharged	☒	☒	☐	☐
22	calculation of dischargeable mass flux (ideal nozzle)	☐	☐	☐	☐
23	calculation methods literature	☐	☒	☐	☐

The results can be visualized intuitively and are listed in a clear manner (criteria 20 fulfilled). The calculated values can be reviewed by simply clicking on the process unit (criteria 21 fulfilled). Literature to the calculation methods can easily be found in the help section (criteria 23 fulfilled).

Table 16: FlowNex requirements evaluation – 3 of 3

	other requirements	SuperChems	FlowNex	ChemCad	ProSar
24	clearly arranged help section	☐	☒	☐	☐
25	well organized example scenarios	☐	☒	☐	☐
26	helpful support	☐	☒	☐	☐
27	user-friendly warnings (phase-change, under sizing, etc.)	☒	☒	☐	☐

The FlowNex help section is well organized and FlowNex also provides well executed trainings and example scenarios. The warning layer gives helpful information on where to look for minor mistakes and the support was always available and intensively looking for a solution (all criteria fulfilled).

5.3 ChemCad (SafetyNet)

ChemCads SafetyNet is a stand-alone program for safety simulations including piping networks, compressor, pumps and valves. ChemCad is a combination of various process simulation software. SafetyNet uses the ChemCad chemical database which provides chemical and thermodynamical data of over 2000 chemicals. For ChemCad, only a free two-week license was available. (ChemStations, 2021)

5.3.1 ChemCad – requirements evaluation

Table 17: ChemCad requirements evaluation – 1 of 3

	software user requirements	SuperChems	FlowNex	ChemCad	ProSar
1	extensive chemicals database	☒	☒	☒	☐
2	dynamic calculation of physical properties at relief/critical conditions	☒	☐	☒	☐
3	one- and two-phase flow calculations	☒	☒	☒	☐
4	forced two phase flow calculations	☐	☐	☐	☐
5	easy scenario creation	☒	☐	☒	☐
6	standard scenario database (physical / chemical)	☐	☐	☐	☐
7	Tempered / gassy / hybrid systems	☒	☐	☒	☐
8	chemical reaction database	☐	☐	☐	☐
9	chemical reaction data user input (VSP)	☐	☐	☒	☐
10	chemical reaction kinetics	☒	☒	☐	☐
11	flow behavior determination	☒	☐	☒	☐
12	PRV user definition	☒	☒	☒	☐
13	PRV manufacturer database	☒	☐	☒	☐
14	BD user definition	☒	☒	☒	☐
15	BD manufacturer database	☒	☐	☒	☐
16	piping pressure loss calculation	☒	☒	☒	☐
17	(Minimum data) calculation of relief area	☒	☐	☒	☐
18	Sizing regarding ISO / API - Norm	☒	☐	☒	☐
19	function stability check	☒	☐	☒	☐

ChemCad provides an extensive chemical database also including some polymers and other special chemicals (criteria 1 fulfilled). ChemCad’s strength clearly lies in the dynamic thermodynamical calculations during the simulation (criteria 2 fulfilled). Basic sizing calculations for one and two-phase flows can be done easily and do not require deep software knowledge (criteria 3 & 5 fulfilled). Chemical reactions (using kinetics) cannot be simulated in the SafetyNet tool of ChemCad but with the complete version of the program (criteria 9 fulfilled, criteria 10 not fulfilled). Relief systems can be defined manually or the next size from a database is chosen (criteria 12-15 fulfilled). Sizing calculations are only done according to the API 520 norm (criteria 18 partly fulfilled).

Table 18: ChemCad requirements evaluation – 2 of 3

	requirements for software evaluation	SuperChems	FlowNex	ChemCad	ProSar
20	understandable visualization of results	☒	☒	☒	☐
21	calculation of mass flow to be discharged	☒	☒	☒	☐
22	calculation of dischargeable mass flux (ideal nozzle)	☐	☐	☐	☐
23	calculation methods literature	☐	☒	☒	☐

ChemCad provides an understandable result layout. Especially within the dynamic tool of ChemCad, all results can be visualized easily in addition to a sizing or simulation report (criteria 20 & 21 fulfilled). Literature for the calculation methods is listed in the respective help section (criteria 23 fulfilled).

Table 19: ChemCad requirements evaluation – 3 of 3

	other requirements	SuperChems	FlowNex	ChemCad	ProSar
24	clearly arranged help section	☐	☒	☒	☐
25	well organized example scenarios	☐	☒	☒	☐
26	helpful support	☐	☒	☒	☐
27	user-friendly warnings (phase-change, under sizing, etc.)	☒	☒	☒	☐

ChemCad has a clearly arranged help section and provide well organized and executed example scenarios. The support team is always available, and support was always very helpful (all criteria fulfilled).

5.4 ProSar

ProSar is a browser-based relief device sizing tool invented by the center of safety excellence (CSE) to provide a fast and easy way to do sizing calculations based on the API 520 as well as the ISO 4126. Once one of three available licenses have been purchased, ProSar can be run from every computer or Laptop using only a browser. The ProSar free license was available for the time of the research. Since the program was just released, the duration of the license was three weeks. (Center of Safety Excellence, 2021)

5.4.1 ProSar – requirements evaluation

Table 20: ProSar requirements evaluation – 1 of 3

	software user requirements	SuperChems	FlowNex	ChemCad	ProSar
1	extensive chemicals database	☒	☒	☒	☐
2	dynamic calculation of physical properties at relief/critical conditions	☒	☐	☒	☐
3	one- and two-phase flow calculations	☒	☒	☒	☒
4	forced two phase flow calculations	☐	☐	☐	☐
5	easy scenario creation	☒	☐	☒	☐
6	standard scenario database (physical / chemical)	☐	☐	☐	☐
7	Tempered / gassy / hybrid systems	☒	☐	☒	☐
8	chemical reaction database	☐	☐	☐	☐
9	chemical reaction data user input (VSP)	☐	☐	☒	☐
10	chemical reaction kinetics	☒	☒	☒	☐
11	flow behavior determination	☒	☐	☒	☐
12	PRV user definition	☒	☒	☒	☐
13	PRV manufacturer database	☒	☐	☒	☒
14	BD user definition	☒	☒	☒	☐
15	BD manufacturer database	☒	☐	☒	☐
16	piping pressure loss calculation	☒	☒	☒	☒
17	(Minimum data) calculation of relief area	☒	☐	☒	☐
18	Sizing regarding ISO / API - Norm	☒	☐	☒	☒
19	function stability check	☒	☐	☒	☒

ProSar is a web-based sizing tool to do quick sizing calculations regarding the ISO 4126-10 and the API 520 for one and two-phase flow (criteria 3 & 18 fulfilled). There is no dynamic tool for dynamic sizing calculations (criteria 2 not fulfilled). The chemical database is rather small and a selection of bursting discs from a manufacturers database is not possible (criteria 1 & 14, 15 not fulfilled).

Table 21: ProSar requirements evaluation – 2 of 3

	requirements for software evaluation	SuperChems	FlowNex	ChemCad	ProSar
20	understandable visualization of results	☒	☒	☒	☒
21	calculation of mass flow to be discharged	☒	☒	☒	☐
22	calculation of dischargeable mass flux (ideal nozzle)	☐	☐	☐	☐
23	calculation methods literature	☐	☒	☒	☐

The results are listed comprehensively in a sizing report (criteria 20 not fulfilled). The sizing calculation is based on the mass flow to be discharged which must be provided by the user (criteria 21 not fulfilled). Literature on calculation methods must be researched by the user since ProSar is a web-based calculation tool (criteria 23 not fulfilled).

Table 22: ProSar requirements evaluation – 3 of 3

	other requirements	SuperChems	FlowNex	ChemCad	ProSar
24	clearly arranged help section	☐	☒	☒	☐
25	well organized example scenarios	☐	☒	☒	☐
26	helpful support	☐	☒	☒	☒
27	user-friendly warnings (phase-change, under sizing, etc.)	☒	☒	☒	☐

The input needed to do the calculations is stated clearly so that there is no need for an extensive help section as well as example scenarios (criteria 24 & 25 not fulfilled). The support was always helpful (criteria 26 fulfilled). Warnings are stated in the sizing report or marked as red crosses.

6 Software application

This chapter describes the workflows of the various tools and the design scenario implementation with the use of screenshots. Basic sizing models are applied and analyzed.

6.1 SuperChems

The following section gives a brief introduction on how to set up steady state and dynamic relief scenarios in SuperChems.

6.1.1 SuperChems flow sheet API 520/ CCPS model implementation

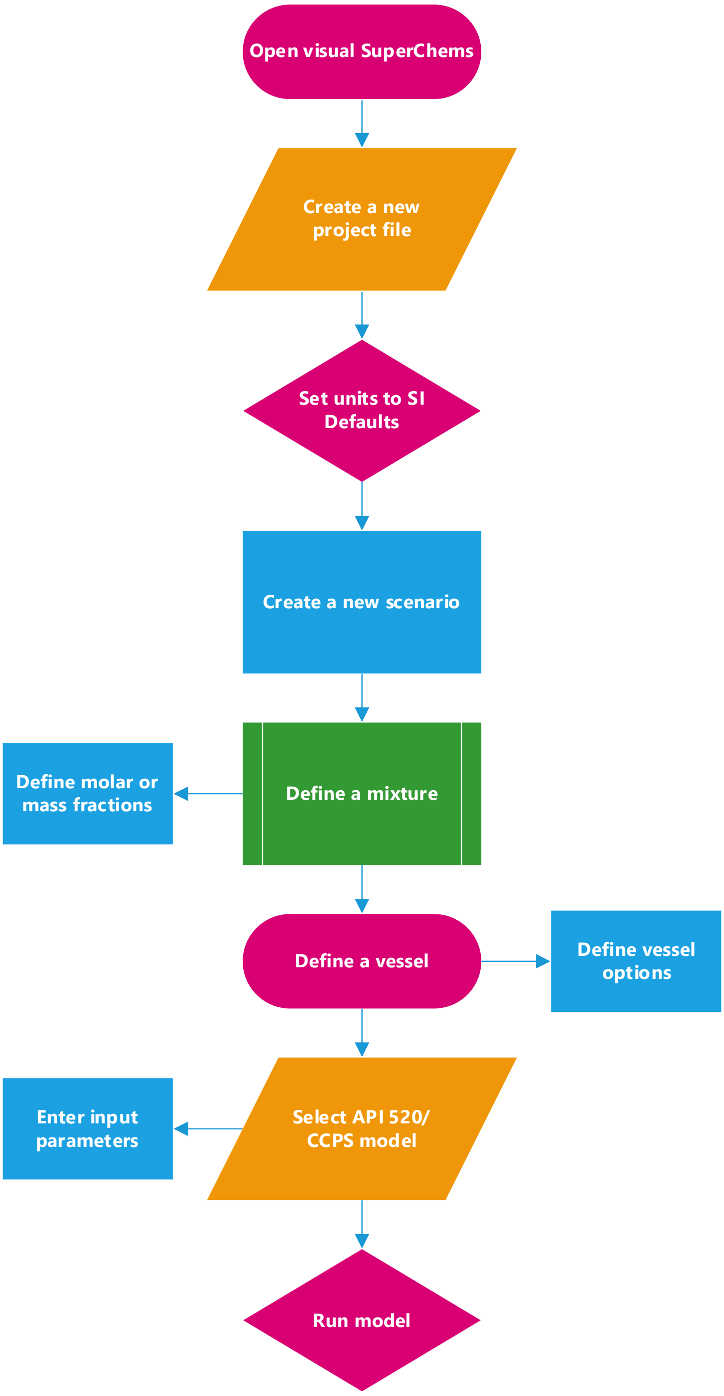


Figure 6: Flow sheet API 520/CCPS model implementation (own drawing)

6.1.2 SuperChems - API 520 / CCPS model

First, a new project is opened and named accordingly. A new scenario is defined and named under the “define – scenario” tab.

The first model to be run is the API 520/CCPS: Abnormal Heat Input. In this case, little information is needed. A mixture must be defined with all its components, which can be chosen from the SuperChems chemical database. Afterwards, mass or mole fractions are defined.

The next step is the equipment definition. A new vessel must be defined under the “define – equipment” tab. Important specification input information are design pressure of the vessel which is higher or at least equal to maximum allowed working pressure, design temperature which is higher or at least equal to the maximum allowed working temperature and normal operating pressure. More important input information are vessel type and geometry including length, inside diameter and liquid pool and grade bottom elevation, which describe the placement of the equipment over ground level. Under the “options” tab in the vessel menu, the external fire box must be checked to account for the external fire option. An external fire tab appears within the specification menu of the vessel. Here, the fire loading methodology must be defined. If the API-521 fire flux methodology is chosen, the liquid level inside the vessel is defined, and a mitigation factor (or environmental factor) is set according to the API 520 norm. SuperChems then calculates the fire flux and the wetted area. The wetted area factor recognizes that large vessels are less likely to be complete engulfed in and open fire than small vessels. A user defined input is also possible.

Afterwards, the model API 520/CCPS: Abnormal heat input can be chosen from the “models – flow and source terms” tab. Within the input section of the model, the relief device type (conventional PRV, balanced bellows PRV or rupture disc) and the heat source is chosen (external fire).

Next essential input information are the relief conditions consisting of initial temperature and initial pressure, set pressure of the relief device, backpressure, allowed percent of overpressure (in Europe 10%, for API fire case 21%) and the device discharge coefficient.

To calculate the required relief flow area, the user can choose the pure component method or the percentage of mass vaporized average method. In the pure component method, SuperChems decides which component will cause the most impact on the relief scenario and calculates the relief area based on solely this component. To do so, the model can be run after the input of the relief conditions.

To use the “% mass vaporized average method”, the “use latent heat at user defined vaporized liquid fraction” checkbox must be checked, and the fraction vaporized must be entered.

In both cases, SuperChems will return a required relief area as well as other output data (see Figure 7).

Output Data		
Latent heat is based on heat required to vaporize 0 % to 10 % of the liquid mass at the relief pressure		
Time required to reach relief pressure	0.0000	h
Average molecular weight	49.3068	
Temperature at maximum pressure	172.3227	°F
Compressibility factor	0.8701	
Density	0.1516	lb/gal
Heat of vaporization	317.4774	BTU/lb
Density correction factor	0.9661	
Correction factor vapor density	0.1516	lb/gal
Correction factor liquid density	4.4706	lb/gal
Evaporation/relief rate	6,463.2568	lb/h
Volumetric flow rate	48,619.3934	SCFH
Flow is critical (choked).		
Relief device orifice area	0.5001	in^2
Exit temperature	143.6530	°F
Exit pressure	64.7843	psig
Exit compressibility factor	0.9156	
Exit density	0.0884	lb/gal
Exit velocity	802.0087	ft/s
Backpressure correction factor	1.0000	
Next size up is G orifice (0.503 in2), 1.5x2.5 or 1.5x3 or 2x3		
Next size down is F orifice (0.307 in2), 1x2 or 1.5x2 or 1.5x2.5		
**NOTE: Actual flow area should be used for all inlet/outlet pressure loss estimates, piping reaction forces, etc.		

Figure 7: API 520/CCPS model output data

Note that in this model, no piping layout was defined. Only data on mixture, vessel, and model input is required. Once the output is created a second model, the “pipes: vapor” model, can be run. For this model, the output from the API/CCPS model can be imported or entered manually. The piping layout must be chosen according to the proposed relief piping which can be imported from other scenarios. Under the user flow options the “calculate maximum flow rate” or “specify user defined flow rate” can be selected. Afterwards, the model can be run, and results can be evaluated. Main parameters to be compared are mass flow rate of the relief piping layout, inlet pressure drop relative to effective set point and backpressure relative to effective setpoint. If the flow rate of the “pipes: vapor” model is higher than the evaporation/relief rate from the API 520/CCPS model, the PRV is sufficient.

6.1.3 SuperChems - External fire (dynamic method with minimum relief area)

For the dynamic method of the fire case a new design scenario must be defined and named accordingly. If the same mixture and equipment is used for the model, they can simply be selected by right-click on the respective tab. For the dynamic model with minimum relief area, a piping layout must be created consisting only of a PRV with the same flow area as obtained from the API 520 model.

Select the external fire case scenario and copy it using right-click. A new piping layout can be created under the “define – piping layout – new layout” tab. Define a new pressure relief device under the “define – piping layout – pressure relief valve” tab. Create a new PRV with the minimum relief area obtained from the API 520 model. Important input information are inlet and outlet pipe schedule as outputted from the API 520 / CCPS model.

Discharge coefficients under the flow section must be set for gas/vapor, liquid and two-phase. The composition of the two-phase flow will change over time; however, this is not accounted for by SuperChems. There is no option in SuperChems that calculates the discharge coefficient of two-phase flow based on composition and discharge coefficients from gas/vapor and liquid. Under the settings menu, a PRV can be chosen from a manufacturers database. Also, the flow area can be manually set. Set pressure and reset pressure must be defined.

The newly defined PRV can be selected in the top primary piping layout section. The new minimum area layout can be chosen here. A rupture disc is set as the default unit. The disc needs to be removed using the left arrow. From the available units list, the newly defined pressure relief valve can be selected using the right arrow. Within the primary piping layout menu, the thermodynamic flow path, and the nozzle flow method is being selected. The thermodynamic flow path is being calculated from the current condition to the final pressure with either a constant entropy (isentropic) or a constant enthalpy (isenthalpic). The nozzle flow method is being calculated either with the use of the specific work of an open system, where the volume changes with the rise of the temperature (VdP integral) or the change of enthalpy in the system (dH). There is an overview of the results of the different combinations of thermodynamic flow path and nozzle flow methods for a simple toluene relief example in the appendix in section 10.1.13.

After the piping layout definition, the model “dynamic vessel: two-phase” can be chosen using right-click on “models – flow and source term – dynamic vessel: two-phase”.

Within the model menu, the initial conditions must be set (temperature, pressure, and contents mass) and the expected fluid phase (one or two-phase) for the modelling is selected. Under relief piping path, the minimum area layout and the flow type is selected (vapor, two-phase, bubbly, churn turbulent or subcooled). For bubbly and churn turbulent flow, the DIERS coupling equation coefficient must be entered. In the time analysis menu, starting and final time can be set. The external fire exposure box under simulation options must be checked to account for the external fire option. Afterwards, the simulation can be started.

Output summary from the dynamic model can be viewed in Figure 8.

Vessel Options & Considerations

External fire exposure

Relief Piping

Vessel Connection	Relief Piping	Backpressure psig	Flow type
TOP: Primary Piping	PSV-2001 - MIN AREA LAYOUT	0	Churn turbulent

Overall Balance

		Initial	Final	Final - Initial
Time	h	0.0000	2.000	2.000
Temperature	°F	74.462	1,234	1,160
Pressure	psig	50.000	107.4	57.440
Vapor mass	lb	37.705	161.7	124.0
Vapor volume	gal	599.6	2,115	1,515
Liquid mass	lb	7,462	0.0000	-7,462
Liquid volume	gal	1,515	0.0000	-1,515
Total mass	lb	7,500	161.7	-7,338
Total volume	gal	2,115	2,115	-0.0200
Volume Full of Liquid	%	71.649	0.0000	-71.649

Design Boundaries

		Maximum	Time h	Point	
Pressure	psig	116.9	0.7920	271	1.17 x DESIGN P
dP/dt	psig/h	1,753	0.8040	290	
Temperature	°F	1,234	1.825	502	2.74 x DESIGN T
dT/dt	°F/h	11,787	0.8210	329	
Impulse	lbf	193.4	0.7920	271	
Fire heating input	BTU/hr	2.12404E+06	0.0000	0	

Composition Balance

		Initial Liquid	Final Liquid	Initial Vapor	Final Vapor	Initial Total	Final Total	Change Total
ETHANE	lb	354.8	0.0000	20.246	0.0000	375.0	0.0000	-375.0
n-BUTANE	lb	3,359	0.0000	15.794	6.226	3,375	6.226	-3,369
n-HEXANE	lb	3,748	0.0000	1.666	155.5	3,750	155.5	-3,594
Totals		7,462	0.0000	37.705	161.7	7,500	161.7	-7,338

Figure 8: dynamic vessel: two-phase model output data

Under the “results – flow” tab the first flow data and the flow at maximum pressure results can be seen. Under the “charts” tab in the result section, various charts can be created for mass flow, pressure and temperature history, phase envelopes and many more.

Flow or relief device opening time	h	0.7921	Data point 271	
Pressure	psig	116.9338		
Temperature	°F	319.5091		
Exit Pressure	psig	67.8078		
Exit Temperature	°F	297.4113		
Liquid flow rate	lb/h	0.0000		
Vapor flow rate	lb/h	17,860.0318		
First flow impulse	lbf	193.4338		
% irreversible inlet pressure loss (1st device)		0.0000		
% backpressure (1st device)		101,325.0000		
% irreversible inlet pressure loss (2nd device)		0.0000		
% backpressure (2nd device)		101,325.0000		
Chemical		Liquid	Vapor	Total
ETHANE	lb/h	0.0000	0.0177	0.0177
n-BUTANE	lb/h	0.0000	687.4452	687.4452
n-HEXANE	lb/h	0.0000	17,172.5690	17,172.5690

Figure 9: dynamic vessel: two-phase model output data at maximum pressure

6.1.4 SuperChems - External fire (dynamic method with actual piping layout)

For the full dynamic simulation, a relief piping path must be created using either MS Visio or the “define – piping layout” section of SuperChems. The piping segments are created with the information given, taking entrances, elbows, and bends into account. The inlet and outlet schedule for the relief valve needs to be the same as for to the pipe schedule. The relief valve can now be chosen from the manufacturers database. Set pressure and reset pressure must be entered.

Under the model menu, the “pipes: vapor” model is chosen. Here, the relief conditions can be either entered manually or can be imported from the API model using the toolbox – import flow data (first flow or maximum pressure flow from dynamic model). If the API/CCPS model was also run in this scenario, this output data can also be imported as a stream (import API/CCPS flow data).

Additionally, a second dynamic vessel model is run, taking the actual relief piping into account.

For a more detailed documentation on how to set up models in SuperChems including screenshots for a better understanding, see appendix section 9.1.

All kind of charts can easily be created within the “charts” tab in the dynamic vessel: two-phase results menu.

Figure 10 shows the venting history as mass flow rate in kg/s over time.

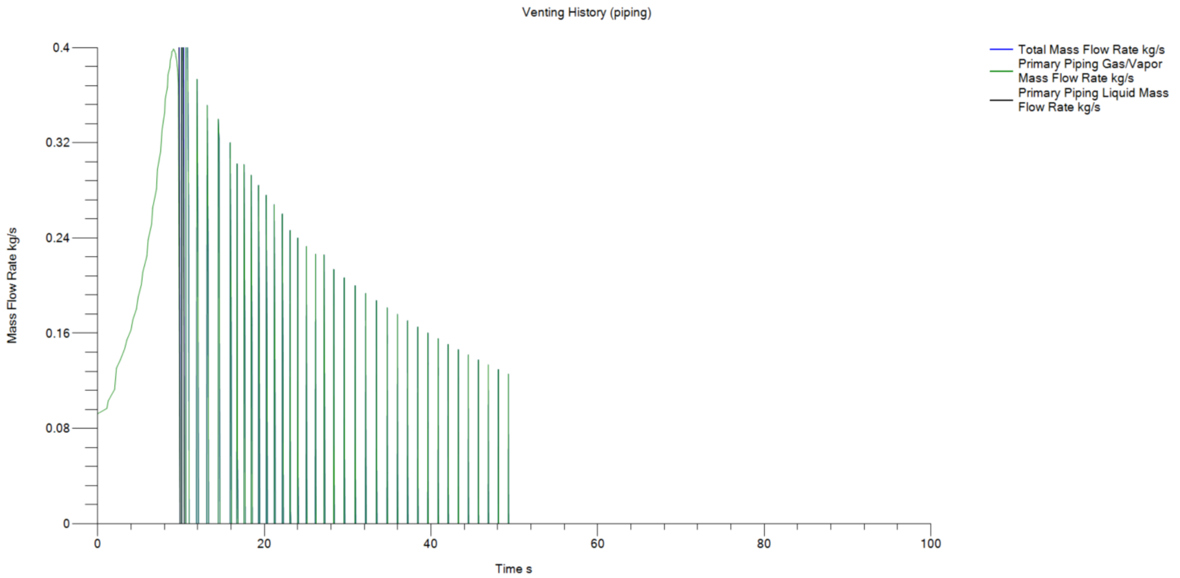


Figure 10: External fire – dynamic method venting history

Figure 11 shows the pressure history as pressure in bar(a) over time.

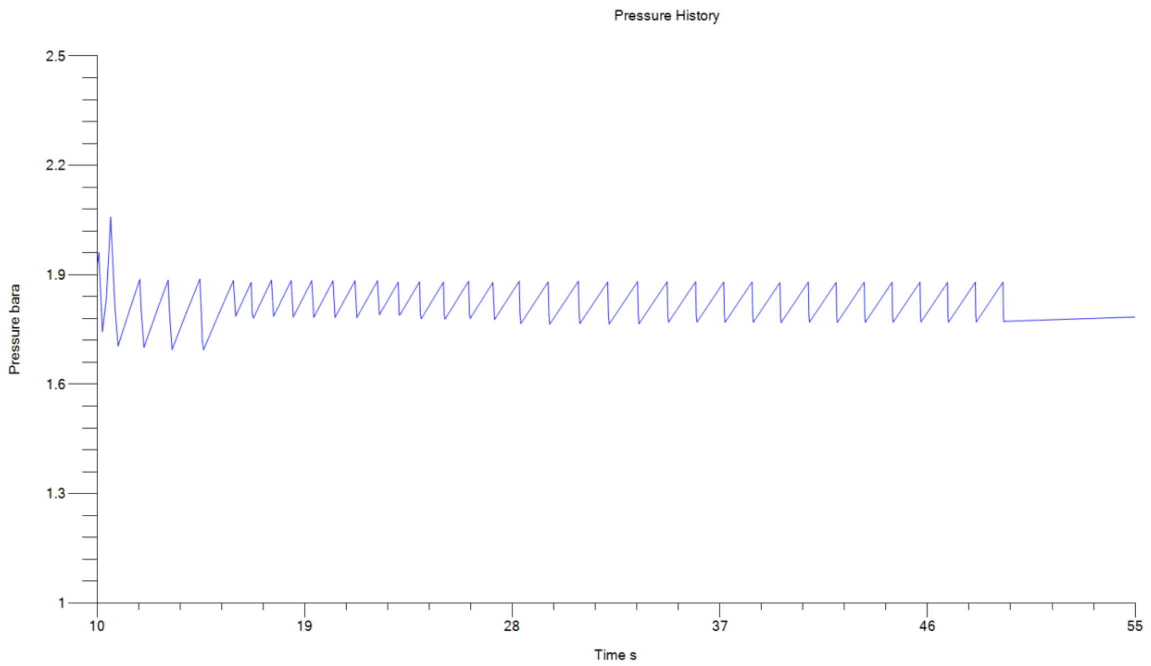


Figure 11: External fire - dynamic method pressure history

Figure 12 shows the pressure in bar(a) over the temperature in degree Celsius.

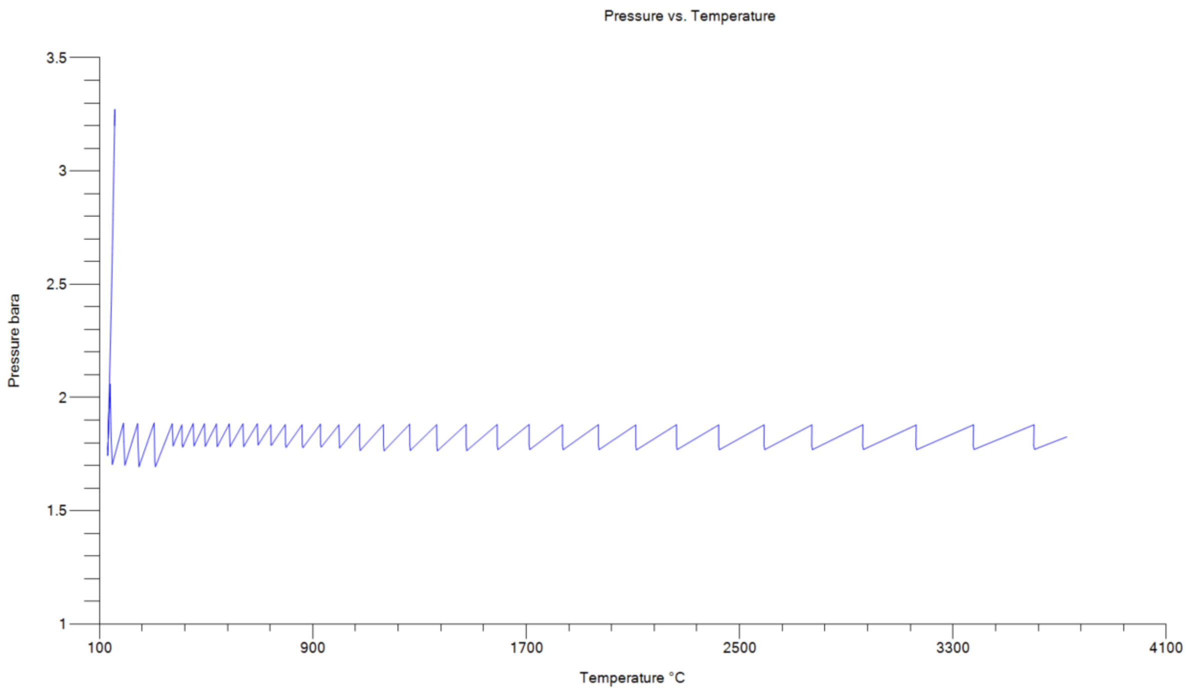


Figure 12: External fire - dynamic method P vs. T

Figure 13 shows the mass history of the vessel content in kg over time.

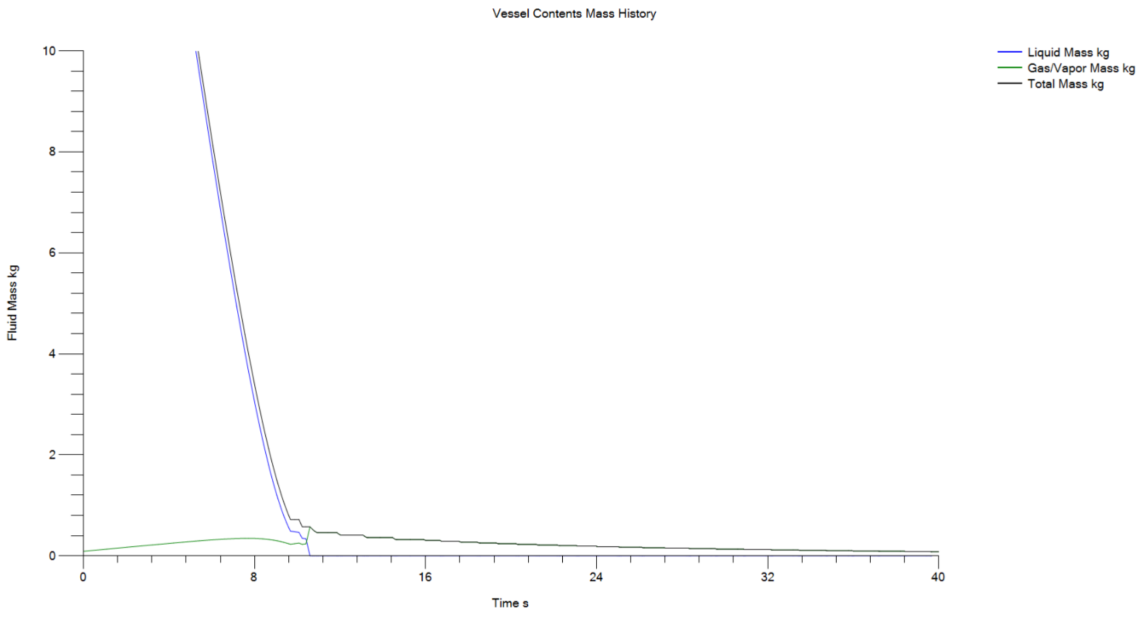


Figure 13: External fire - dynamic method vessel content mass history

6.1.5 SuperChems – Dynamic simulation conclusion

The output of the dynamic model in SuperChems is an overall balance as well as temperature and pressure rate at the highest-pressure point. During the dynamic simulation, SuperChems switches to the “classic” version, which can be confusing for the user. Dynamic simulation can take up to 30 minutes. In the results overview, the user can create various charts like pressure and temperature history, flow compositions and many more. Nevertheless, the data output is not dynamic. The user must wait for the program to finish the simulation and evaluate the results afterwards.

6.1.6 SuperChems – Validation of results for selected cases

For the calculation of the required relief device orifice area for the external fire case using SuperChems, one of TÜV SÜD's project data is implemented. Table 23 shows a summary of the input data provided by TÜV SÜD. For this calculation, toluene was used as a solvent for the fire case scenario.

Table 23: Reactor input data

Parameter		
Nominal volume	100	L
Maximum volume	143	L
Internal diameter	0.61	m
Heat Exchange Area	0.55	m^2
Heat transfer coefficient	1000	W/m^2*K
External surface (reactor)	0.81	m^2
MAWP	6	bar(a)
Insulation type	Rockwool	
Insulation thickness	50	mm

Table 24: Relief parameters

Parameter		
T_{set}	132	°C
T_{max}	192	°C
P_{set}	1.8	bar(a)
Discharge Coefficient (gas)	0.7	
Discharge Coefficient (liquid)	0.45	
Thermal power (q_{set})	6.76	kW
Type of flow	1	phase

The results for the relief system sizing calculation as provided by TÜV SÜD can be viewed in Table 255.

Table 25: Sizing results TÜV SÜD – external fire case

Parameter		
Discharge rate	0.02	kg/s
Mass flux / capacity	589	$kg/(m^2*s)$
Required relief area	0.47	cm^2
Required relief diameter	8	mm

6.1.6.1 SuperChems – External Fire Case scenario set up

For the external fire case calculations in SuperChems, first a new scenario must be defined and named accordingly. Also, toluene must be defined as the scenario's mixture.

Afterwards, the vessel geometry must be defined. Geometrical data is entered in the basic menu (Figure 14).

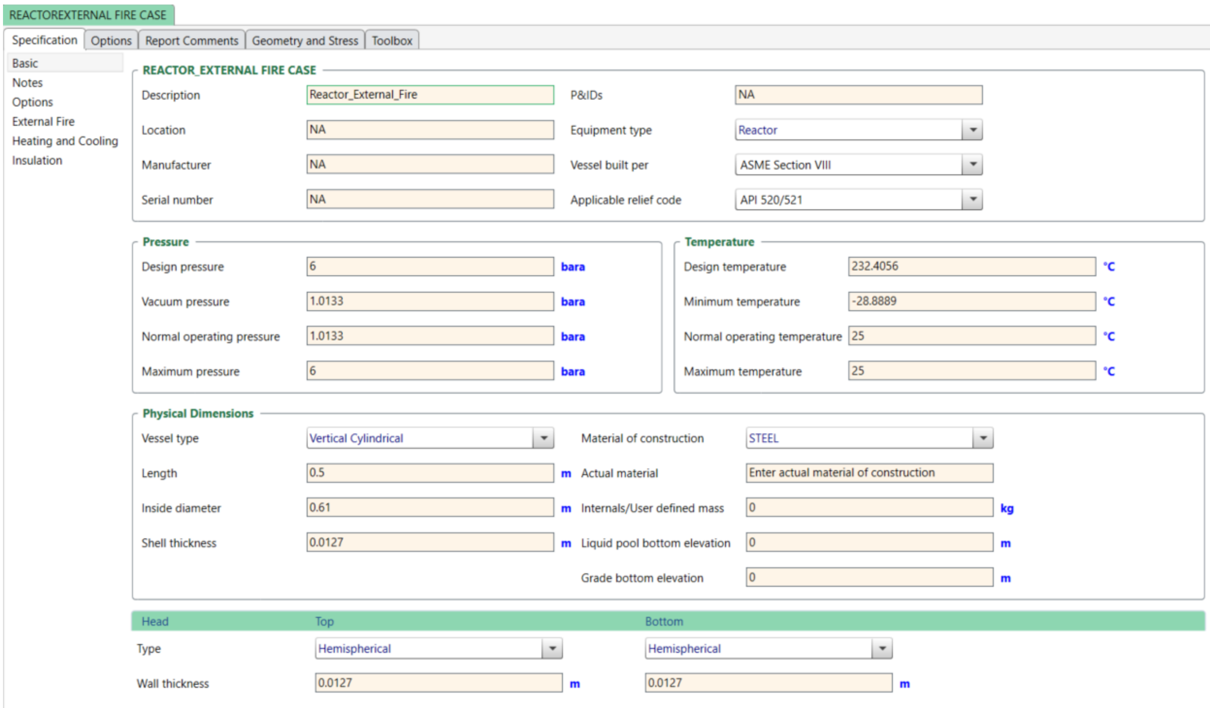


Figure 14: SuperChems vessel menu

To account for the external fire case, the external fire case checkbox under the options tab must be checked, and the fire methodology must be selected. The user-defined fire loading was selected in this scenario as Figure 15 shows.

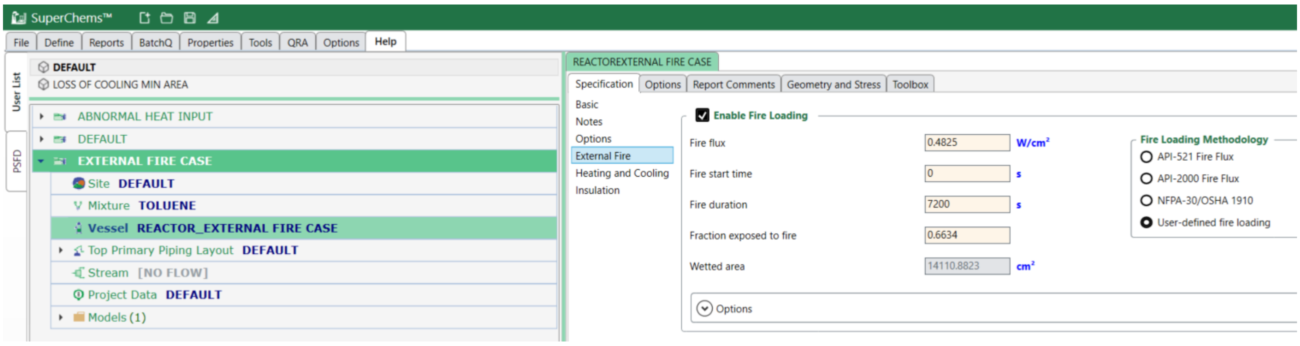


Figure 15: SuperChems External fire menu

After selecting the API 520/CCPS: Abnormal Heat Input model, the heat source “external fire” must be selected, and the relief conditions must be entered as shown in Figure 16

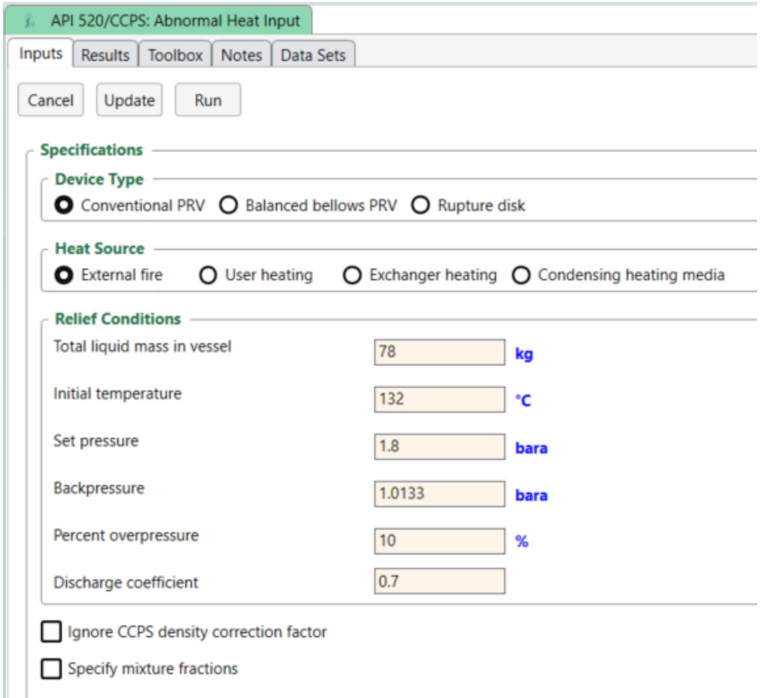


Figure 16: API 520/CCPS: Abnormal heat input model - external fire

6.1.6.2 SuperChems – External Fire Case output data

Input Data		
Liquid Density = Databank, Thermo = Equation of state		
Vessel is under fire exposure		
PRV is Conventional		
Determine relief flow area		
Average molecular weight	92.1405	
Total liquid mass in vessel	78.0000	kg
Initial vessel liquid temperature	132.0000	°C
Vessel wetted surface area	14,110.8823	cm^2
Additional wetted surface area	0.0000	cm^2
Heating load	6,808.5007	W
Set pressure	1.8000	bara
Backpressure	1.0133	bara
Percent overpressure	10.0000	%
Discharge coefficient	0.7000	

Figure 17: SuperChems Input data overview external fire case

The heat load is automatically calculated by SuperChems depending on the input information provided.

Output Data		
Relief requirement will be set by evaporation of TOLUENE		
Time required to reach Pset (lightest component)	45.2085	s
Average molecular weight	92.1405	
Temperature at maximum pressure	133.9118	°C
Compressibility factor	0.9465	
Density	5.4037	kg/m^3
Heat of vaporization	348,374.7412	J/kg
Density correction factor	0.9932	
Correction factor vapor density	5.1146	kg/m^3
Correction factor liquid density	754.0437	kg/m^3
Evaporation/relief rate	0.0194	kg/s
Volumetric flow rate	588.3344	SCFH
Flow is critical (choked).		
Relief device orifice area	0.4433	cm^2
Exit temperature	121.7388	°C
Exit pressure	1.1138	bara
Exit compressibility factor	0.9661	
Exit density	3.2354	kg/m^3
Exit velocity	193.3470	m/s
Backpressure correction factor	1.0000	
Next size up is D orifice (0.110 in2), 1x2 or 1.5x2 or 1.5x2.5		
Next size down is less than D orifice (0.11 in2) 1x2, 1.5x2, or 1.5x2.5		

Figure 18: SuperChems output data external fire case

The API 520/CCPS model does not give information about the flow regime. The SuperChems output data is compiled in Figure 18. A comparison of TÜV SÜD calculation and the SuperChems results are shown in Table 26.

Table 26: comparison of sizing results

Parameter	TÜV SÜD	SuperChems	
Discharge rate	0.02	0.019	kg/s
Required relief area	0.47	0.4433	cm^2

With small deviations, the results of the two calculation methods are comparable.

6.1.6.3 SuperChems – External Fire Case conclusion

The API 520/CCPS Abnormal Heat Input model – external fire case can be used as for quick calculations regarding the external fire, especially when the API fire flux methodology is used. The input data is equivalent to the API 520 norm. Output data can be reviewed in Figure 18. Most essential output data is the required relief area, the evaporation/relief rate, and the volumetric flow rate. Additional output information is the time to reach set pressure, temperature at maximum pressure as well as exit conditions. Information about the flow regime is not available – also forced two-phase flow calculations for the sizing of a pressure relief device under the external fire case using the API norm are not available.

6.1.7 SuperChems - Abnormal Heat Input

For the calculation of the required relief device orifice area for the maximum heating scenario using SuperChems, one of TÜV SÜD's project data is implemented. In this scenario, the used mixture and vessel are the same as in the external fire case scenario.

Table 27 shows a summary of the input data regarding the heating system as provided by TÜV SÜD. For this calculation, toluene was used as a solvent for the fire case scenario.

Table 27: Heating system data

Parameter		
Heat transfer coefficient	1000	W/m^2*K
Flow of heating medium	4.7	kg/s
heating medium temperature	189	°C

The results for TÜV SÜD's calculation method are listed in Table 28.

Table 28: Sizing results TÜV SÜD - maximum heating case

Parameter		
Discharge rate	0.09	kg/s
Mass flux / capacity	589	kg/(m2*s)
Required relief area	2.19	cm2
Required relief diameter	17	mm

6.1.7.1 SuperChems – Abnormal Heat Input scenario set up

To account for the heating and cooling, the required information must be entered in the vessel menu as shown in Figure 19.

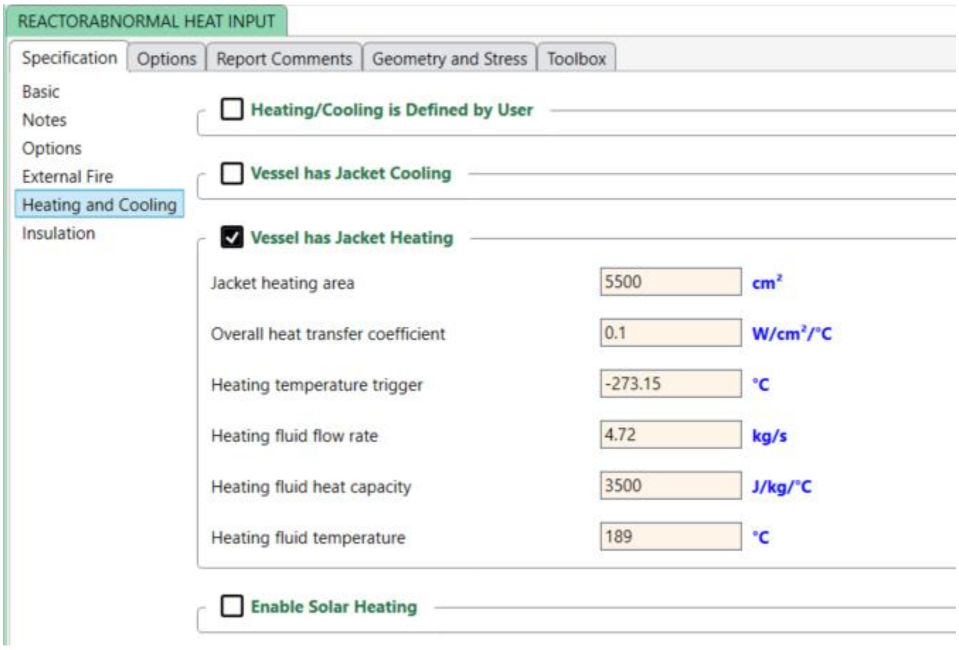


Figure 19: SuperChems heating and cooling menu

Also, the information given on insulation must be entered in the respective menu (Figure 20).

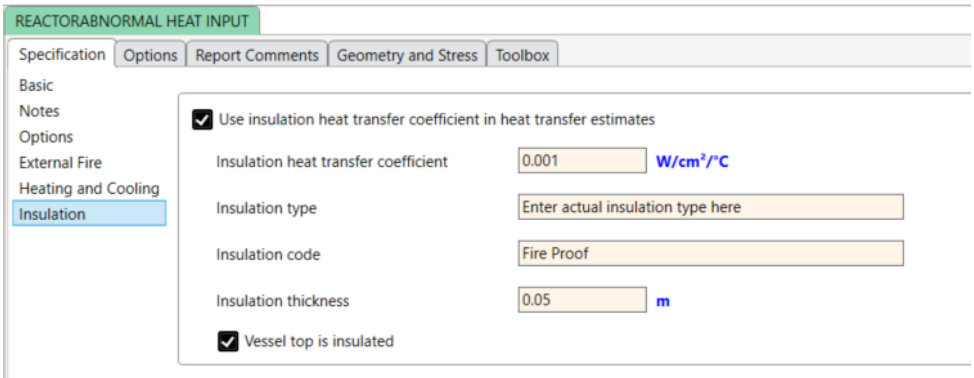


Figure 20: SuperChems insulation menu

To run the API 520/CCPS: Abnormal heat input model with the exchanger heating option, the respective model must be selected, and the input data must be entered.

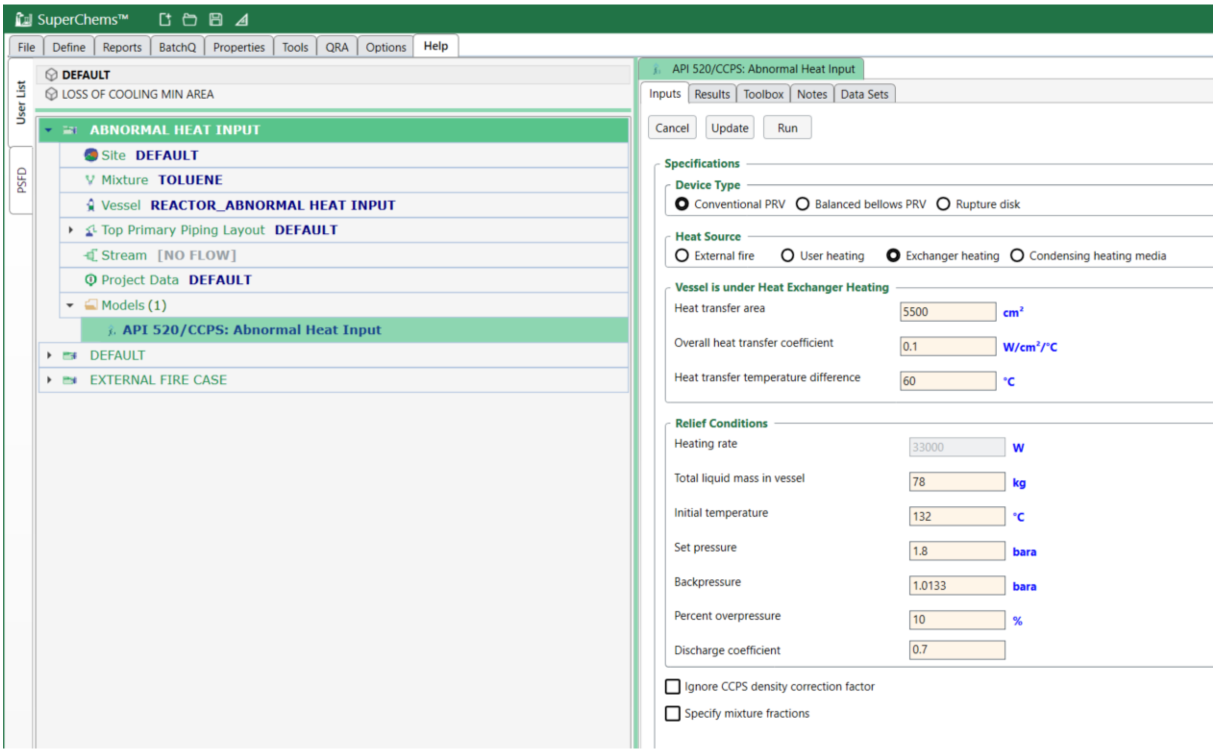


Figure 21: SuperChems API 520/CCPS model - exchanger heating

6.1.7.2 SuperChems – Abnormal Heat Input output data

The heating rate is automatically calculated by SuperChems with the input information provided in the vessel menu. The heat transfer temperature difference is the difference between T_{max} and T_{set}.

Input Data		
Liquid Density = Databank, Thermo = Equation of state		
Vessel is under heat exchanger heating		
PRV is Conventional		
Determine relief flow area		
Heat transfer area	5,500.0000	cm^2
Overall heat transfer coefficient	0.1000	$W/cm^2/°C$
Heat transfer temperature difference	60.0000	°C
Average molecular weight	92.1405	
Total liquid mass in vessel	78.0000	kg
Initial vessel liquid temperature	132.0000	°C
Vessel wetted surface area	14,110.8823	cm^2
Additional wetted surface area	0.0000	cm^2
Heating load	33,000.0000	W
Set pressure	1.8000	bara
Backpressure	1.0133	bara
Percent overpressure	10.0000	%
Discharge coefficient	0.7000	

Figure 22: SuperChems input data summary - API 520/CCPS: Abnormal Heat Input - exchanger heating

Output Data		
Relief requirement will be set by evaporation of TOLUENE		
Time required to reach Pset (lightest component)	9.3273	s
Average molecular weight	92.1405	
Temperature at maximum pressure	133.9118	°C
Compressibility factor	0.9465	
Density	5.4037	kg/m^3
Heat of vaporization	348,374.7412	J/kg
Density correction factor	0.9932	
Correction factor vapor density	5.1146	kg/m^3
Correction factor liquid density	754.0437	kg/m^3
Evaporation/relief rate	0.0941	kg/s
Volumetric flow rate	2,851.5872	SCFH
Flow is critical (choked).		
Relief device orifice area	2.1486	cm^2
Exit temperature	121.7388	°C
Exit pressure	1.1138	bara
Exit compressibility factor	0.9661	
Exit density	3.2354	kg/m^3
Exit velocity	193.3470	m/s
Backpressure correction factor	1.0000	
Next size up is G orifice (0.503 in2), 1.5x2.5 or 1.5x3 or 2x3		
Next size down is F orifice (0.307 in2), 1x2 or 1.5x2 or 1.5x2.5		

Figure 23: SuperChems output data summary - API 520/CCPS: Abnormal Heat Input - exchanger heating

Table 29 shows the results of the sizing calculation for each method. The results are comparable.

Table 29: comparison of sizing results

Parameter	TÜV SÜD		SuperChems	
Discharge rate	0.09	kg/s	0.0941	kg/s
Required relief area	2.19	cm^2	2.1486	cm^2

6.1.7.3 SuperChems – Abnormal Heat Input conclusion

To account for the maximum heating case, also the API 520/CCPS model is used in SuperChems. Again, the API 520/CCPS Abnormal Heat Input model gives no information about the flow regime and no forced two-phase flow calculations are available within this model. Since the same model is used, the output parameters are the same as in the external fire case.

6.1.8 SuperChems - Ideal Nozzle

The ideal nozzle model can be used to rate an existing ERS. To run the ideal nozzle model, first the mixture and vessel must be defined. Since the same mixture and vessel as in the previous cases are being used, these steps can be reviewed in the external fire case scenario.

6.1.8.1 SuperChems – Ideal Nozzle scenario set up

The required input information for the ideal nozzle model is shown in Figure 24.

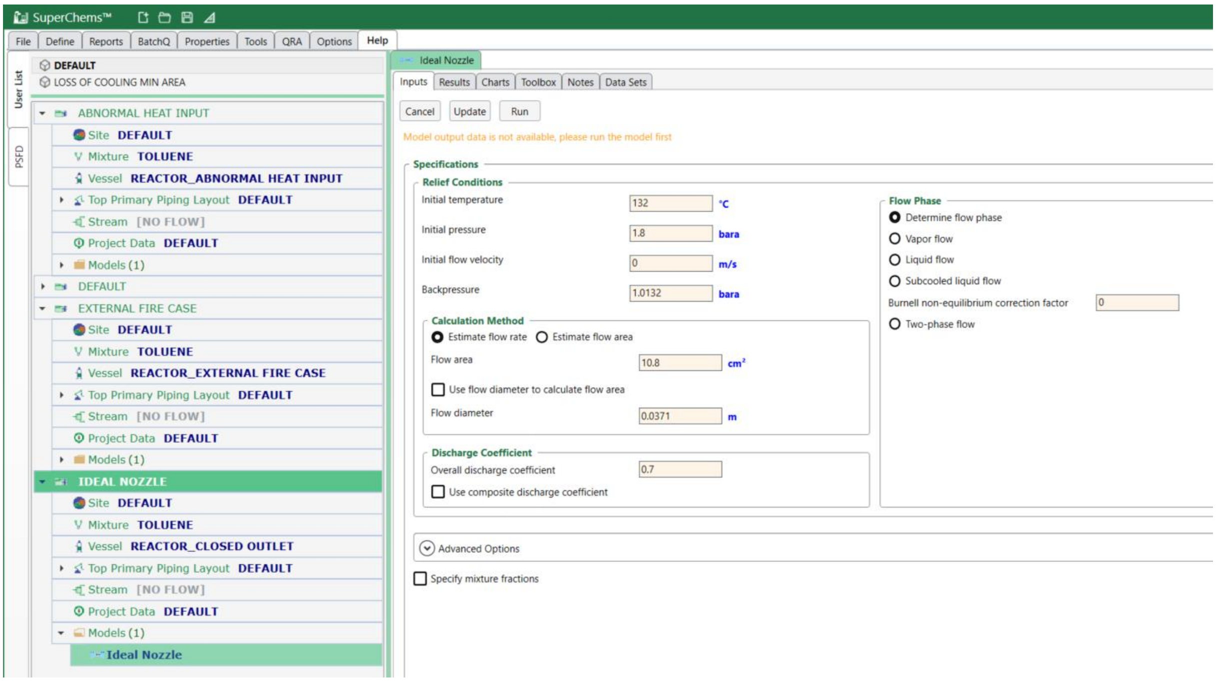


Figure 24: SuperChems Ideal Nozzle model input requirements

In the flow phase section, different flow regimes can be selected for the simulation. In this case, the determine flow case option is selected.

6.1.8.2 SuperChems – Ideal Nozzle output data

Input Data			
Liquid Density Method	Databank		
VLE/PVT Method	Equation of state		
Flow Method	Use VdP		
Initial State	Vapor		
Temperature	132.20	°C	
Pressure	1.80	bara	
Initial flow velocity	0.00	m/s	
Ambient pressure	1.01	bara	
Flow area	1.0800E+01	cm^2	
Flow diameter	3.7082E-02	m	
Overall discharge coefficient	0.70		
Output Data			
Final State	Vapor		
Discharge temperature	118.82	°C	
Discharge pressure	1.06	bara	Flow is Choked
Flow Pressure differential	0.74	bara	
Mass flow rate	0.45	kg/s	
Mass flux	0.06	$kg/cm^2/s$	
Velocity	191.61	m/s	
Density	3.090	kg/m^3	
V / F molar ratio	1.0000		
Flow impulse	199.91	N	
Reaction force	90.47	N	
rho*u*u	113,431.44	Pa	
Upstream sound power level	120.08	dB	
Upstream acoustic efficiency	0.01	%	Carucci and Mueller
Downstream sound power Level	119.15	dB	
Downstream acoustic efficiency	0.01	%	Carucci and Mueller

Figure 25: SuperChems Ideal Nozzle model output data

A summary of the SuperChems Ideal Nozzle model input and output data is shown in Figure 25. The output data gives information about discharge temperature and pressure, flow pressure differential as well as mass flow rate and mass flux. The mass flux rate can easily be compared with the results from TÜV SÜD's calculations as Table 30 shows.

Table 30: Comparison of mass flux

Parameter	TÜV SÜD		SuperChems	
Mass flux / capacity	589	$kg/(m^2*s)$	600	$kg/(m^2*s)$

6.1.8.3 SuperChems – Ideal Nozzle conclusion

The ideal nozzle model is easy to implement and generates important output data quickly. The model gives information about the flow regime as well as discharge conditions and the mass flux through the nozzle. Therefore, an existing ERS can easily be rated for suitability.

6.1.9 SuperChems - Loss of cooling

The loss of cooling model describes the relief need generated by an exothermal reaction once a cooling failure occurs. The implementation of reaction modelling in SuperChems can only be done using kinetic data.

6.1.9.1 SuperChems – Loss of cooling scenario set up

To implement a chemical reaction in SuperChems, the reactive modelling options must be selected in the main menu under the option tab as Figure 26 shows.

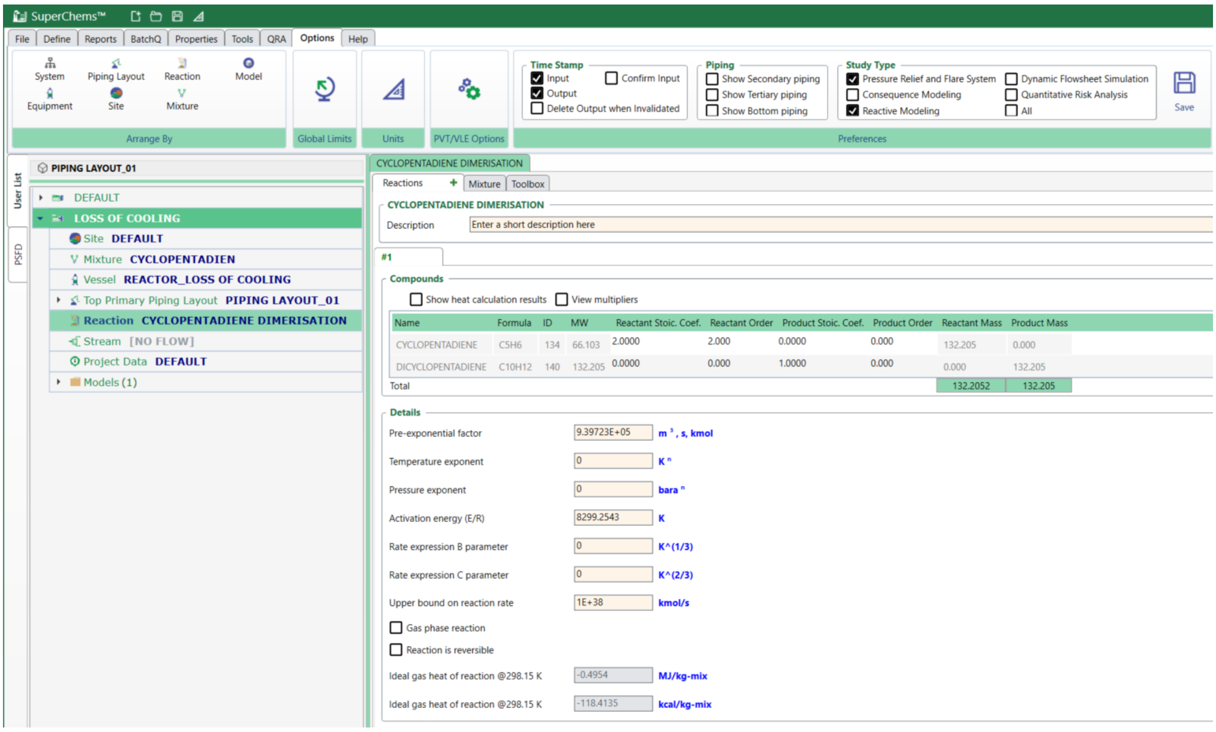


Figure 26: SuperChems reaction modelling menu

6.1.9.2 SuperChems – Loss of cooling conclusion

Reactive modelling in SuperChems is only possible using reaction kinetics. As Figure 26 shows, only very basic kinetic data can be entered. Kinetic data is available very rarely and if kinetic data is available, the kinetic models are of higher order and more complex than those used in SuperChems. The reaction shown above describes a dimerization of cyclopentadiene. The kinetic model behind this reaction cannot be implemented in SuperChems and therefore the results of the dynamic model are not usable. Furthermore, catalytic reaction forces cannot be considered in SuperChems. To be of use for TÜV SÜD, an implementation of VSP data is a must, which SuperChems does not support.

6.2 FlowNex

The following section describes briefly how to set up a flowsheet using FlowNex. Since FlowNex only meets a few software requirement criteria, there will be no detailed description for FlowNex.

6.2.1 FlowNex – Flow sheet creation and simulation

After starting the FlowNex software, the drawing page appears where the flowsheet will be created. Using the drag and drop option of FlowNex, all the process units are being dragged into the drawing page. The program connects most process units automatically, other must be connected using “nodes”. Every process must have boundary conditions (pressure and temperature at beginning/end).

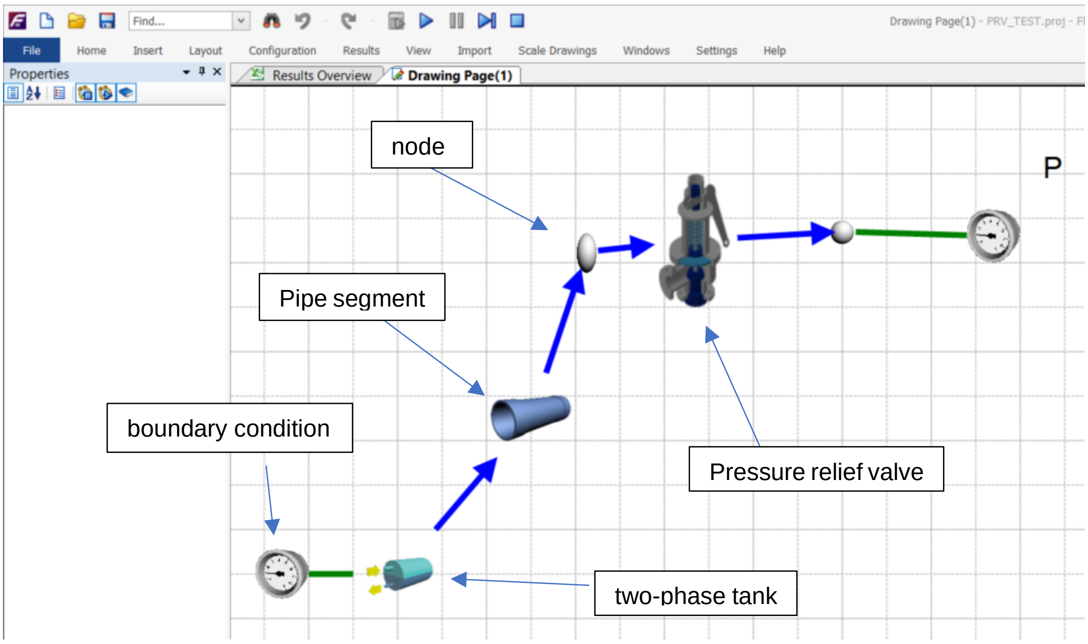


Figure 27: FlowNex flowsheet

Once the flowsheet is created a steady state calculation can be performed using the “solve steady state” button in the “home” menu. Dynamic simulations are being created in the “action” menu where the user defines a parameter that needs action and the respective action.

Action	Trig..	Stop T..	Target	Value	ValueType	
Abn. Heat	**0**	**Never**				
start of heat input	5	Never	{COMPONENT}Two Phase Tank - 24|:|{Heat Transfer}Heat input	60	CONSTANT	[kW]
inlet quality	0	Never	{COMPONENT}Boundary Condition - 20|:|{Boundary Conditions}Quality bou...	Not specified		
inlet pressure	0	Never	{COMPONENT}Boundary Condition - 20|:|{Boundary Conditions}Pressure bo...	Not specified		
stop of heat input	600	Never	{COMPONENT}Two Phase Tank - 24|:|{Heat Transfer}Heat input	0	CONSTANT	[kW]
outlet quality	0	Never	{COMPONENT}Boundary Condition - 21|:|{Boundary Conditions}Quality bou...	Not specified		

Figure 28: FlowNex "action menu"

Figure 28 shows the FlowNex action menu to simulate a relief scenario. In this example, the heat input of 60kW was chosen to be active from t = 5s to t= 600s. Also, the inlet pressure and quality were set to change over time (value is “not specified”). The heat input specified in the action menu shall simulate an external fire case with a heat load of 60kW. This is not a realistic value but was chosen to trigger a viewable reaction in FlowNex. The charts regarding this scenario can be viewed in Figure 29.

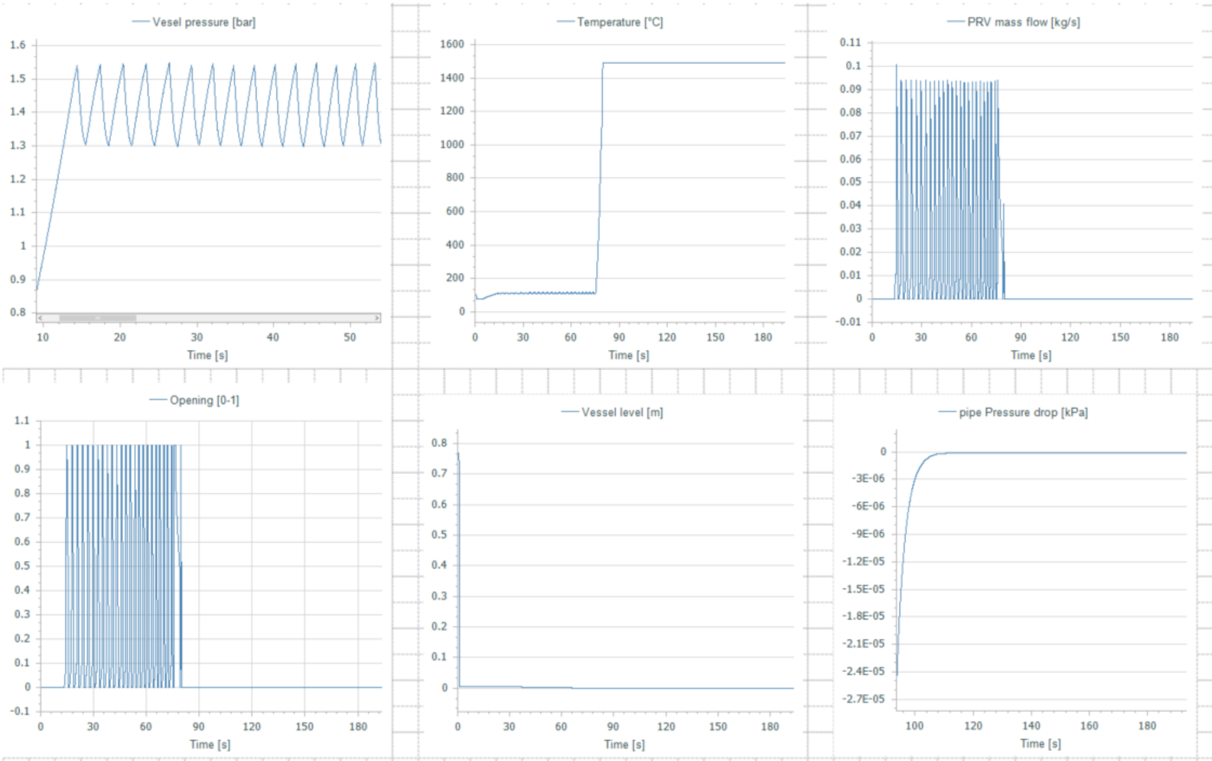


Figure 29: FlowNex dynamic charts

Dynamic charts can easily be created by clicking on the parameters to be plotted and dragging it into a line graph. The vessel pressure chart on the top left shows the pressure curve due to the external heating as specified in the action menu (Figure 29). After the set pressure is reached the valve opens and closes, once the pressure is below set pressure. Other charts show the vessel temperature (top middle), the mass flow through the opened pressure relief valve (top right), if the valve is open (bottom left), the liquid level inside the vessel (bottom middle) and the calculated pressure drop in the pipe (bottom right).

6.2.2 FlowNex – conclusion

FlowNex is not capable of doing steady state sizing calculations regarding the ISO or API norms since it was not invented to fulfill that purpose. Flowsheet creation can be done intuitively, and the creation of charts can be done by dragging the respective parameter into a line graph. This way diagrams can be easily created to visualize the simulation. FlowNex is a code-based simulation software than can be extended by the user. With deep programming knowledge, sizing calculation processes could be programmed and implemented in the software. In addition to a rather small chemical database, chemical runaway reactions cannot be simulated using FlowNex.

6.3 ChemCad / SafetyNet

The following section gives a brief introduction on how to set up steady state and dynamic relief scenarios in ChemCad.

6.3.1 ChemCad - Flow sheet relief device sizing

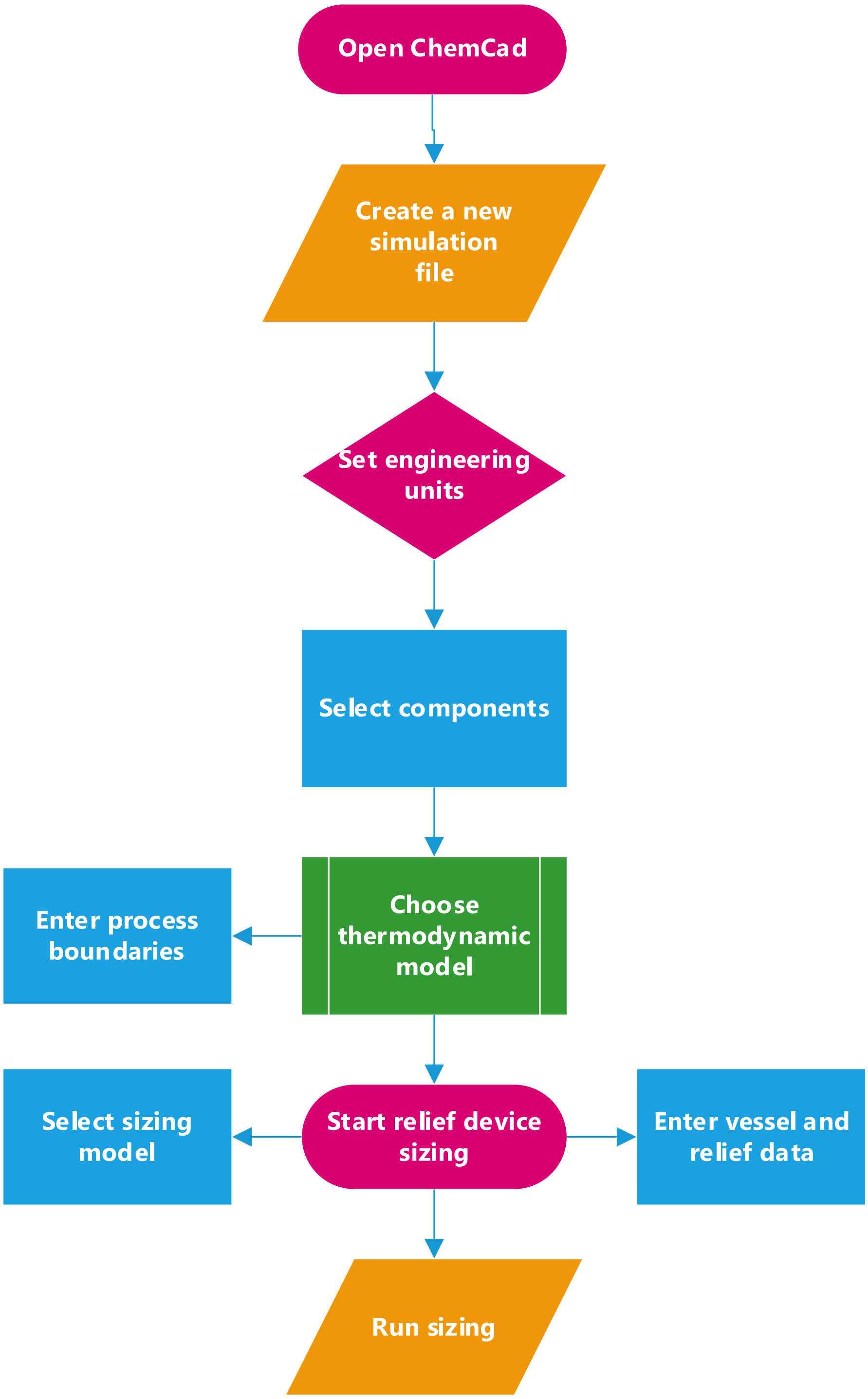


Figure 30: ChemCad flowsheet relief sizing model implementation

6.3.2 ChemCad – Basic sizing procedure

After opening the ChemCad program, the engineering units must be selected under the “home – engineering units” tab. It is possible to create a user specific profile. In this case, the units were adapted to fit TÜV SÜD’s project units. Units can also be changed into English units, common SI-units, formal SI-units or the metric units’ systems. Afterwards, the components must be selected under the “home – select components” tab. The components are selected from the ChemCad components database. Also, own databases can be created and used in ChemCad.

The next step is the selection of a thermodynamical model. ChemCad suggests a thermodynamical model based on minimum and maximum process temperature and pressure which are entered by the user. For single component systems, the thermodynamical model will be the ideal vapor model. The choice of a thermodynamical model for mixtures depends on binary interaction parameters (BIP). Depending on the BIPS available for the components, ChemCad normally chooses between the NRTL and the UNIFAC model. Detailed information about the NRTL and UNIFAC models can be reviewed in the literature. (Bruce E. Poling, 2000, p. 8.75)

After selecting the thermodynamical models, a feed and product stream must be created using the drag and drop option of ChemCad. By clicking on the “sizing” tab, the relief device sizing can be started by entering the vessel geometrical data and relief conditions. For a relief device sizing, the “use calculated size only” option must be selected for the calculation. In the next step, the sizing model must be chosen by selecting the design method (short cut or rigorous integral) and the latent heat option (average or rigorous values) as well as the vessel flow model (bubbly, churn-turbulent or homogenous). For a basic relief device sizing, the information provided is sufficient.

Additionally, piping information can be entered in the “inlet/outlet piping” section. By clicking on “ok” the sizing calculations are performed.

```
Relief Device Sizing for Stream 1

Device type: Relief valve
Valve type: Conventional valve
Vent model: HEM (Homogeneous Equilibrium Model)
Vessel model: Bubbly model
Design model: Specify heat rate
Specified heat rate:                      6.67 kJ/sec
Design, Pressure vessels.
Rigorous integral analysis used for design case.
Vertical vessel
Head type: Flat
Head K factor (dpth / R):                    0

Vessel dimensions:
Diameter:                                 0.61 m
Length (T to T):                          0.49 m
Vessel volume:                          0.1432 m3
Liquid level:                             0.34 m
Initial vapor volume fraction:         0.30612
Height above ground:                         0 m

Fluid properties:
Vapor mass:                            0.23631 kg
Liquid mass:                            75.026 kg
Vapor density:                          5.3907 kg/m3
Liquid density:                         755.07 kg/m3
Surface tension:                      0.015687 N/m
Liquid viscosity:                   0.00019485 N-s/m2
Vapor Z factor:                        0.94879
Cp/Cv:                                  1.0817
Vapor MW                                92.141
Liquid heat capacity:                   2.0968 kJ/kg-K
Latent heat:                            346.26 kJ/kg

Relief device analysis:
Set pressure:                              1.8 bar
Back pressure:                          1.0132 bar
% Overpressure                              10
Temperature:                            133.91 C
Discharge coefficient:                     0.7
C0 radial distribution parameter:          1.2
* Pb/Pmax > 0.5 for conventional valve.
Kb Backpressure corr. factor:          0.99337
Heat rate:                                6.67 kJ/sec
Vent area based on all vapor vent is used.

Calculated nozzle area:                0.44033 cm2
Rate based on area:                    0.44033 cm2
Calculated vent rate                  0.019244 kg/sec
Calc critical rate                    0.019244 kg/sec
Calc critical press                     1.1057 bar
Nozzle inlet vap. mass fraction:             1
Device inlet density:                   5.3907 kg/m3
Nozzle inlet vap. vol. fraction:             1
```

Figure 31: Basic sizing output data

Figure 31 shows the output data of the basic sizing procedure using a specified user heat input. The report summarizes all the input data and the calculated output data such as calculated nozzle area, calculated vent rate, critical rate and pressure, relief stream quality and density.

6.3.3 ChemCad – External fire (dynamic method)

For a dynamic simulation of the external fire case a flowsheet consisting of a dynamic vessel must be created. Using the drag and drop option of ChemCad, the dynamic vessel is placed on the drawing sheet. By right-clicking on the “dynamic vessel” symbol, a vertical dynamic vessel with relief valve can be chosen and dragged into the flowsheet. Also, one feed as well as three product streams must be created. One product stream represents the vapor outlet stream on top of the vessel, one stream represents the liquid outlet stream on the vessel bottom and the third and last stream represents the vent stream through the safety valve.

The feed and product streams are connected with the dynamic vessel by clicking on the red dot and dragging it to the blue dot on the vessel. The auto-hold function of ChemCad displays an anchor if the stream and the vessel are connected properly.

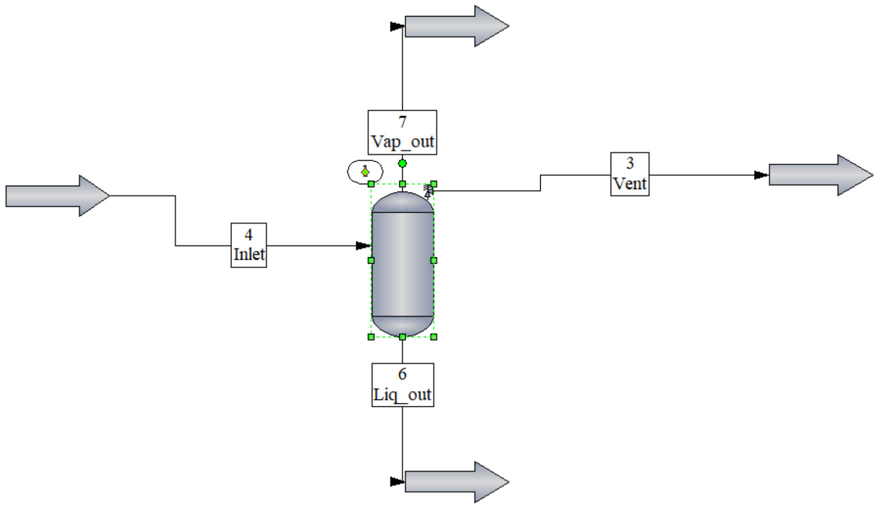


Figure 32: Flowsheet of the external fire case (dynamic method)

If a closed vessel shall be simulated, the outgoing streams for vapor and liquid are set to zero, so that no flow leaves the vessel. For the external fire case, the inlet and charge stream of the vessel must be specified. A stream is specified by temperature, pressure, and vapor fraction. Two of the named properties must be set to flash the missing property.

After selecting the dynamic option in ChemCad, the run time and the streams to be recorded must be specified for detailed dynamic stream tracking. Vessel and relief data must be inputted in the next step. By double-clicking on the vessel symbol in the workspace, the dynamic vessel menu opens and geometrical data as well as the vessel thermal mode must be entered. Also, output flow and relief device information obtained from the basic sizing procedure must be entered within the dynamic vessel menu. The dynamic simulation can now be run by clicking on the “run” button. Dynamic output data mainly consist of a pressure curve, but also other curves can be created within in the dynamic stream menu.

6.3.4 ChemCad – External fire (dynamic method) output data

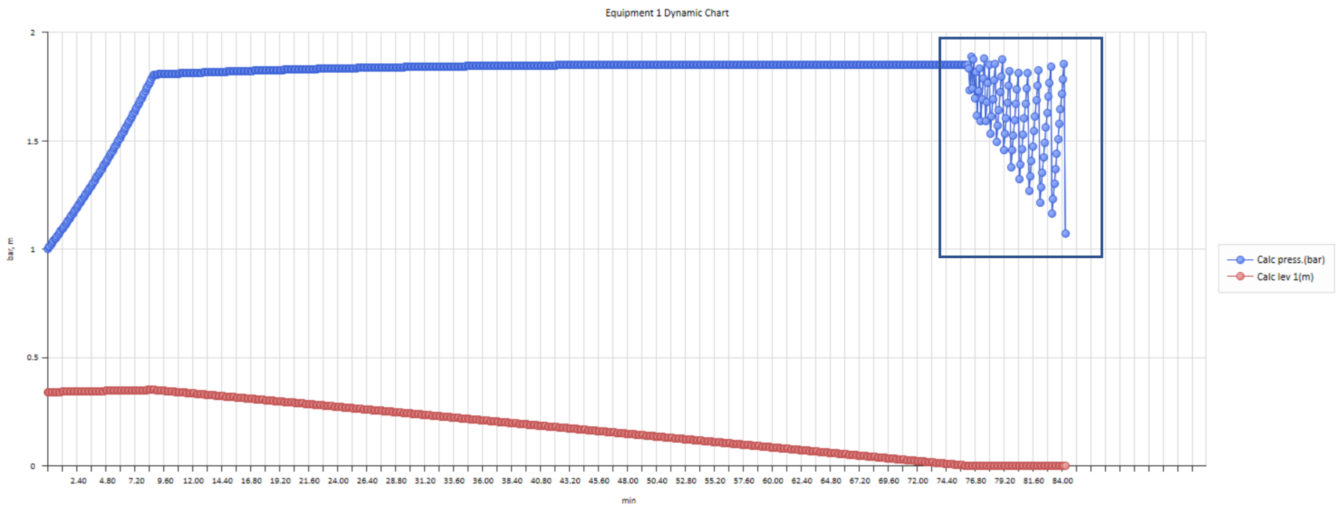


Figure 33: Dynamic sizing output data

Figure 33 shows the dynamically tracked pressure and level of the vessel during the relief scenario. The pressure rises due to the heat input until the set pressure (+10%) is reached. Afterwards, the relief valve opens and the level sinks due to the venting process (see box in Figure 33). Once the vessel level is almost empty, the valve opens and closes several times (see the end of the curve). After the vessel is completely empty, the valve stays closed, and the simulation stops.

Simulation: External Fire Case

STREAM PROPERTIES				
Stream No.	3	4	6	7
Name	Vent	Inlet	Liq_out	Vap_out
- - Overall - -				
Molar flow kmol/sec	0.0000	0.0000	0.0000	0.0000
Mass flow kg/sec	0.0000	0.0000	0.0000	0.0000
Temp C	8434.2715	**25.0000**	8433.5967	8433.5967
Pres bar	1.0130	**1.0130**	0.5264	0.5264
Vapor mole fraction	1.000	0.0000	0.0000	1.000
Enth kJ/sec	3.4686E-008	1.3204E-010	0.00000	7.9621E-010
Tc C	318.6400	318.6400	0.0000	318.6400
Pc bar	41.0800	41.0800	0.0000	41.0800
Std. sp gr. wtr = 1	0.872	0.872	0.000	0.872
Std. sp gr. air = 1	3.181	3.181	0.000	3.181
Degree API	30.8079	30.8079	0.0000	30.8079
Average mol wt	92.1410	92.1410	0.0000	92.1410
Actual dens kg/m3	0.1289	863.9382	0.0000	0.0670
Actual vol m3/h	0.0000	0.0000	0.0000	0.0000
Std liq m3/h	0.0000	0.0000	0.0000	0.0000
Std vap 0 C m3/h	0.0000	0.0000	0.0000	0.0000
- - Vapor only - -				
Molar flow kmol/sec	0.0000			0.0000
Mass flow kg/sec	0.0000			0.0000
Average mol wt	92.1410			92.1410
Actual dens kg/m3	0.1289			0.0670
Actual vol m3/h	0.0000			0.0000
Std liq m3/h	0.0000			0.0000
Std vap 0 C m3/h	0.0000			0.0000
Cp kJ/kg-K	3.7214			3.7214
Z factor	1.0000			1.0000
Visc N-s/m2	7.433e-005			7.433e-005
Th cond W/m-K	2.2601			2.2599
- - Liquid only - -				
Molar flow kmol/sec		0.0000	0.0000	
Mass flow kg/sec		0.0000	0.0000	
Average mol wt		92.1410		
Actual dens kg/m3		863.9382		
Actual vol m3/h		0.0000		
Std liq m3/h		0.0000		
Std vap 0 C m3/h		0.0000		
Cp kJ/kg-K		1.6979		
Z factor		0.0049		
Visc N-s/m2		0.0005543		
Th cond W/m-K		0.1323		
Surf. tens. N/m		0.0279		
Flow rates in kg/sec				
Toluene	0.0000	0.0000	0.0000	0.0000

Figure 34: Dynamic simulation stream properties - external fire case

In addition to the dynamic curve, ChemCad outputs a stream properties report of the individual streams (Figure 34).

6.3.5 ChemCad – Maximum heating case (dynamic method with piping)

This section gives an overview on how to set up a dynamic simulation in ChemCad. For a more detailed documentation including screenshots of every step, see appendix section 9.2.

For the simulation of the maximum heating case with the dynamic method in ChemCad, an additional utility stream must be created and connected to the existing flowsheet. Figure 35 shows the flowsheet for the maximum heating case (dynamic method) with the additional utility stream. To also account for pressure losses in the relief piping path, a vent piping was created within the flowsheet for the maximum heating case. The piping is being created using the drag and drop option of ChemCad. Bends and fittings are being added by double-clicking on the pipe segment. In the piping menu, the fittings can be added.

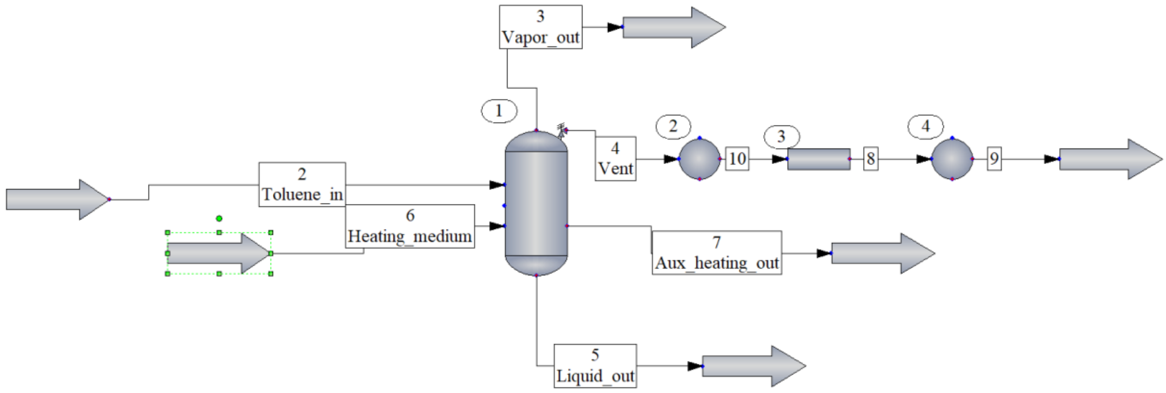


Figure 35: Flowsheet maximum heating case with utility steam (dynamic method)

The additional utility stream represents the heating medium. In this case, water is chosen as the heating medium and the temperature is set to fit the values provided by TÜV SÜD ($q_{max\ heating}$=31 kW). Afterwards, the vessels thermal mode must be changed to “flash with UA & utility” in the vessel menu and the values for heat transfer coefficient and area must be provided (see Table 23). Also, the relief device parameters must be adapted to the maximum heating case within the relief device tab in the dynamic vessel menu (relief device area must be changed to the respective value). Afterwards, the dynamic simulation can be run. For a more detailed documentation for the maximum heating case see appendix section 10.2.10.

6.3.6 ChemCad – Maximum heating case (dynamic method) output data

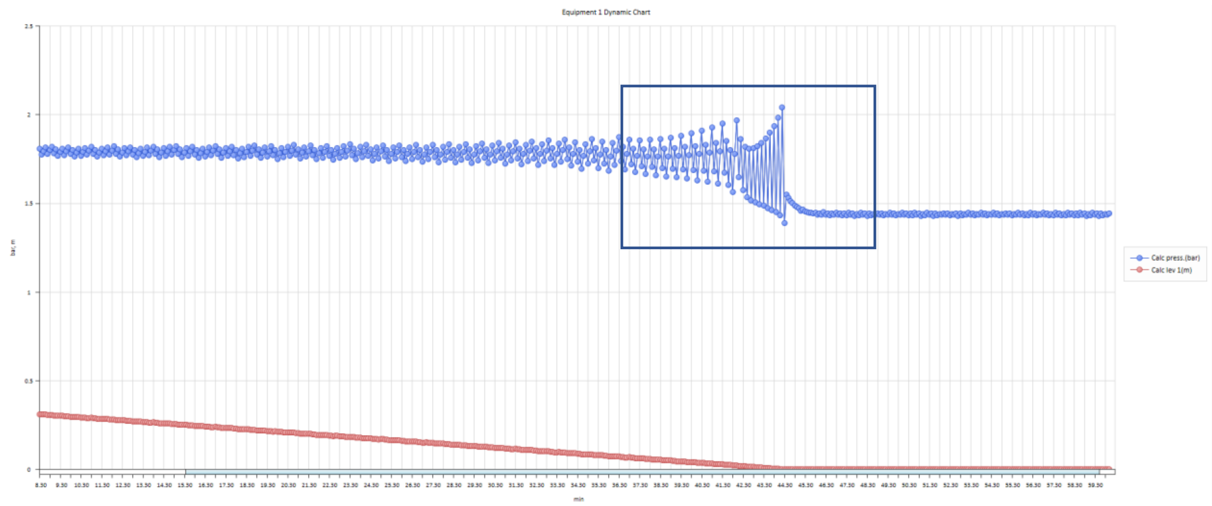


Figure 36: Maximum heating case pressure and level curve (dynamic method with piping)

The pressure rises due to the heat input caused by the heating medium. Once the set pressure is reached, the safety valve opens and the pressure decreases. Since there is still a heat input, the vessel pressure rises and the valve opens again. This happens until the vessel is completely empty as the box in the graph highlights.

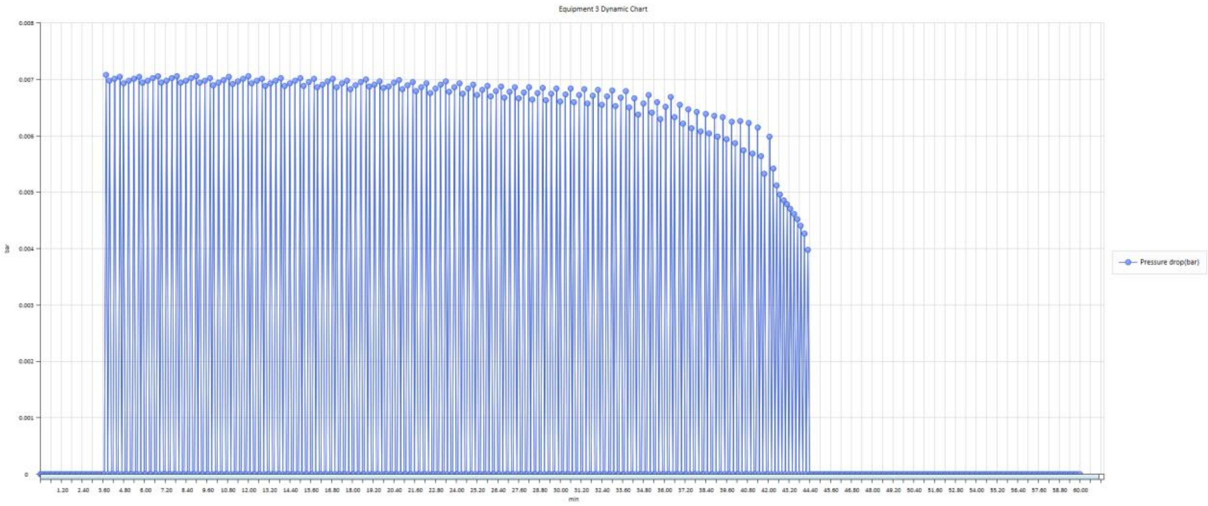


Figure 37: Maximum heating case pressure drop curve (dynamic method with piping)

Figure 37 shows the pressure loss of the relief piping path downstream of the safety valve. The alternating values for the pressure drop result from the opening and closing of the safety valve. Once the piping is created and the stream is being tracked, the pressure loss can easily be displayed in a curve. Also, all curves can be exported to MS Excel for further use.

6.3.7 ChemCad – Dynamic methods conclusion

Once the user knows its way around the software, ChemCad can be used to simulate any kind of process not limited to emergency relief sizing. Dynamic simulations can be visualized quite easily in the dynamic mode of ChemCad. The user decides what kind of streams or utilities shall be plotted. This way, an overload of plots can be avoided. Also, the curves to be plotted are created dynamically. This makes it possible for the user to evaluate the relief scenario during simulation.

6.3.8 ChemCad – External fire case (steady state)

To compare the different software used in this thesis, the same reactor data and relief parameters are used as listed in Table 23 and Table 24.

6.3.8.1 ChemCad – External fire case scenario set up

To simulate the external fire case in ChemCad, toluene is selected as the only compound. Afterwards, ChemCad automatically sets the thermodynamical model to the ideal vapor model and the enthalpy model is set to latent heat. A feed and product arrow must be created and connected with a stream using the drag and drop option of ChemCad. After clicking on the “relief device” sizing tab, vessel and relief device data must be entered as in Figure 38.

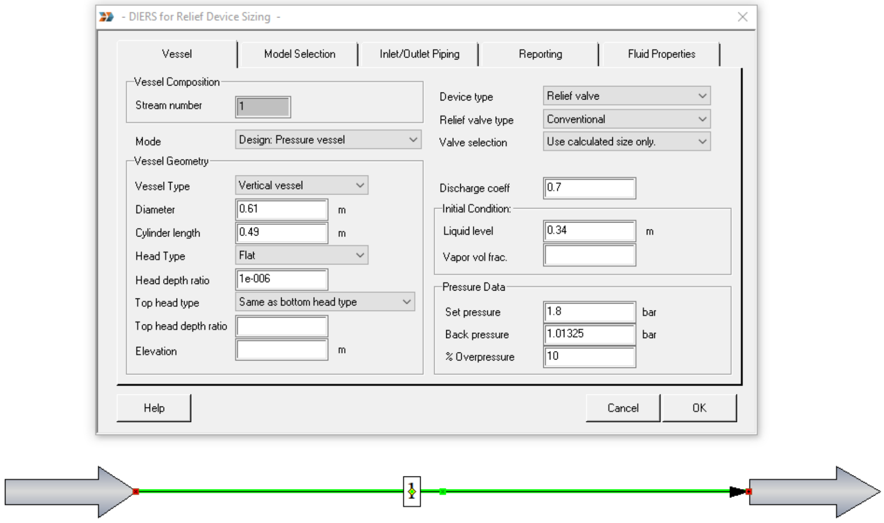


Figure 38: Relief device menu: vessel data

Under the “model selection” tab, the design method, latent heat option, vessel model, vent flow model and heat model are selected. For a quick sizing calculation, the “specify heat rate” heat model is chosen, and the respective heat rate is entered. In this case, the external fire heat rate is 6.67 kW as in Figure 39.

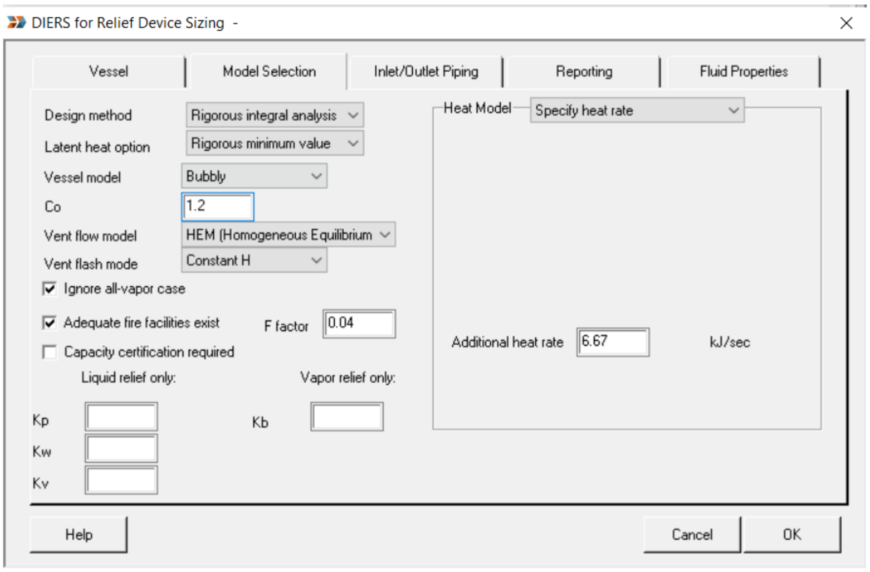


Figure 39: Relief device menu - model selection menu

Since no piping is involved in this step, the calculation can be run by clicking the “ok” button.

6.3.8.2 ChemCad – External fire case output data

ChemCad creates a sizing report as output with a summary of all the input and the calculated output information (Figure 40).

```
Relief Device Sizing for Stream 1

Device type: Relief valve
Valve type: Conventional valve
Vent model: HEM (Homogeneous Equilibrium Model)
Vessel model: Bubbly model
Design model: Specify heat rate
Specified heat rate:                        6.67 kJ/sec
Design, Pressure vessels.
Rigorous integral analysis used for design case.
Vertical vessel
Head type: Flat
Head K factor (dpth / R):                      0

Vessel dimensions:
Diameter:                                   0.61 m
Length (T to T):                            0.49 m
Vessel volume:                            0.1432 m3
Liquid level:                               0.34 m
Initial vapor volume fraction:           0.30612
Height above ground:                           0 m

Fluid properties:
Vapor mass:                              0.23631 kg
Liquid mass:                              75.026 kg
Vapor density:                            5.3907 kg/m3
Liquid density:                           755.07 kg/m3
Surface tension:                        0.015687 N/m
Liquid viscosity:                    0.00019485 N-s/m2
Vapor Z factor:                          0.94879
Cp/Cv:                                    1.0817
Vapor MW                                  92.141
Liquid heat capacity:                     2.0968 kJ/kg-K
Latent heat:                              346.26 kJ/kg

Relief device analysis:
Set pressure:                                1.8 bar
Back pressure:                            1.0132 bar
% Overpressure                                10
Temperature:                              133.91 C
Discharge coefficient:                       0.7
C0 radial distribution parameter:            1.2
* Pb/Pmax > 0.5 for conventional valve.
Kb Backpressure corr. factor:            0.99337
Heat rate:                                  6.67 kJ/sec
Vent area based on all vapor vent is used.

Calculated nozzle area:                  0.44033 cm2
Rate based on area:                      0.44033 cm2
Calculated vent rate                    0.019244 kg/sec
Calc critical rate                      0.019244 kg/sec
Calc critical press                       1.1057 bar
Nozzle inlet vap. mass fraction:               1
Device inlet density:                     5.3907 kg/m3
Nozzle inlet vap. vol. fraction:               1
```

Figure 40: ChemCad external fire output data

Furthermore, the compositions of the stream are being displayed in the output report.

Relief Device Outlet Compositions

Stream No.	10104	10105
Name	Total	Vapor
- - Overall - -		
Molar flow kmol/sec	0.0002	0.0002
Mass flow kg/sec	0.0192	0.0192
Temp C	131.6579	131.6579
Pres bar	1.0132	1.0132
Vapor mole fraction	1.000	1.000
Enth kJ/sec	13.152	13.152
Tc C	318.6400	318.6400
Pc bar	41.0800	41.0800
Std. sp gr. wtr = 1	0.872	0.872
Std. sp gr. air = 1	3.181	3.181
Degree API	30.8079	30.8079
Average mol wt	92.1410	92.1410
Actual dens kg/m3	2.8522	2.8522
Actual vol m3/h	24.2888	24.2888
Std liq m3/h	0.0795	0.0795
Std vap 0 C m3/h	16.8519	16.8519

Figure 41: Relief device outlet composition - external fire case

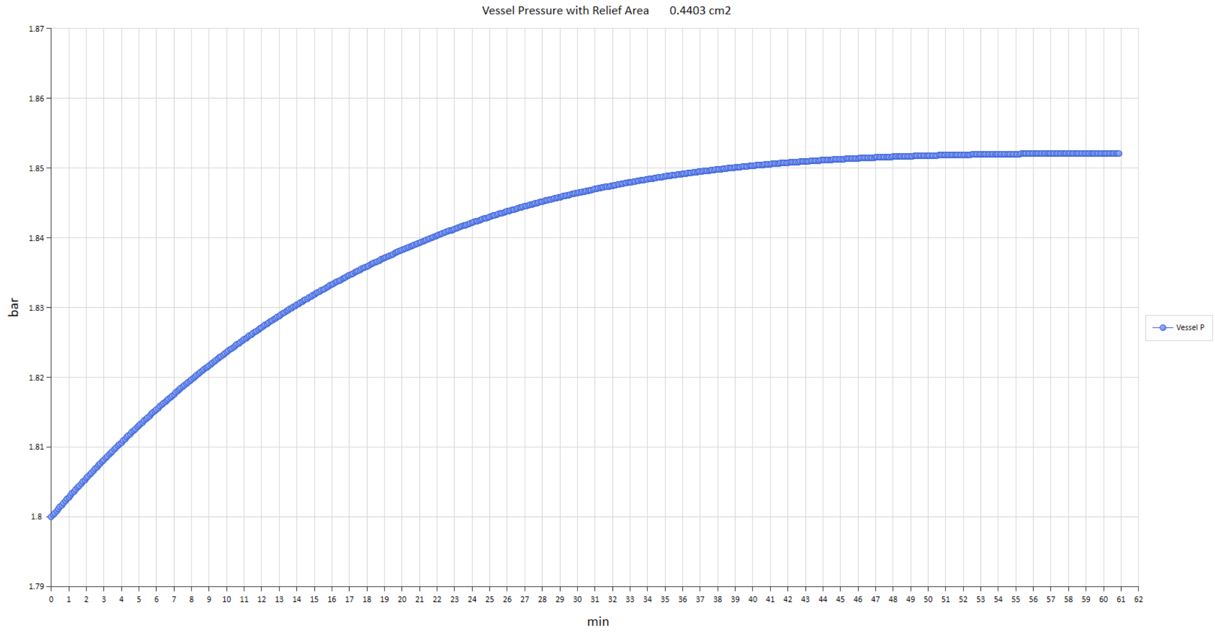


Figure 42: ChemCad external fire pressure curve output

Output data includes relief temperature, calculated nozzle area and vent rate, critical flow rate and pressure as well as device inlet density and relief device stream composition. Also, a pressure curve is being generated.

Table 31: comparison of sizing results – external fire case

Parameter	TÜV SÜD		ChemCad	
Discharge rate	0.02	kg/s	0.019244	kg/s
Required relief area	0.47	cm^2	0.44033	cm^2

With small deviations, the results are comparable to the results from TÜV SÜD.

6.3.8.3 ChemCad – External fire case conclusion

ChemCad is a capable of doing all sorts of process simulations and relief device sizing is only a small part of it. ChemCad is suitable to do quick sizing calculations with little program knowledge necessary. Nevertheless, not all the work can be done by the program. The heat rate must be calculated beforehand. If the heat rate is known, the calculation can be done quickly. The result layer is constructed simply and is easy to understand. Also, the results of the sizing calculation are equal (or at least very close) to the hand-calculations done by TÜV SÜD.

6.3.9 ChemCad – Maximum heating case (steady state)

To simulate the maximum heating case in steady state, the same input information is being entered in the respective menu. Only the heat rate and the vessel model are changed to the new value (in this example 31 kW) and the new vessel model (churn-turbulent).

6.3.9.1 ChemCad – Maximum heating case scenario set up

For the calculation of the relief area for the maximum heating case, a new feed and product arrow is created and connected with a stream using the drag and drop option of ChemCad. The steps for the external fire case are being repeated since the same vessel is used. The respective changes are being made under the “model selection” tab as seen in Figure 43.

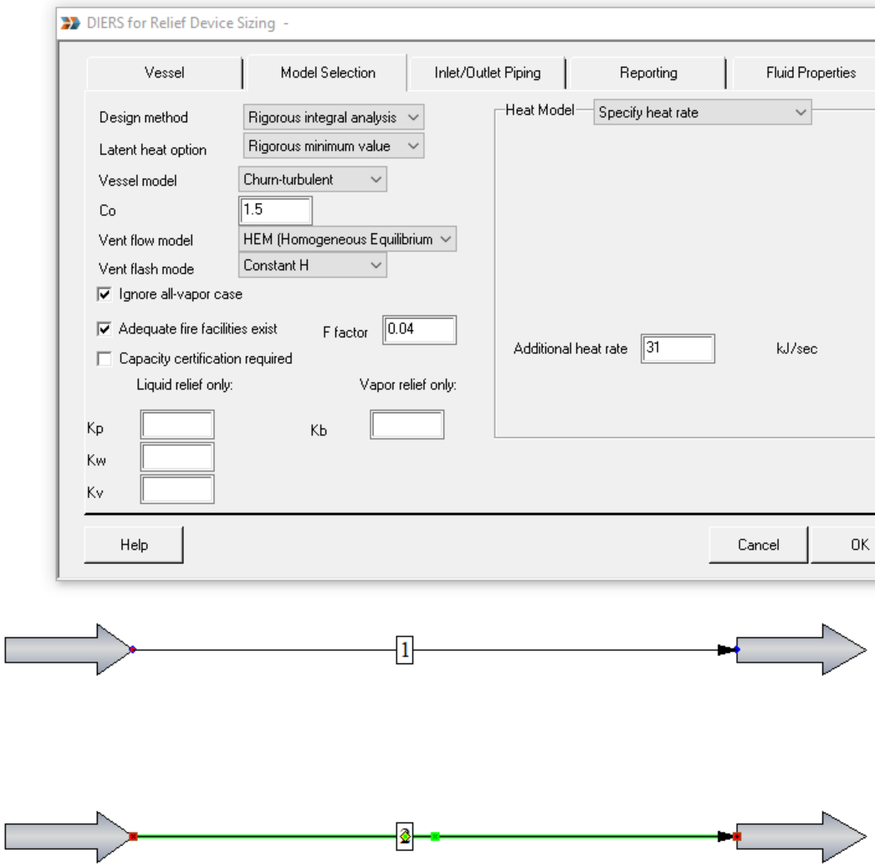


Figure 43: Maximum heating case - model selection menu

6.3.9.2 ChemCad – Maximum heating case output data

For every calculation, ChemCad creates a new report summarizing all the input and output information.

```
Relief Device Sizing for Stream 2

Device type: Relief valve
Valve type: Conventional valve
Vent model: HEM (Homogeneous Equilibrium Model)
Vessel model: Churn turbulent model
Design model: Specify heat rate
Specified heat rate:                          31 kJ/sec
Design, Pressure vessels.
Rigorous integral analysis used for design case.
Vertical vessel
Head type: Flat
Head K factor (dpth / R):                      0

Vessel dimensions:
Diameter:                                   0.61 m
Length (T to T):                            0.49 m
Vessel volume:                            0.1432 m3
Liquid level:                               0.34 m
Initial vapor volume fraction:           0.30612
Height above ground:                           0 m

Fluid properties:
Vapor mass:                              0.23631 kg
Liquid mass:                              75.026 kg
Vapor density:                            5.3907 kg/m3
Liquid density:                           755.07 kg/m3
Surface tension:                        0.015687 N/m
Liquid viscosity:                     0.00019485 N-s/m2
Vapor Z factor:                          0.94879
Cp/Cv:                                    1.0817
Vapor MW                                  92.141
Liquid heat capacity:                     2.0968 kJ/kg-K
Latent heat:                              346.26 kJ/kg

Relief device analysis:
Set pressure:                                1.8 bar
Back pressure:                            1.0132 bar
% Overpressure                                10
Temperature:                              133.91 C
Discharge coefficient:                       0.7
C0 radial distribution parameter:            1.5
* Pb/Pmax > 0.5 for conventional valve.
Kb Backpressure corr. factor:            0.99337
Heat rate:                                    31 kJ/sec
Vent area based on all vapor vent is used.

Calculated nozzle area:                   2.0465 cm2
Rate based on area:                       2.0465 cm2
Calculated vent rate                    0.089438 kg/sec
Calc critical rate                      0.089438 kg/sec
Calc critical press                       1.1057 bar
Nozzle inlet vap. mass fraction:               1
Device inlet density:                     5.3907 kg/m3
Nozzle inlet vap. vol. fraction:               1
```

Figure 44: Maximum heating case output data

Also, the relief device outlet stream composition is being displayed in the report.

Relief Device Outlet Compositions

Stream No.	10104	10105
Name	Total	Vapor
- - Overall - -		
Molar flow kmol/sec	0.0010	0.0010
Mass flow kg/sec	0.0894	0.0894
Temp C	131.6579	131.6579
Pres bar	1.0132	1.0132
Vapor mole fraction	1.000	1.000
Enth kJ/sec	61.125	61.125
Tc C	318.6400	318.6400
Pc bar	41.0800	41.0800
Std. sp gr. wtr = 1	0.872	0.872
Std. sp gr. air = 1	3.181	3.181
Degree API	30.8079	30.8079
Average mol wt	92.1410	92.1410
Actual dens kg/m3	2.8522	2.8522
Actual vol m3/h	112.8864	112.8864
Std liq m3/h	0.3693	0.3693
Std vap 0 C m3/h	78.3221	78.3221

Figure 45: relief device outlet composition - maximum heating case

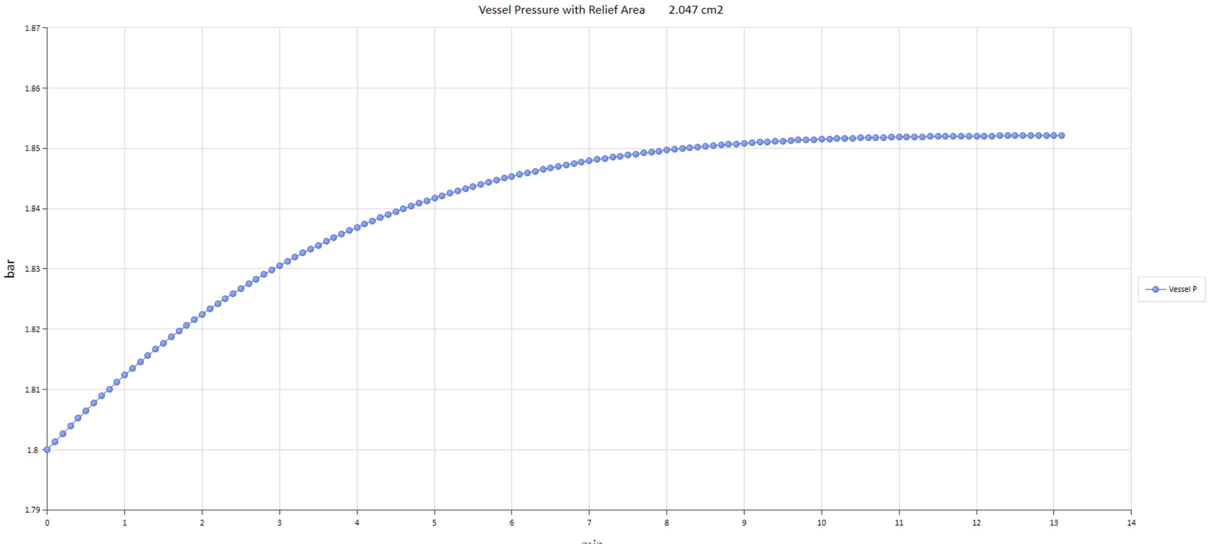


Figure 46: Maximum heating case pressure curve output

Table 32: comparison of sizing results - maximum heating case

Parameter	TÜV SÜD		ChemCad	
Discharge rate	0.09	kg/s	0.089438	kg/s
Required relief area	2.19	cm^2	2.0465	cm^2

As listed in Table 32, the results are comparable with only small deviations.

6.3.9.3 ChemCad – Maximum heating case conclusion

As in the external fire case simulation, not all the work can be done by ChemCad. The user must provide certain information. For example, the heat rate must be entered by the user. If all information needed is available, ChemCad provides a simple and fast way to do steady state sizing calculations for cases with a known heat rate. Maximum heating scenarios where heat exchange area and heat transfer coefficients shall be considered cannot be calculated in steady state. The creation of the dynamic flowsheet requires deeper software knowledge.

6.3.10 ChemCad – Adiabatic runaway reaction (steady state)

Within the steady state simulations, ChemCad also has a sizing option for an adiabatic runaway reaction. Only input information is the temperature increase rate at set pressure and at maximum pressure (p_{set}+10%). No additional reaction data is needed.

6.3.10.1 ChemCad – Adiabatic runaway reaction output data

```
Relief Device Sizing for Stream 1

Device type: Relief valve
Valve type: Balanced valve
Vent model: HEM (Homogeneous Equilibrium Model)
Vessel model: Homogeneous vessel model
Design model: Tempered runaway reaction
Design, Pressure vessels.
Vertical vessel
Head type: Flat
Head K factor (dpth / R):                     0

Vessel dimensions:
Diameter:                                  0.61 m
Length (T to T):                           0.49 m
Vessel volume:                           0.1432 m3
Liquid level:                              0.34 m
Initial vapor volume fraction:          0.30612
Height above ground:                          0 m

Fluid properties:
Vapor mass:                             0.77989 kg
Liquid mass:                             60.982 kg
Vapor density:                           17.791 kg/m3
Liquid density:                          613.73 kg/m3
Surface tension:                       0.008029 N/m
Liquid viscosity:                    0.00014938 N-s/m2
Vapor Z factor:                         0.87571
Cp/Cv:                                   1.1144
Vapor MW                                  80.76
Liquid heat capacity:                    2.6985 kJ/kg-K
Latent heat:                             360.96 kJ/kg

Relief device analysis:
Set pressure:                               1.8 bar
Back pressure:                           1.0132 bar
% Overpressure                              600
Temperature:                             133.38 C
Discharge coefficient:                    0.953
C0 radial distribution parameter:           1.5
Kb Backpressure corr. factor:                 1
dT/dt rate of T rise at Pset K/s:     0.0066667
dT/dt rate of T rise at P    K/s:         0.727
Length/Diameter of pipe:                      0

Calculated nozzle area:                 0.44987 cm2
Rate based on area:                     0.44987 cm2
Calculated vent rate                    0.18789 kg/sec
Calc critical rate                       0.1879 kg/sec
Calc critical press                      5.5638 bar
Nozzle inlet vap. mass fraction:       0.012627
Device inlet density:                     431.3 kg/m3
Nozzle inlet vap. vol. fraction:        0.30612
```

Figure 47: Adiabatic runaway output data

As for all basic sizing methods in ChemCad, the results can be seen in Figure 47 including calculated nozzle area, vent rate, critical pressure and critical rate, vapor quality and density. Furthermore, ChemCad outputs the relief device outlet compositions (Figure 48).

Relief Device Outlet Compositions

Stream No.	100	101	102
Name	Total	Vapor	Liquid
- - Overall - -			
Molar flow kmol/sec	0.0026	0.0012	0.0014
Mass flow kg/sec	0.1879	0.0951	0.0927
Temp C	65.4540	65.4540	65.4540
Pres bar	1.0132	1.0132	1.0132
Vapor mole fraction	0.4449	1.000	0.0000
Enth kJ/sec	-748.91	-318.50	-430.42
Tc C	232.0785	226.6430	237.6787
Pc bar	49.6162	43.1661	49.2221
Std. sp gr. wtr = 1	0.756	0.749	0.764
Std. sp gr. air = 1	2.490	2.834	2.214
Degree API	55.5469	57.3896	53.6565
Average mol wt	72.1167	82.0907	64.1241
Actual dens kg/m3	5.9959	3.0489	710.7956
Actual vol m3/h	112.8140	112.3442	0.4697
Std liq m3/h	0.8942	0.4572	0.4369
Std vap 0 C m3/h	210.2300	93.5221	116.7080

Figure 48: Adiabatic runaway relief device outlet compositions

6.3.10.2 ChemCad – Adiabatic runaway reaction conclusion

The sizing calculations done by TÜV SÜD are done with the temperature increase rate at maximum allowed working pressure (and not at set pressure). To compare the results with those from the adiabatic runaway reaction in ChemCad, the values from TÜV SÜD must be recalculated at set pressure. Since no further information about the chemical reaction is needed, the results are not quite descriptive for the case. There is no additional fire simulation possible within the adiabatic runaway reaction sizing and the heat rate used for calculation is not visible in the results report. Also, the size of the relief area does not change for different flow models.

6.4 ProSar

6.4.1 ProSar – Safety valve sizing

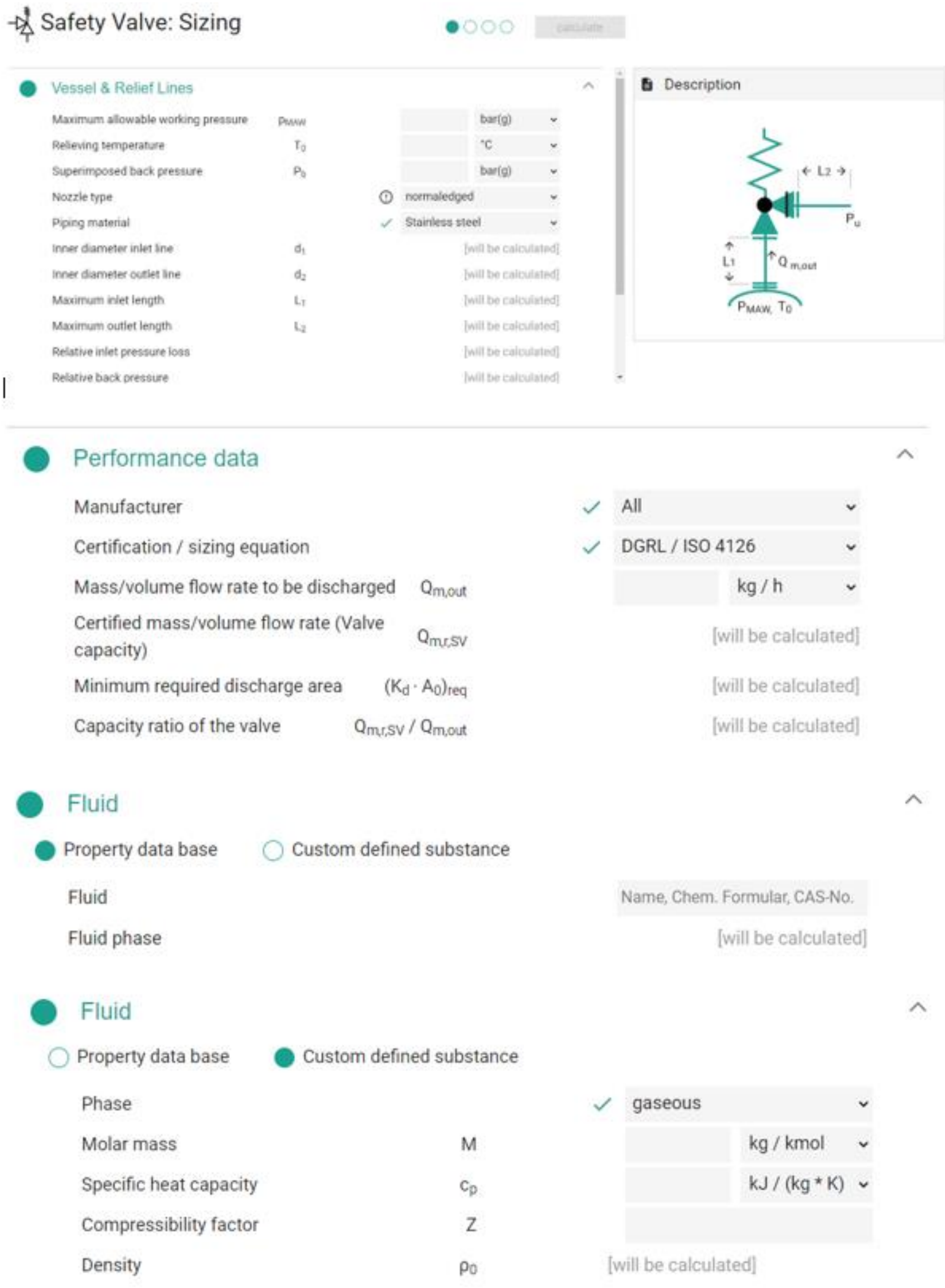


Figure 49: ProSar input menu

To do sizing calculations using ProSar, the user must provide data on the vessel and relief line, the norm that shall be used for sizing, the mass flow to be discharged as well as the fluid definition.

6.4.2 ProSar – Safety valve sizing output data

Sizing Input Data

Calculation standard			ISO 4126
Relieving temperature	T_0	132	C
Maximum allowable working pressure	p_{MAW}	0.8	bar(g)
Massflow	$Q_{m,out}$	0.019	kg/s
Piping material			Stainless steel
Superimposed back pressure	p_b	0	bar(g)

Safety Valve (Type)

Valve series	GOETZE	461	
Nominal diameter (inlet - outlet)	DIN flange	DN15	DN15
Nominal pressure (inlet - outlet)	DIN flange	PN100	PN100

Safety Valve (Process)

Set pressure	p_{set}	0.8	bar(g)
Discharge pressure	p_0	0.88	bar(g)
Back pressure valve outlet	p_{bb}	0.12	bar(g)
Pressure at end of outlet line	$p_{u,e}$	0	bar(g)
Pressure ratio	p_b/p_0	0.53513	
Capacity ratio of the valve	$Q_{m,r,SV}$ / $Q_{m,out}$	126.6	%
Effective discharge area required	$(K_d \cdot A_0)_{req}$	38.3	mm²
Discharge area chosen	A_0	78.5	mm²
Seat diameter	d_0	10	mm
Discharge capacity (pressure loss calculation)	$Q_{m,r,SV}$	0.025	kg/s
Dischargeable massflow	$Q_{m,SV}$	0.027	kg/s
Certified discharge coefficient liquid (valve)	$K_{dr,l}$	0.47	
Certified discharge coefficient gaseous (valve)	$K_{dr,g}$	0.71	

Figure 50: ProSar valve sizing report

ProSar generates a sizing report consisting of an overview of the input data, the safety valve type and detailed safety valve parameters. Furthermore, the report consists of corrected discharge coefficients, important fluid properties, geometrical data regarding the vessel and relief line as well as comments on critical flow.

Corrected discharge coefficient

Certified discharge coefficient	K_{dr}	0.618	
Discharge coefficient	K_d	0.687	
Back pressure dependency (gas) considered			Yes

Fluid properties (discharge conditions)

Name			Acetone
CAS registry number			67-64-1
Fluid phase			gaseous
Molecular mass	M	0.05808	kg/mol
Isentropic exponent	κ	1.119	
Real gas factor	Z	0.962	
Density	ρ_0	3.393	kg/m³
Reduced pressure	p_{red}	0.04028	
Reduced temperature	T_{red}	0.79738	

Vessel & Relief Lines

Nozzle type			normal edged
Inner diameter inlet	d_1	0.0173	m
Inlet length	L_1	0.6	m
Relative inlet pressure loss		3	%
Minor loss coefficient inlet line	ζ_1	1.15886	
Inner diameter outlet	d_2	0.0173	m
Outlet length	L_2	2.7	m
Relative back pressure		15	%
Minor loss coefficient outlet line	ζ_2	4.37176	
Sound power level	P_{WL}	59.28823	dB
Reaction force	F	4.59353	N

Details

Critical flow safety valve	No
Critical flow at end of outlet line	No
Recommendation: heating	No
Recommendation: bellow	No
Recommendation: friction damper	No

Figure 51: ProSar valve sizing report

6.4.3 ProSar – Safety valve sizing conclusion

With ProSar the Center of Safety Excellence provides a fast-sizing tool once the mass flow to be discharged is known. The calculation of the mass flow is an essential and elaborate part of the sizing-process and must be done by the software to be of value for TÜV SÜD.

7 Discussion

7.1 Overview

According to the outcome of this thesis, the perfect software to satisfy all TÜV SÜD's needs does not exist – yet. Before applying all software, SuperChems seemed to be the top player. But drawbacks in the isometric drawings of relief lines and non-existing European valve manufacturer databases as well as European sizing norms gave another impression. Furthermore, SuperChems requires some dedication from the user to be able to fully handle the program since there was no satisfying support for SuperChems.

FlowNex provides a great range of simulation opportunities and with the help of the support, there was a (more or less complex) solution for most problems. Even if the program is not designed to do special sizing calculations and simulations, its code can always be adapted to do so. Unfortunately, FlowNex was not invented to do emergency relief sizing calculations and the given alternatives were too complex for beginners to handle in that short amount of time. Even with those alternatives, an actual sizing of relief devices according to ISO 4126-10 and/or API 510 is not possible.

ChemCad/SafetyNet seemed to be the next top player for relief device sizing calculation since it provides a fast, intuitive way to do steady state sizing calculations according to API 520 norm. Unfortunately, the program does not take the European norms or safety valve manufacturers into account. With the help of the support team, the two-week trial was stressful but sufficient to deal with most problems and to evaluate the software.

After some drawbacks, ProSar, a newly invented web-based sizing tool, came into view. The major drawback concerning ProSar is that the user must provide the mass flow to be discharged through the safety valve, which is basically the main work of the whole sizing process.

7.2 SuperChems

SuperChems is an American software and was programmed to fit the American market needs. As the requirements evaluation shows, SuperChems seems to be covering a lot of these criteria. An advantage of SuperChems is the new visual software surface makes sizing for beginners easier in comparison to the classic layout. SuperChems strength lies in the models provided for the sizing and rating of emergency relief systems according to the API 520 norm. The user input required to do these calculations are equal to those needed in the API 520 norm. Another strength is the possibility to draw the relief piping path using MS Visio. This provides a simple way of constructing the relief piping path and overall a simple way to do sizing calculations. Also, running a dynamic simulation of created scenarios is easy and therefore a strength of SuperChems. The dynamic simulation models provide a variety of visualized charts for the rating of the used system.

One of SuperChems weaknesses are the missing European norms and European safety valve databases. With the use of MS Visio, relief piping can easily be dragged and dropped into the flowsheet but these drawing are no actual isometric piping layouts since elbows, bends, and tees are not visualized in the technical drawing of the relief piping. Another weakness is the first impression of the user interface. To be able to use SuperChems effectively, the user needs a training beforehand since it is not possible to use the software intuitively with the use of the help section.

Since a significant part of TÜV SÜD Process Safety's customers are from Europe, the sizing using European norms like the ISO 4126-10 is essential. Also, a European safety valve manufacturer database would be of great help. SuperChems cannot provide these essential requirements. Furthermore, to use SuperChems properly, a training is necessary to fully understand what the program does. Unfortunately, the help section and the support team of SuperChems where not helpful during the duration of this thesis.

7.3 FlowNex

FlowNex strength lies in the opportunities to do all kinds of process simulations. Another strength is a highly motivated support team and a very supportive help section. But as the requirements evaluation in section 5.2.1 shows, it does not cover enough evaluation criteria which is a significant drawback. The program was not invented to fit the special needs of TÜV SÜD regarding the relief device sizing process. Even with the constant help of the FlowNex support team, some major points including sizing according to European norm ISO 4126-10 could not be sorted out which is a great weakness of the program regarding the requirements.

7.4 ChemCad/SafetyNet

As the requirements evaluation in chapter 5 shows, ChemCad SafetyNet covers a significant amount of the pre-defined evaluation criteria. ChemCads strength lies in quick state sizing calculations and a highly sophisticated dynamic thermodynamical simulation tool. The dynamic part needs a little more user commitment to fully take advantage of. One drawback is that ChemCad does not provide a pressure relief device manufacturer database and the sizing calculations are only possible regarding the API 520 norm. Since for TÜV SÜD it is also important to simulate and calculate dynamic scenarios including chemical runaway reactions, the SafetyNet tool is not the right choice for TÜV SÜD. To be fully of use, the complete ChemCad program must be purchased. Still then, reactions must be described using reaction kinetics and the sizing will still be done regarding American norms only, which is another drawback. Another significant strength is the ChemCads help section and its support team.

7.5 ProSar

The strength of ProSar is, that it is a web-based sizing tool for quick sizing calculations. As the only program evaluated it accounts for the ISO 4126-10 which also is its greatest strength. On the downside, ProSar did not match on various of the evaluation criteria in chapter 5. The main drawback is that the mass flow to be discharged must be known before the sizing calculation. The calculation of this mass flow is associated with a great deal of effort. To be of value for TÜV SÜD, the mass flow calculation is a must-have in a sizing program.

8 Outlook

Up to now, TÜV SÜD does its emergency relief device sizing calculations with a highly sophisticated Excel sheet which covers all the requirements from chapter 5. Even though some of the software tools evaluated in this thesis do partly cover most of the requirements stated in chapter 5, there are still some major drawbacks to each software. This makes it impossible for TÜV SÜD to not make use of the Excel sheet – up to now. Most of the software are American made and therefore only cover American norms or simply have not been invented to fit these requirements. But with a chance, these programs will stock up on European norms and manufacturer databases making it interesting for TÜV SÜD.

SuperChems is always developing its software to make it more user-friendly and to fit more customer needs. In the future, SuperChems might also adapt to the European market (ISO 4126-10 and manufacturer databases for more adequate sizing)

ChemCads SafetyNet is the most promising software due to its strong thermodynamic simulation tools and an easy sizing procedure. Unfortunately, SafetyNet is also not suitable for the European market until now. ChemCad's complete version of the software seems to be able to handle most of TÜV SÜD's sizing challenges including an adequate dynamic simulation of runaway reactions.

FlowNex support is always trying to find a solution for every individual problem. Regarding FlowNex one could think about adapting the program's code together with the FlowNex team to make it more suitable for emergency relief system sizing and chemical reaction simulation.

ProSar has just released its software recently and so far, its functions are not sufficient to do the job. But on the other hand, ProSar is the only (web-based) software taking European norms and manufacturers into account. Also, the developers of the software want to make ProSar the leading software on the market and are already highly motivated to present a more sophisticated version of the program soon.

Summarized, TÜV SÜD will still have to use their Excel spreadsheet for accurate ERS sizing It might be of value to keep an eye on the software evaluated in this thesis and check for updates and extensions frequently to make sure to not miss a major improvement.

One software to come is FAUSKE'S FERST, which will be a replacement for their current software PrEVent. FERST will use the ChemCad interface with a reduced menu for emergency relief systems sizing only. The program is momentarily not ready for testing but should be tested by TÜV SÜD once it is available.

9 Appendix

9.1 SuperChems – Step-by-step scenario documentation

To follow this documentation, the SuperChems V10.0 software and the Microsoft Visio desktop version must be installed on the computer.

9.1.1 Open SuperChems visual and press run!

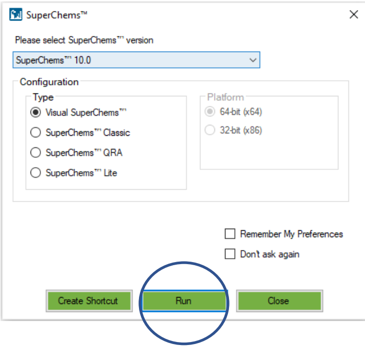


Figure 52: opening SuperChems

9.1.2 Create a new project file

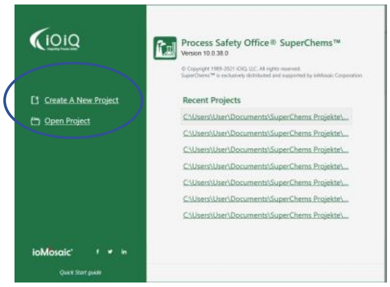


Figure 53: creating a new project

Note the default setup!

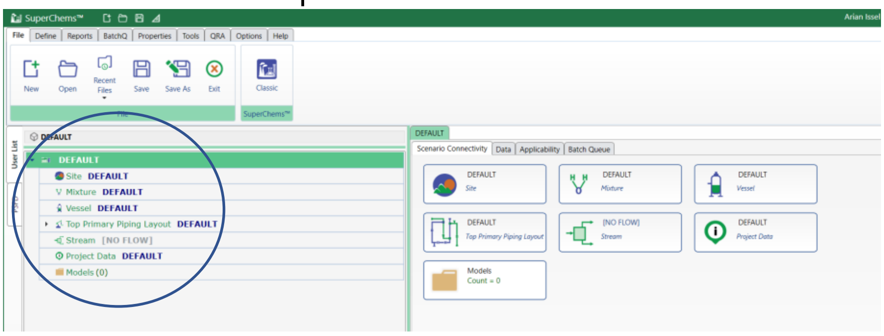


Figure 54: default scenario menu

NOTE: The "site" menu is only important for information in the report and for consequence analysis. For ERS sizing, this part is not of importance and can be left out completely.

NOTE: Units can be changed any time! By right-clicking on the specific unit, single units can be changed to the desired unit!

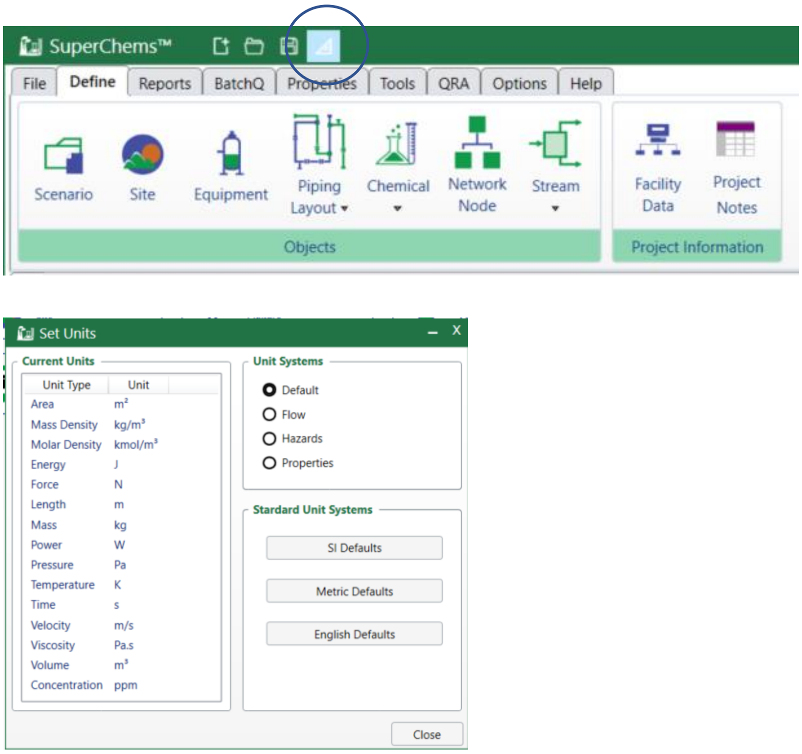


Figure 55: change units

9.1.3 Create a new scenario

A new scenario can be created by simply right clicking on the left-hand side and select "new scenario". Name the scenario as desired.

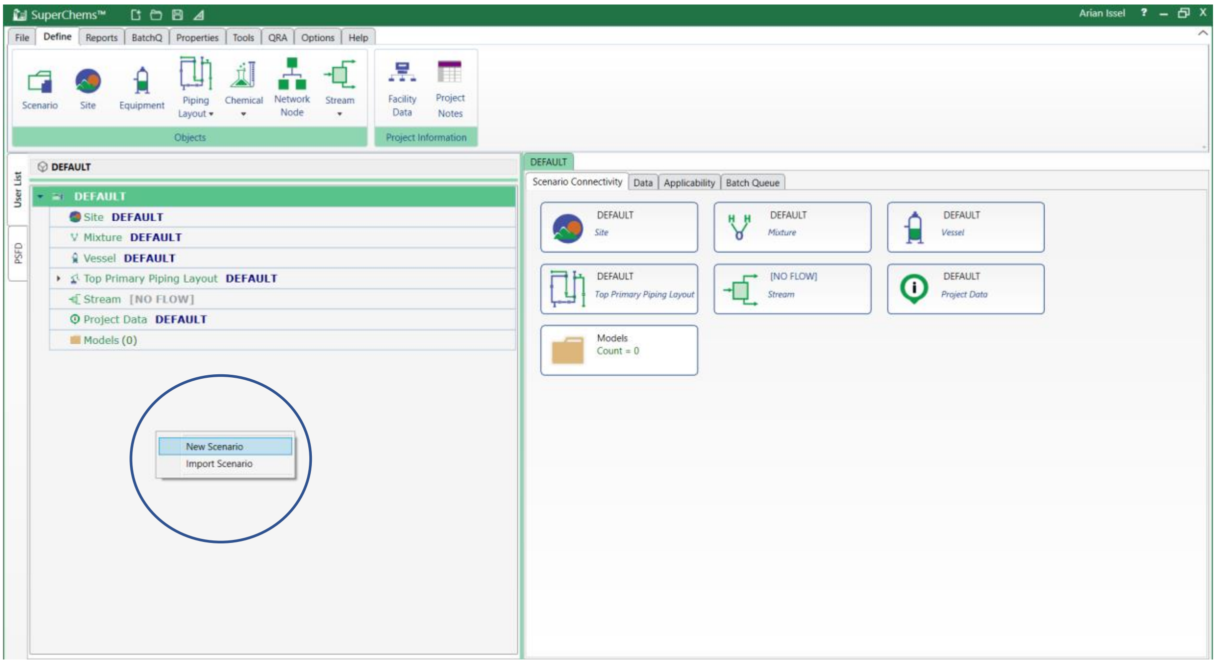


Figure 56: alternative way of creating a new scenario

Note the newly created scenario named “DOCUMENTATION ONLY”.

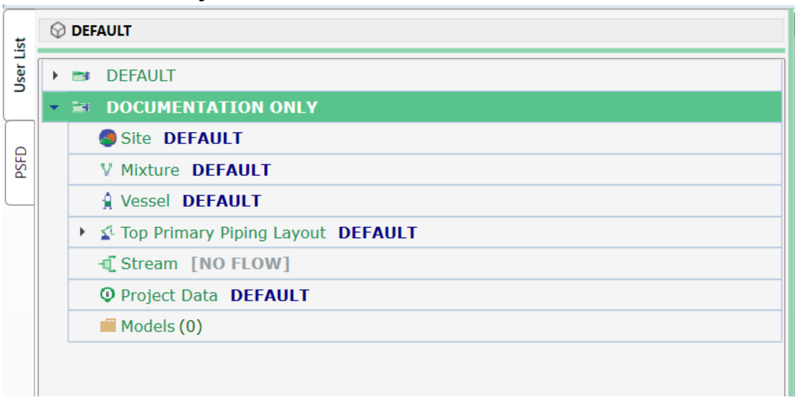


Figure 57: newly created scenario

9.1.4 Create a new mixture

A new mixture can be created by clicking on the “define – chemical” tab.

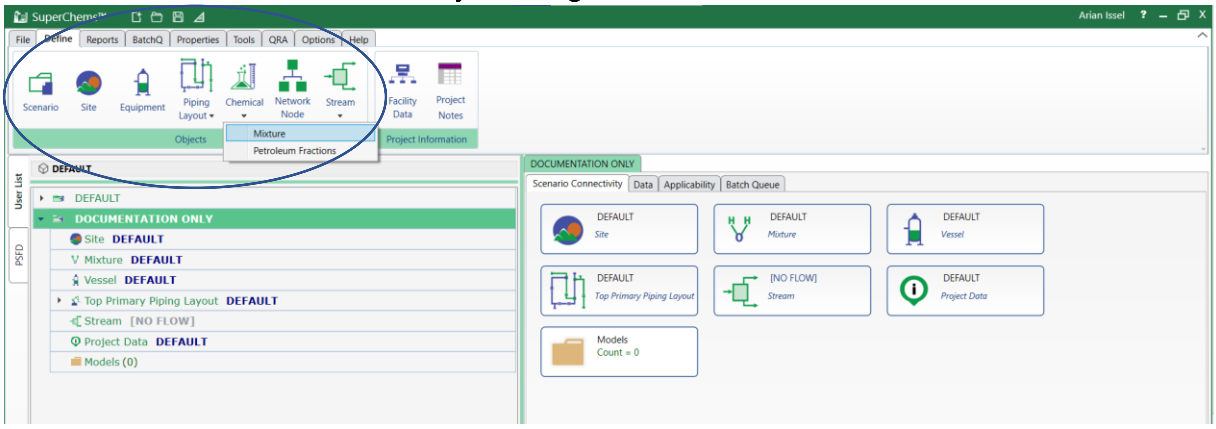


Figure 58: creating a new mixture

Click on the “add one unit” tab on the top left and name the mixture. The mixture in this example is named “DOCUMENTATION MIX”.

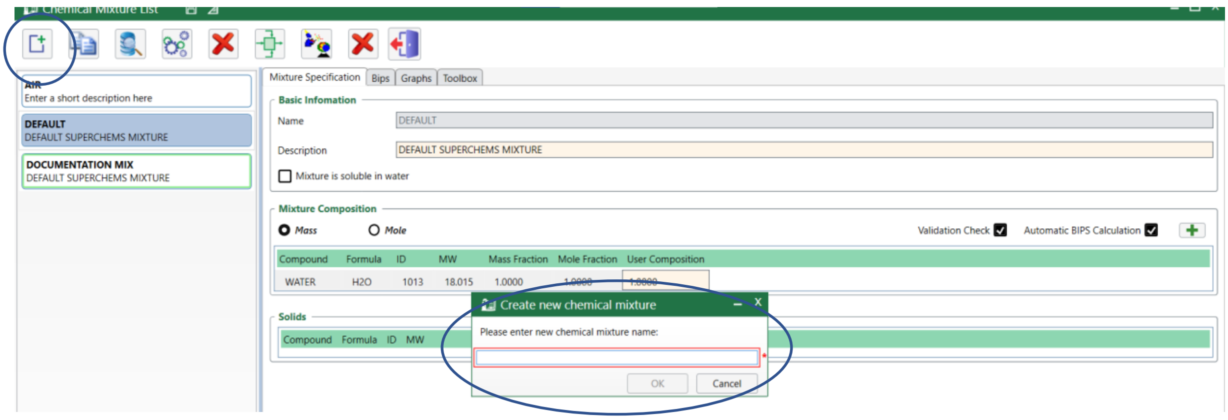


Figure 59: creating a new mixture

A mixture can also be created by right clicking on “mixture” on the scenario overview.

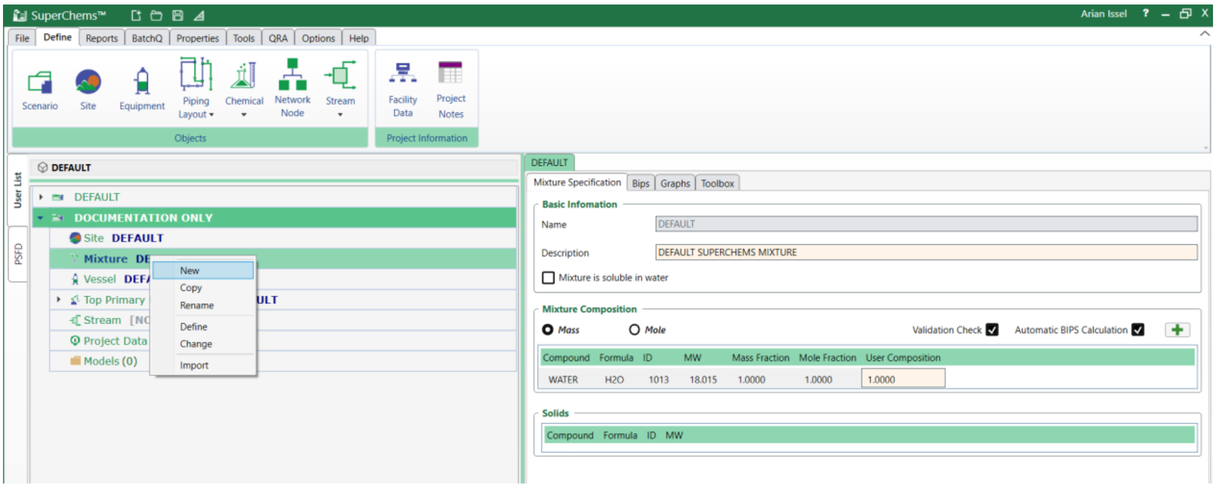


Figure 60: alternative way to create a new mixture

Within the mixture menu, compounds can be removed, added, or replaced from the SuperChems database. Simply right click on the default compound (water) and select “add”, “remove”, or “replace”.

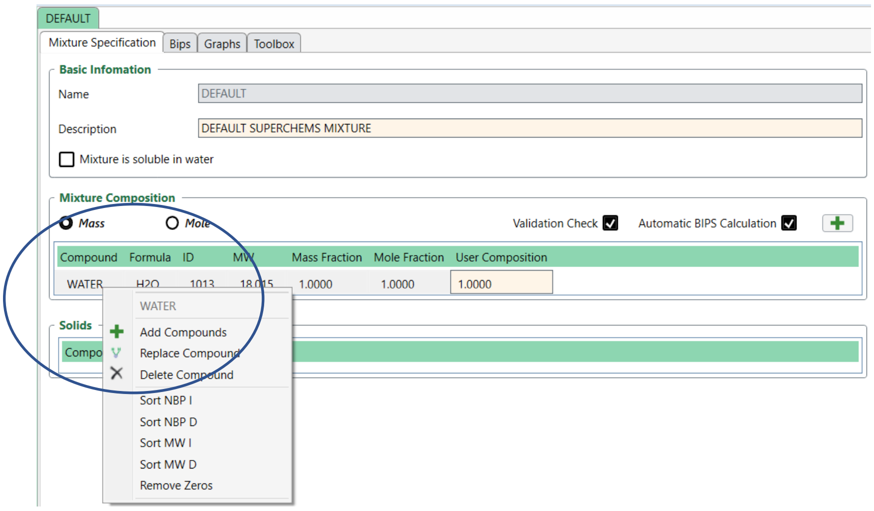


Figure 61: Adding compounds to a mixture

The compounds database will open to select the components of the mixture. The database provides approx. 3000 chemicals to choose from. They can be searched by name, CAS, Formula but also molar weight.

Figure 62: compound database

After selecting the compounds for the mixture, the mole or mass fraction must be defined.

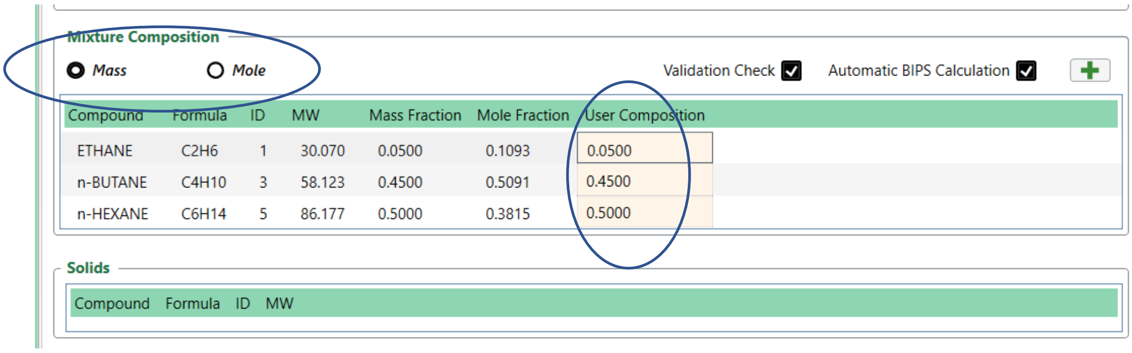


Figure 63: defining the mole or mass fractions

After the creation of the mixture, click on the door symbol. A mixture can be changed by right-clicking on the default mixture and selecting the desired mixture from the list.

9.1.5 Define a vessel

The next step is the definition of a vessel. Again, one can use the “define – equipment – new” tab.

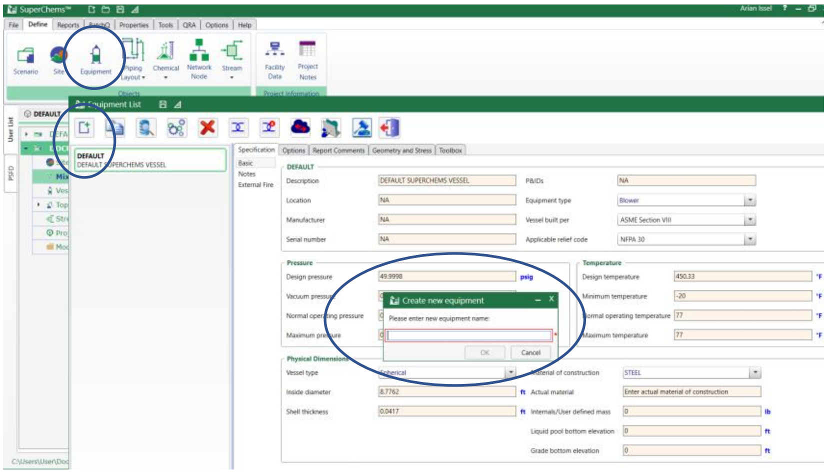


Figure 64: creating a new vessel

Also, a new vessel can be created by right clicking on the default vessel within the scenario and click on “new”. The vessel must be named afterwards. In this example, the vessel is named “DOCUMENTAITION VESSEL”.

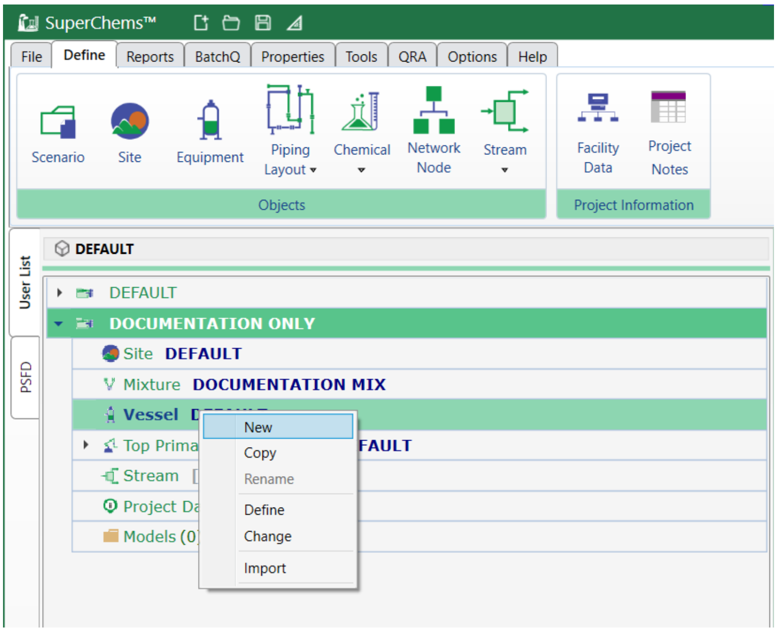


Figure 65: alternative way to create a new vessel

Within the vessel menu there are various tabs to enter information (Specification, Options, Report comments, Geometry and Stress, Toolbox).
The main information is entered in the specification tab.

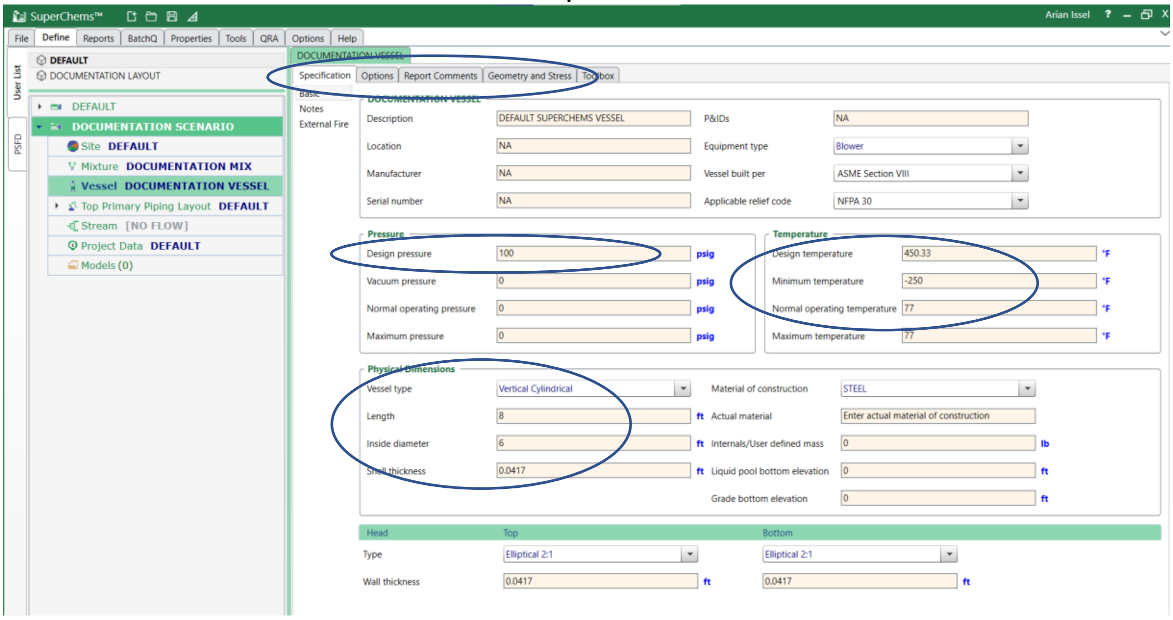


Figure 66: the vessel menu

Essential information is design pressure, design and operation temperature, vessel type and diameter (and length, depending on vessel type). The documentation part for the vessel is only for information in the report.

Some scenarios must be enabled within the options section of the vessel.

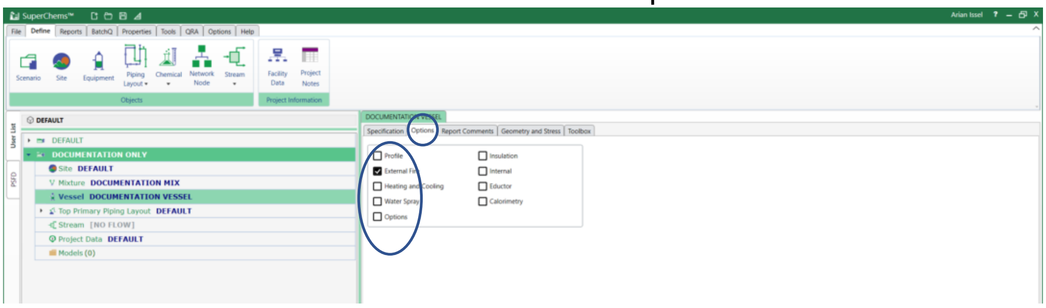


Figure 67: vessel - external fire option

Click on the “external fire” tab within the documentation vessel menu.

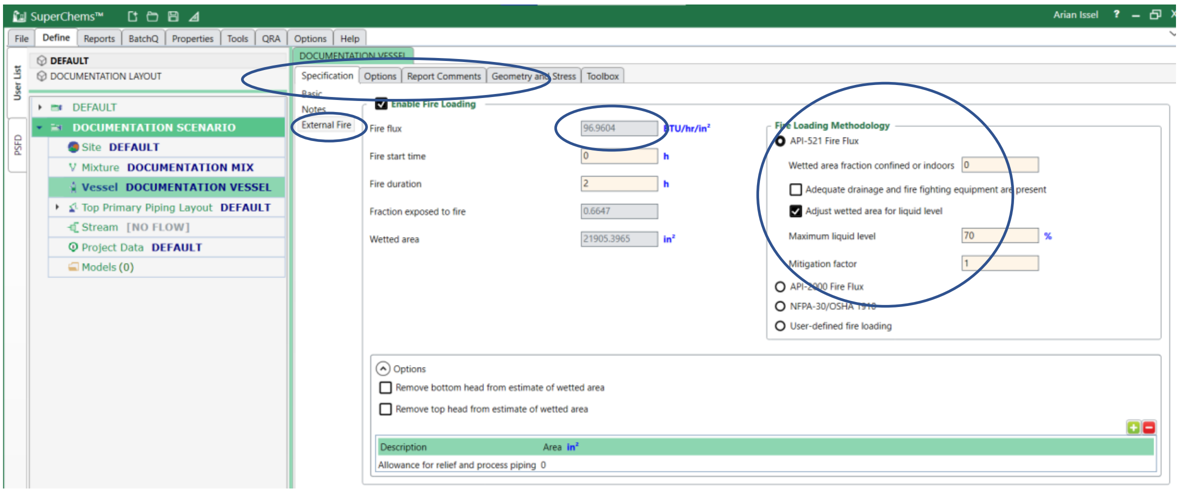


Figure 68: vessel - external fire definition

Choose the desired Fire loading methodology and enter the mitigation factor and in this case (API 521 fire flux) also enter the filling level of the vessel. SuperChems will then calculate the fire flux.

NOTE: Different models need certain input. The information provided at this point is enough to run the first API 520/CCPS model.

9.1.6 API 520/CCPS model

To choose a model, right click on the model menu within the scenario. Click on “Flow and source term” or “network flow”, depending on the desired model.

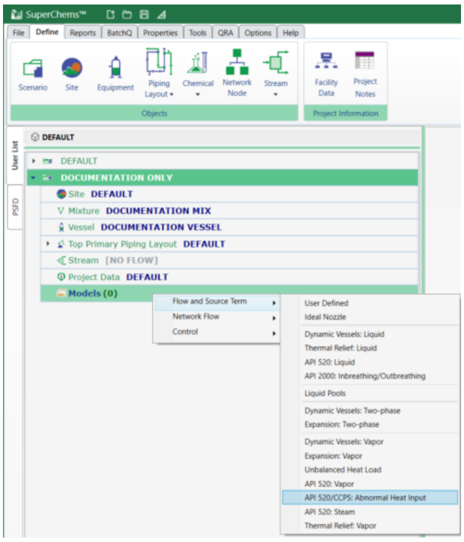


Figure 69: API 520/CCPS: Abnormal Heat Input model

Note the newly created model and its input parameters.

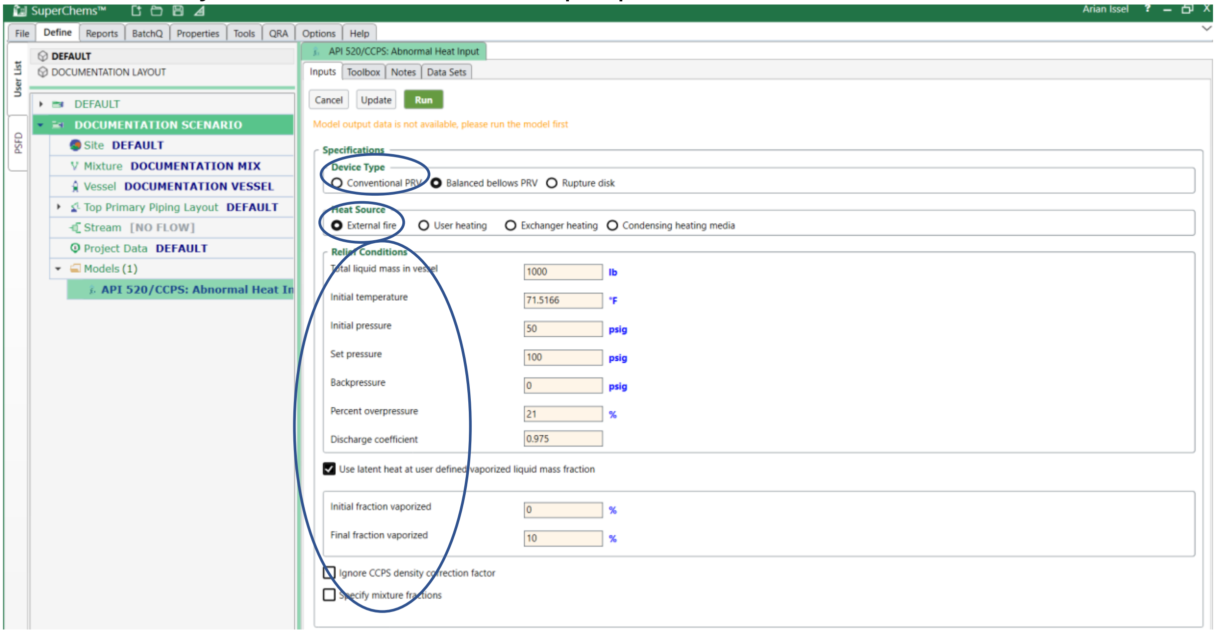


Figure 70: API 520/CCPS input parameters (pure components method)

The input parameters within the model menu are all essential, except for the total liquid mass in vessel (this will be calculated using the mixture properties, vessel geometry and the filling degree as defined in the external fire section).

Device type must be chosen (conventional PRV, balanced bellows PRV or rupture disk).
Heat source must be chosen (external fire in this case).
Relief conditions must be entered (initial temp, initial pressure, set pressure of the ERS, backpressure if applicable, precent overpressure and the discharge coefficient.
Initial temperature and initial pressure are the standard process conditions in the vessel.

NOTE: The piping layout is of no importance at this point (for the CCPS method). The default piping layout always only consist of a default rupture disk!

The model can now be run!
NOTE: SuperChems will use the pure component method by default! SuperChems decides which compound has the most relief need and uses this component as the pure component.

By clicking on the “update”-tab the input parameters will be saved.

To choose the “% mass vaporized average method” the “use latent heat at user defined vaporized liquid mass fraction” box needs to be checked and initial and final fraction vaporized must be entered.

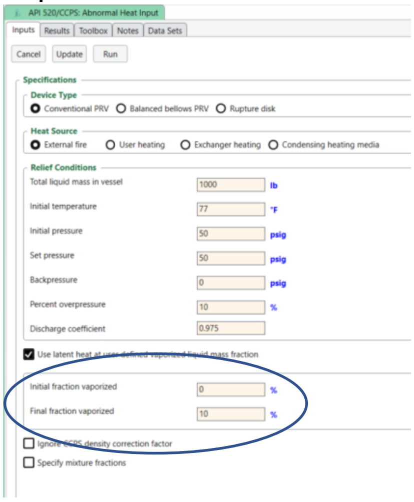


Figure 71: API 520/CCPS input parameters (% mass vaporized average method)

In both cases, SuperChems will return a required relief area! But the values will be different! Choose wisely!

9.1.7 Output data for the pure component method!

Output Data		
Relief requirement will be set by evaporation of n-HEXANE		
Time required to reach Pset (lightest component)	0.0003	h
Average molecular weight	86.1772	
Temperature at maximum pressure	324.8746	°F
Compressibility factor	0.7776	
Density	0.2388	lb/gal
Heat of vaporization	103.8113	BTU/lb
Density correction factor	0.9557	
Correction factor vapor density	0.1857	lb/gal
Correction factor liquid density	4.1903	lb/gal
Evaporation/relief rate	19,553.1014	lb/h
Volumetric flow rate	80,253.5512	SCFH
Flow is critical (choked).		
Relief device orifice area	1.2267	in²
Exit temperature	307.8600	°F
Exit pressure	66.2638	psig
Exit compressibility factor	0.8682	
Exit density	0.1304	lb/gal
Exit velocity	670.2654	ft/s
Backpressure correction factor	1.0000	
Next size up is J orifice (1.287 in2), 2x3 or 2.5x4 or 3x4		
Next size down is H orifice (0.785 in2), 1.5x3 or 2x3		

Figure 72: output data pure components method

9.1.8 Output data for the “% mass vaporized average method”.

Output Data		
Latent heat is based on heat required to vaporize 0 % to 10 % of the liquid mass at the relief pressure		
Time required to reach relief pressure	0.0343	h
Average molecular weight	49.3068	
Temperature at maximum pressure	172.3227	°F
Compressibility factor	0.8701	
Density	0.1516	lb/gal
Heat of vaporization	317.4774	BTU/lb
Density correction factor	0.9661	
Correction factor vapor density	0.1516	lb/gal
Correction factor liquid density	4.4706	lb/gal
Evaporation/relief rate	6,463.2568	lb/h
Volumetric flow rate	48,619.3934	SCFH
Flow is critical (choked).		
Relief device orifice area	0.5001	in²
Exit temperature	143.6530	°F
Exit pressure	64.7843	psig
Exit compressibility factor	0.9156	
Exit density	0.0884	lb/gal
Exit velocity	802.0087	ft/s
Backpressure correction factor	1.0000	
Next size up is G orifice (0.503 in2), 1.5x2.5 or 1.5x3 or 2x3		
Next size down is F orifice (0.307 in2), 1x2 or 1.5x2 or 1.5x2.5		
**NOTE: Actual flow area should be used for all inlet/outlet pressure loss estimates, piping reaction forces, etc.		

Figure 73: output data “% mass vaporized average method”

NOTE: the smaller required relief area!

NOTE: SuperChems automatically returns the orifice one size up and one size down!
NOTE: To make things easier, write down or export the output data to use them for the next models!

9.1.9 Define minimum relief area PRV from the API 520/CCPS method

Prior to the set-up of a new piping layout, right-click on the scenario and select “copy”. Within the newly created scenario, right-click on “top primary piping layout” and select “new”. Give it a suitable name and click “Ok”. To add a new layout, click on the “add 1 unit” tab on the top left. In this example it is named “MIN DOCUMENTATION LAYOUT”.

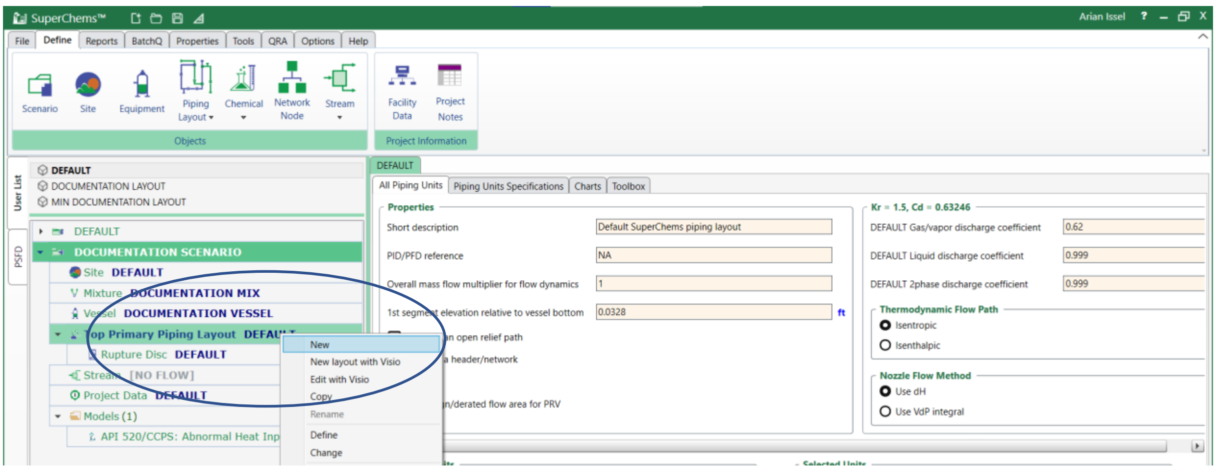


Figure 74: Defining a new piping layout with a PRV

To define a PRV with the minimum relief area obtained from the CCPS method, go to the “define – piping layout – pressure relief valve” tab.

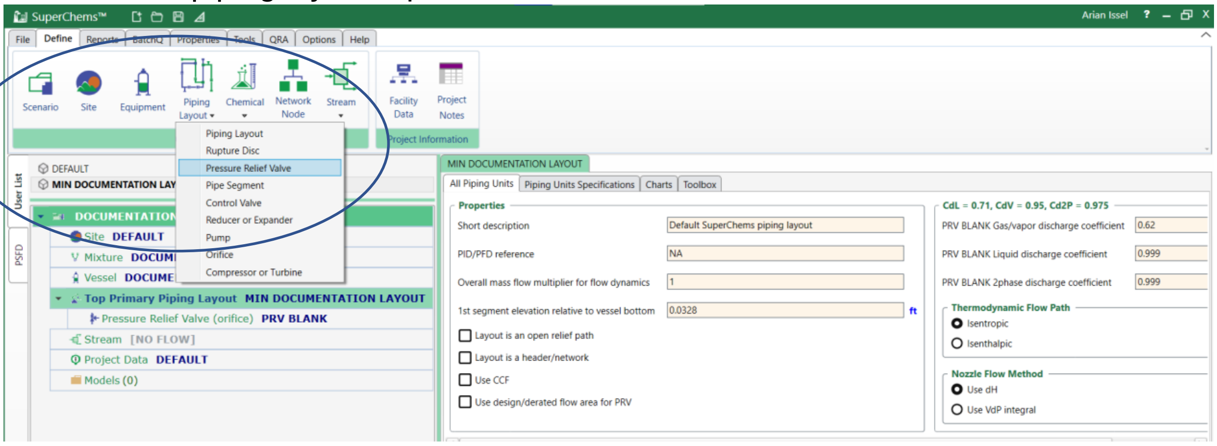


Figure 75: by hand definition of a PRV

Select “add 1 unit” and name the pressure relief valve. In this case, the PRV is named “MIN PRV DOCUMENTATION”.

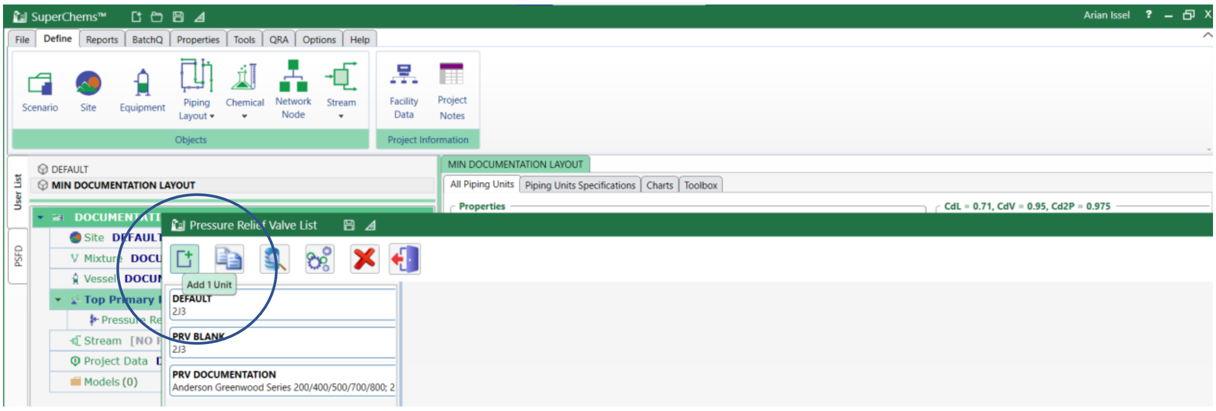


Figure 76: Add a PRV to the piping layout

In the PRV menu, enter the minimum relief area obtained from the API 520/CCPS method. In this case 1.23 in^2. Afterwards, click on the door symbol to return to the piping layout menu.

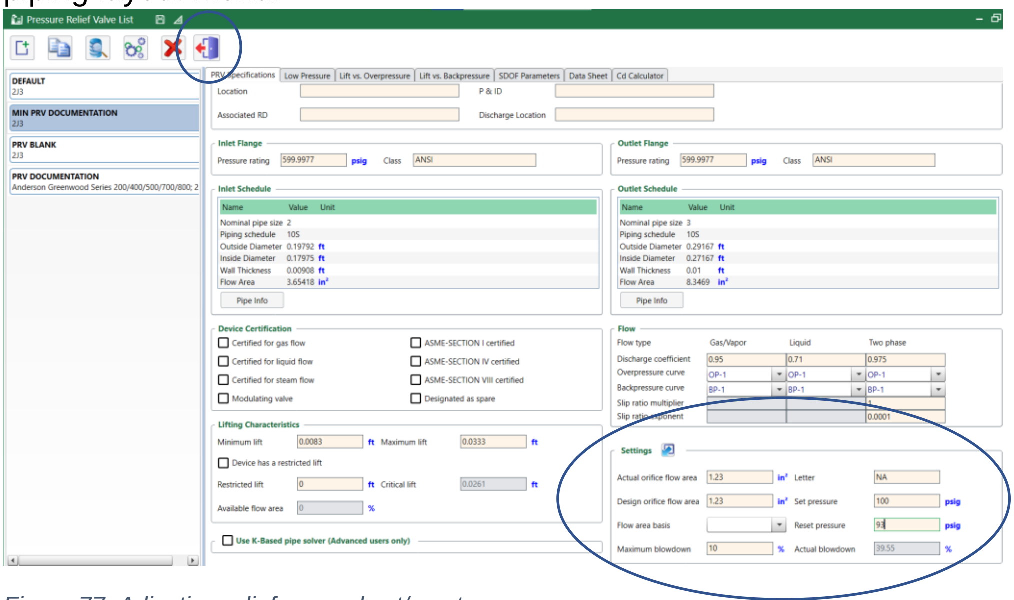


Figure 77: Adjusting relief are and set/reset pressure

To select the newly created PRV, first the default rupture disc must be removed from the piping layout. Choose the newly created PRV from the drop-down list and move it to the “selected units” side.

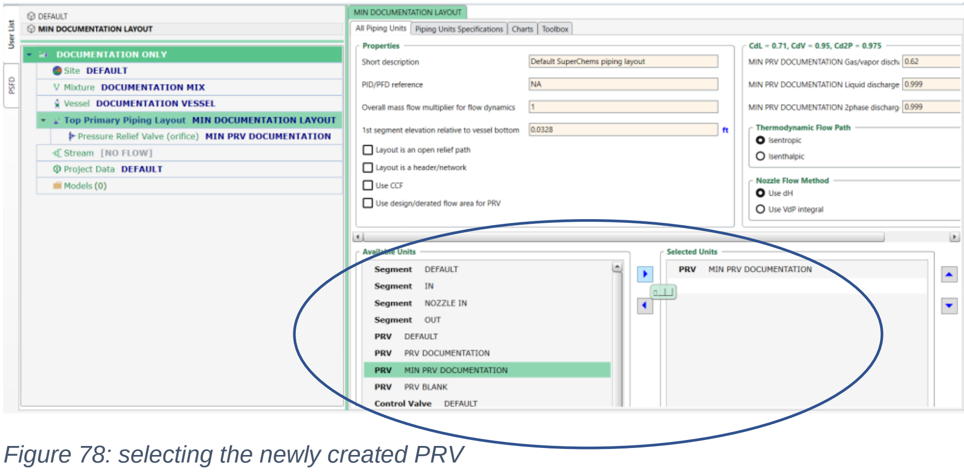


Figure 78: selecting the newly created PRV

Make sure to enter proper discharge coefficients for gas/vapor, liquid and two-phase.

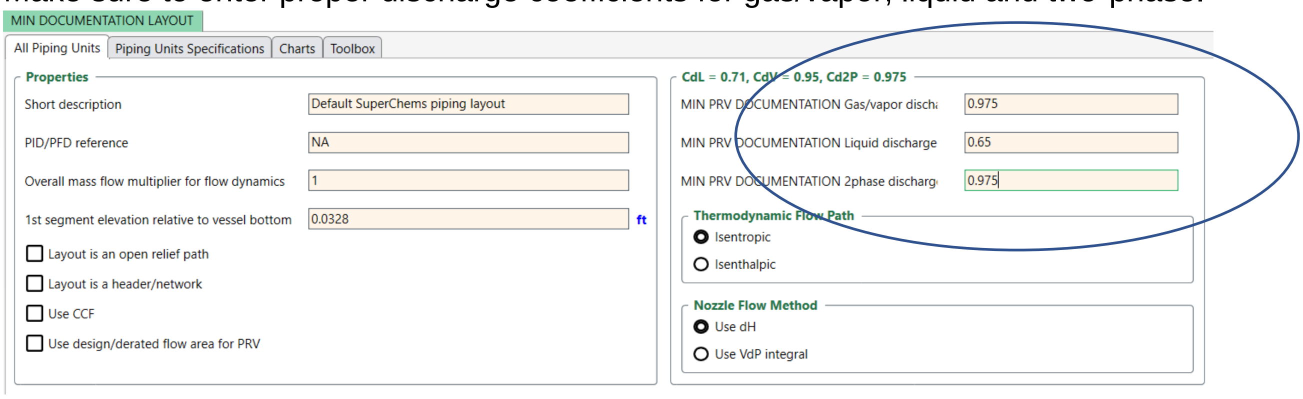


Figure 79: discharge coefficients in the piping layout menu

The input data is now sufficient to run a dynamic model.

9.1.10 Dynamic vessel: two-phase

Right-click on model and select “flow and source term – dynamic vessel: two-phase”.

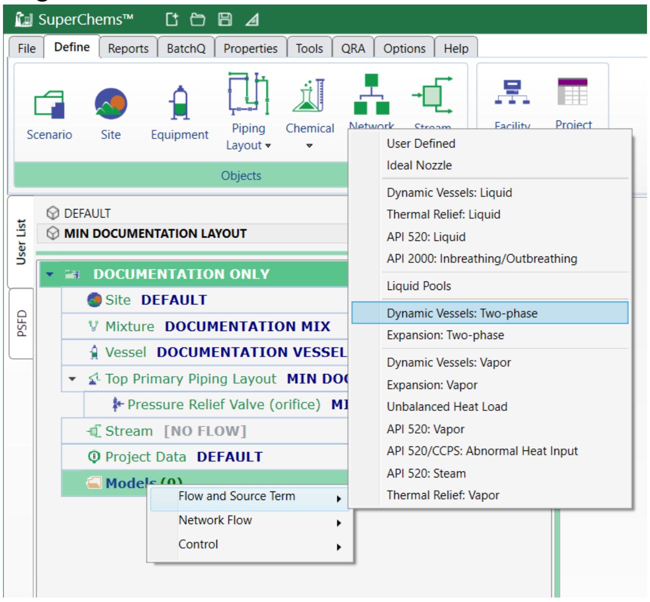


Figure 80: Dynamic vessel: two-phase model

Enter the initial conditions and a flow type for the relief piping path. Make sure the checkbox for external fire is checked. Depending on the flow type, a DIERS coupling equation coefficient must be entered.

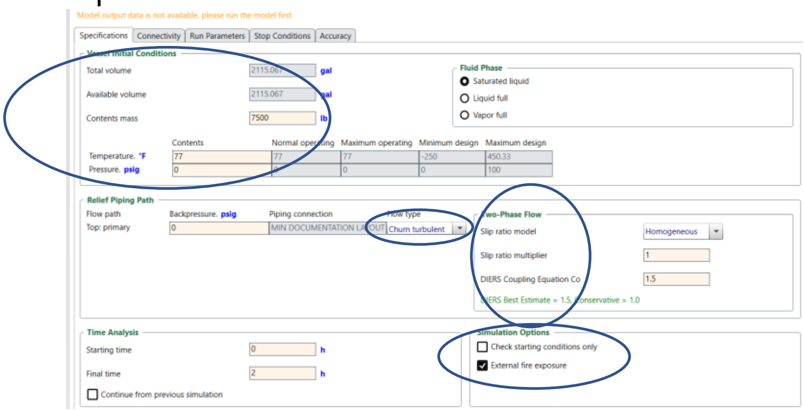


Figure 81: input data for the dynamic simulation

The simulation can now be run.
NOTE: SuperChems returns to the classical layout for the simulation!

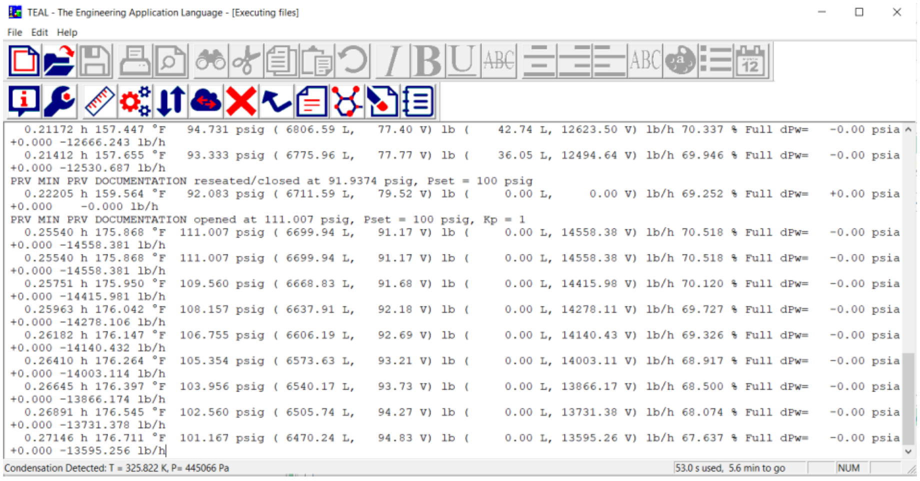


Figure 82: classical layout simulation progress

NOTE: The summary section of the results menu.

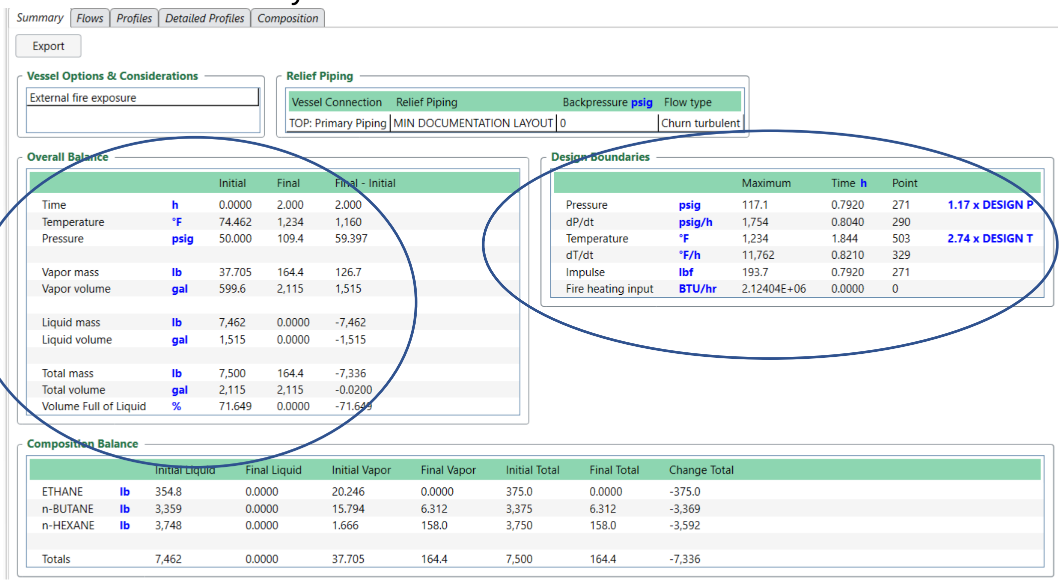


Figure 83: summary of the result menu

Under the header “flows” SuperChems returns output data for the “first flow” and “flow at maximum pressure”.

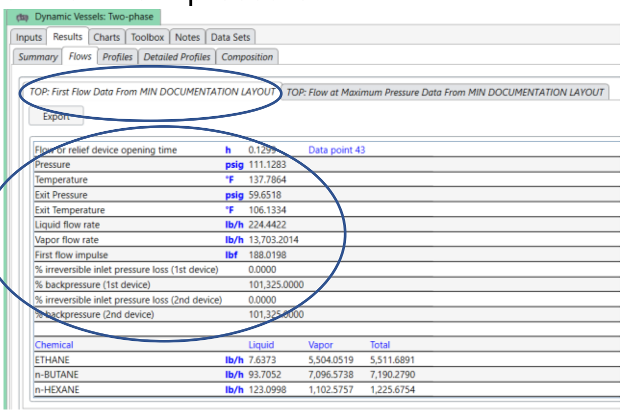


Figure 84: Output data "first flow"

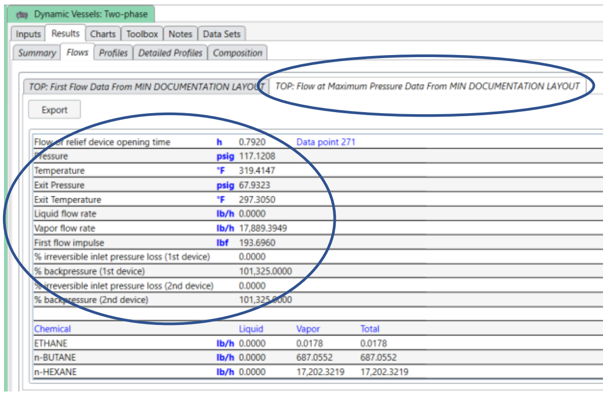


Figure 85: output data "flow at maximum pressure"

Under the “charts” tab within the results menu of the model, a variety of charts can be created.

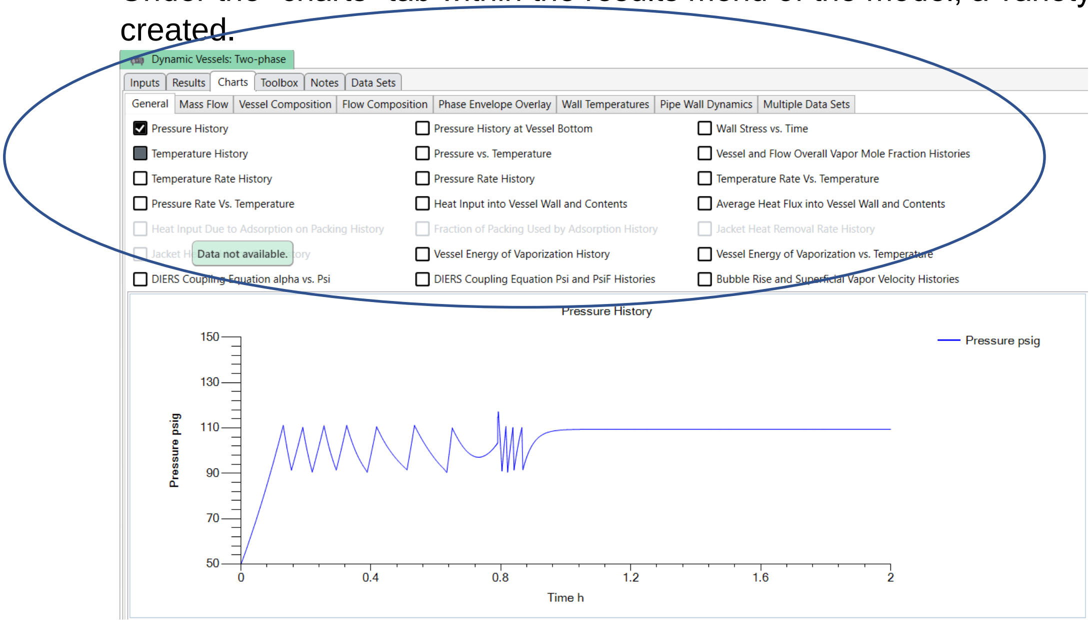


Figure 86: Charts tab in the result menu

9.1.11 Define a detailed piping layout for the dynamic simulation.

Since the following models are based on the previous simulation, the scenario can be copied and renamed.

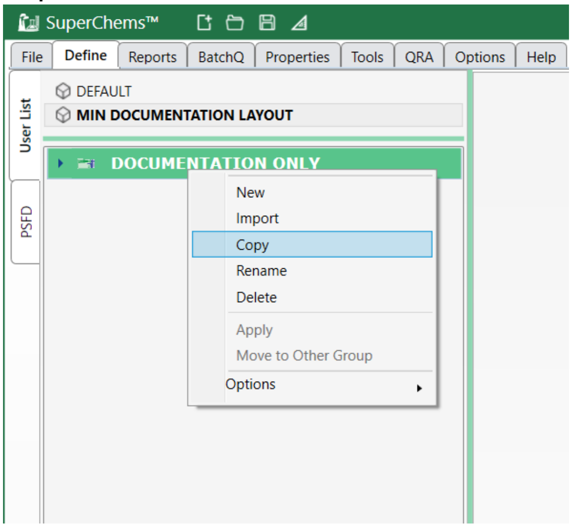


Figure 87: copying a complete scenario

NOTE: the newly created scenario by copying the old one.

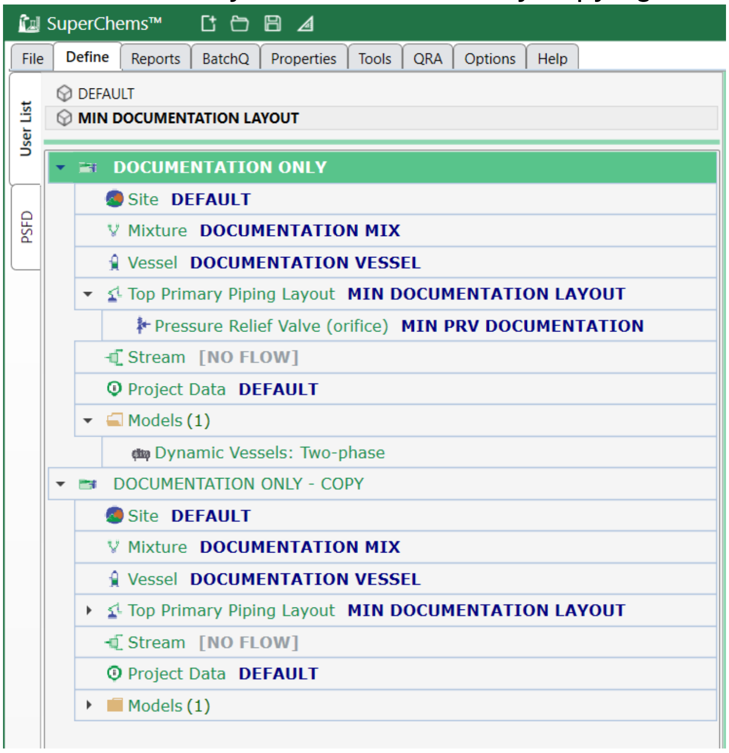


Figure 88: Copying a scenario

For the definition of a new detailed piping layout, MS Visio can be used. Right click on the “top primary layout” menu and select “new design with Visio”.

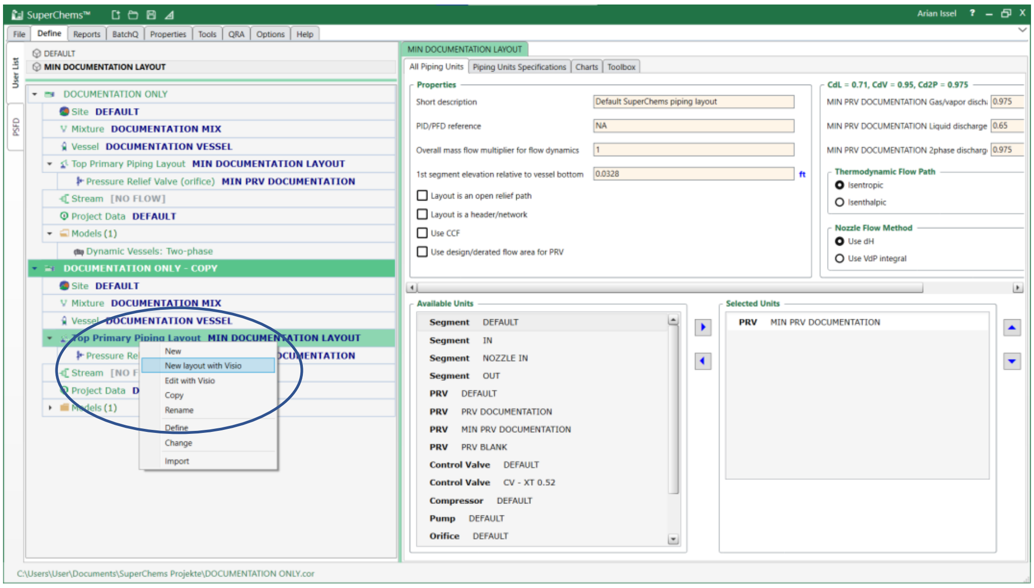


Figure 89: creation of a new piping layout

NOTE: MS Visio must be installed as a desktop version on your PC!

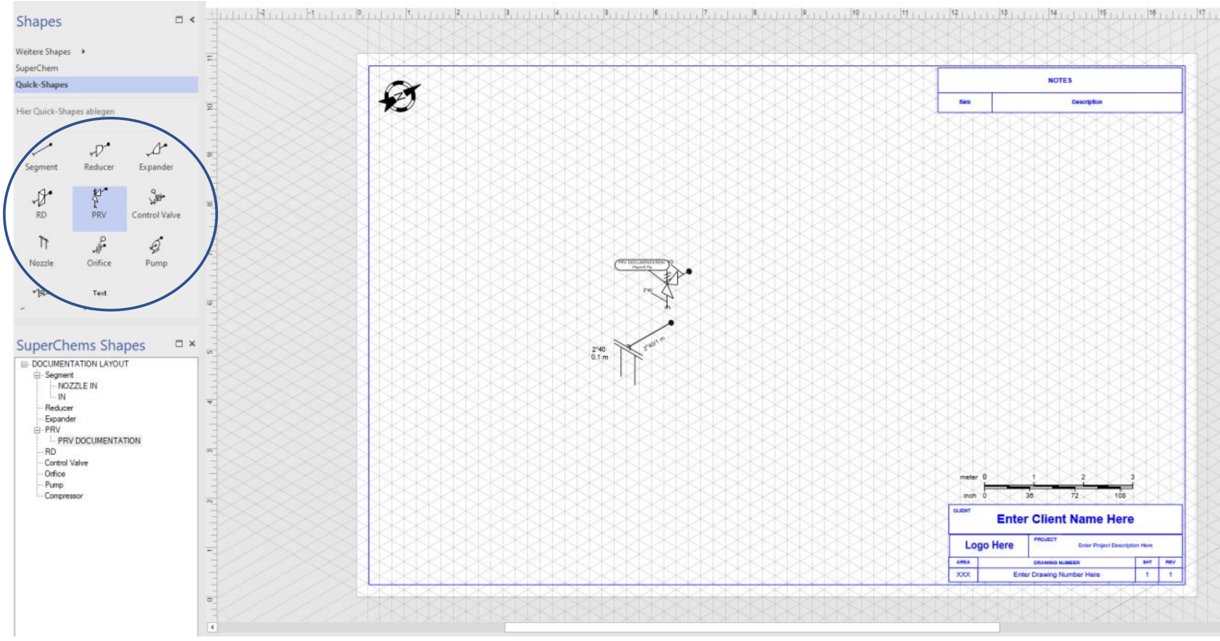


Figure 90: MS Visio piping layout surface

Once MS Visio opened, the piping layout can simply be constructed “drag and drop”. By double clicking on the items, a sub menu opens where all the parameters and fittings can be entered (pipe schedule, length, etc.).

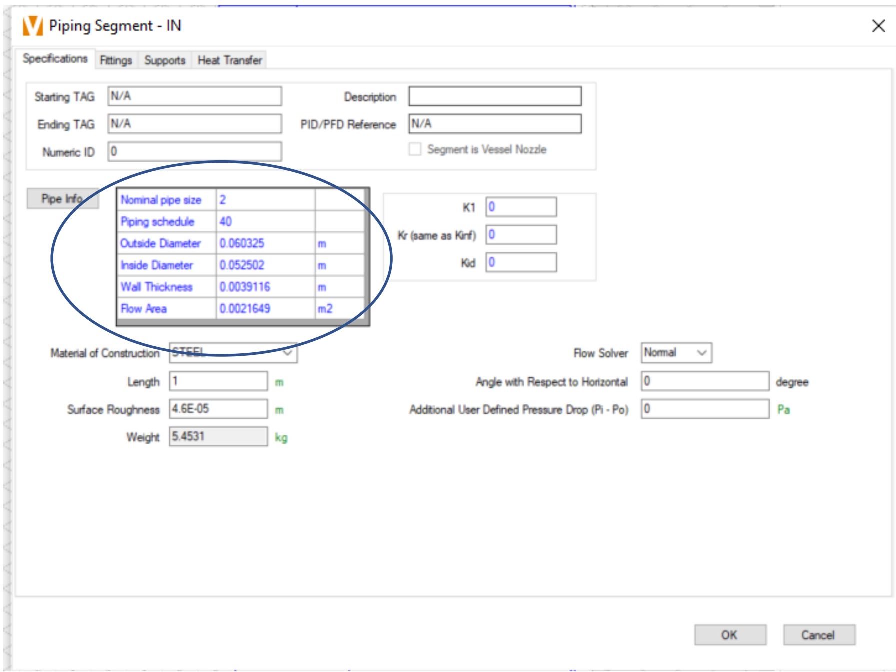


Figure 91: pipe segment menu

A PRV can be dragged into the drawing, but the inlet piping segment and the relief valve are not yet connected. They need to be connected manually as shown in Figure 92 by clicking on the pipe segment, holding the shift key, and then clicking on the PRV. By clicking on "connect" in the top section of the screen, these elements will be connected.

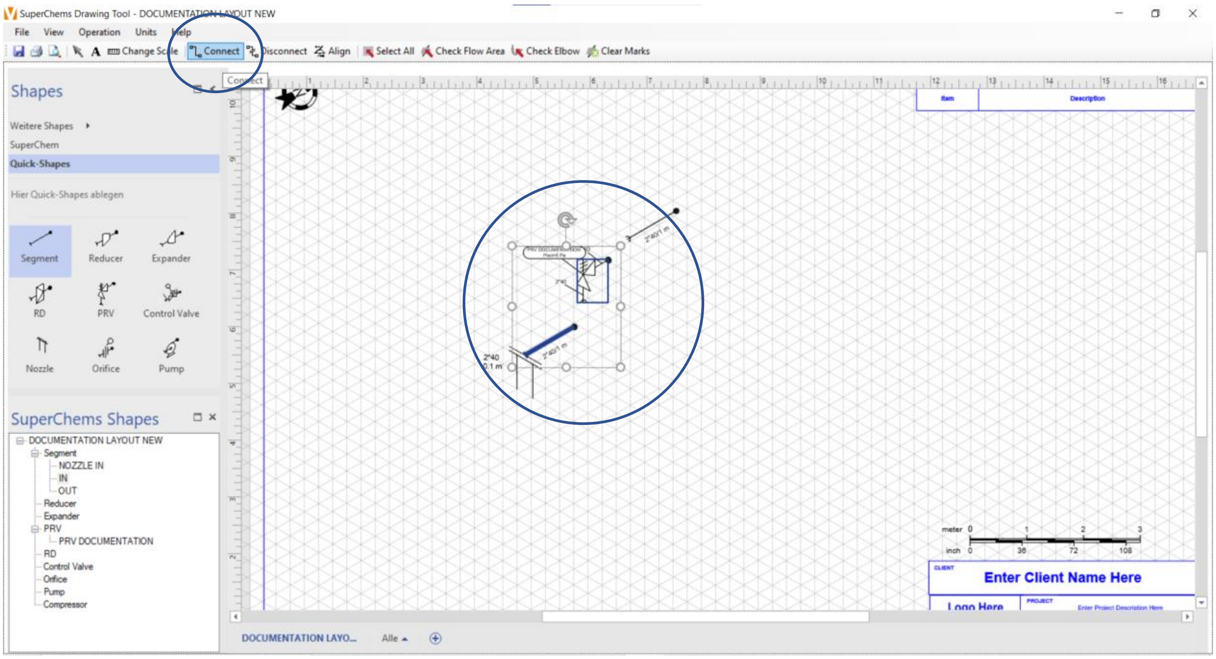


Figure 92: connecting a PRV and pipe segments

The same procedure must be repeated for the downstream pipe segment. Afterwards, the PRV must be defined.

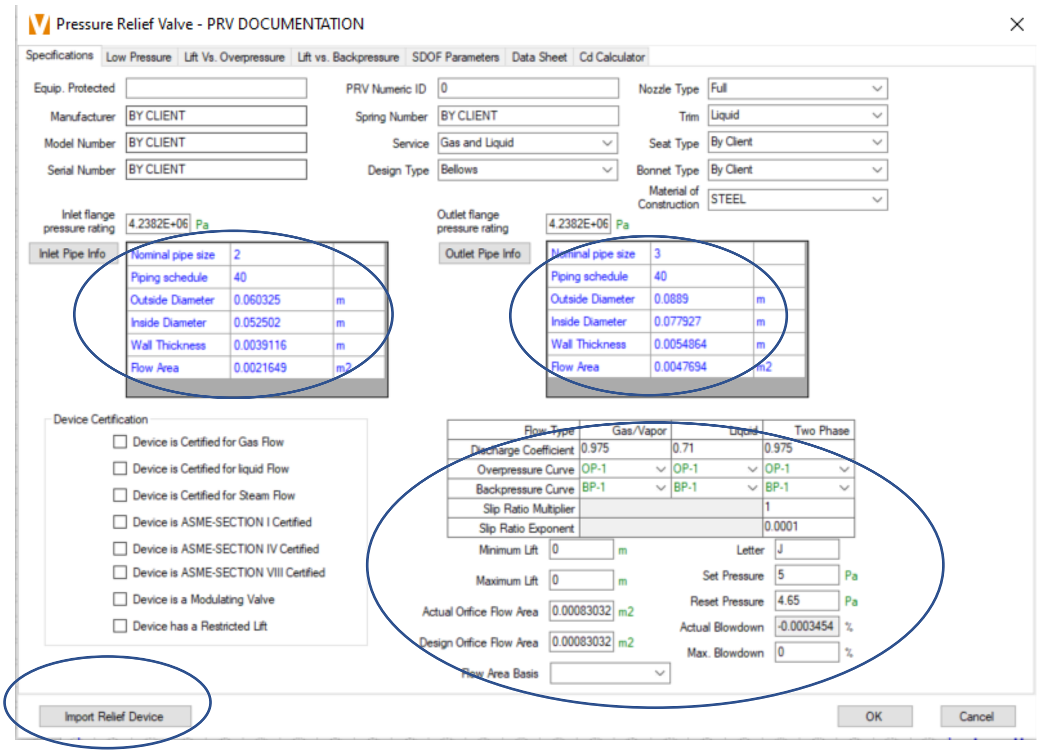


Figure 93: Pressure relief valve definition menu

A PRV can also easily be imported from a manufacturers database. Essential information is set pressure, reset pressure and orifice area.

By clicking on “import relief device” the database opens.

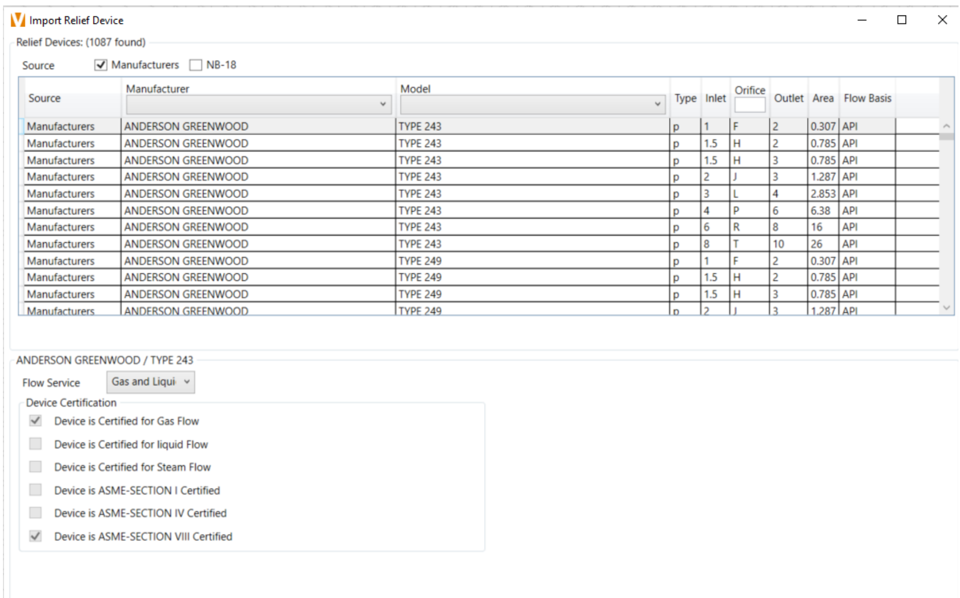


Figure 94: PRV manufacturer list

NOTE: The pipe schedule before and after the PRV must fit the PRV size! EXAMPLE: 2J3 PRV needs a pipe schedule 2 inlet, and a pipe schedule 3 outlet! This must be adapted manually!

After successfully implementing the piping layout, click on “save” and “exit”. SuperChems will now update the piping schedule in the scenario menu.

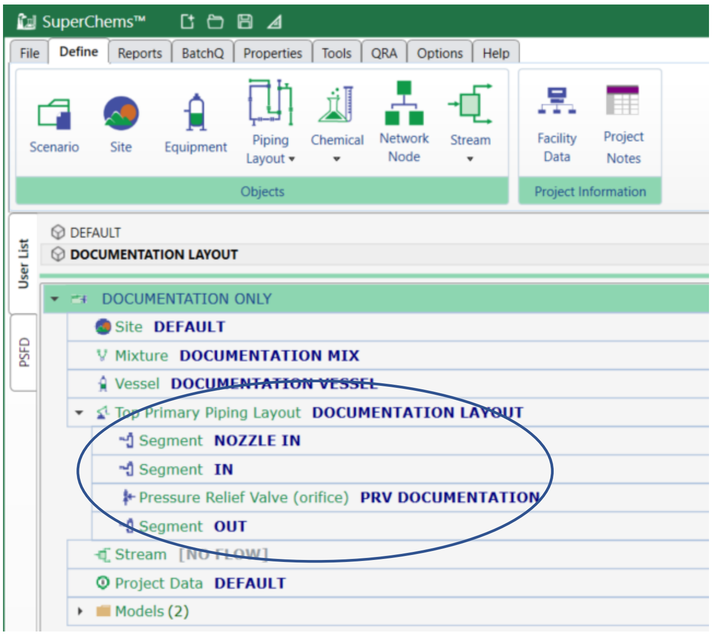


Figure 95: updated scenario menu

Any parameters can also be changed here (e.g., pipe schedule, PRV size, etc.) by clicking on the piping segment.

9.1.12 Dynamic vessel: two-phase

After creation of the piping layout, a dynamic method can be run.
Right click on the models, choose “flow and source term” and choose “dynamic vessel: two-phase”.

The input parameters stay the same to the previous dynamic model, since only the piping layout has changed!

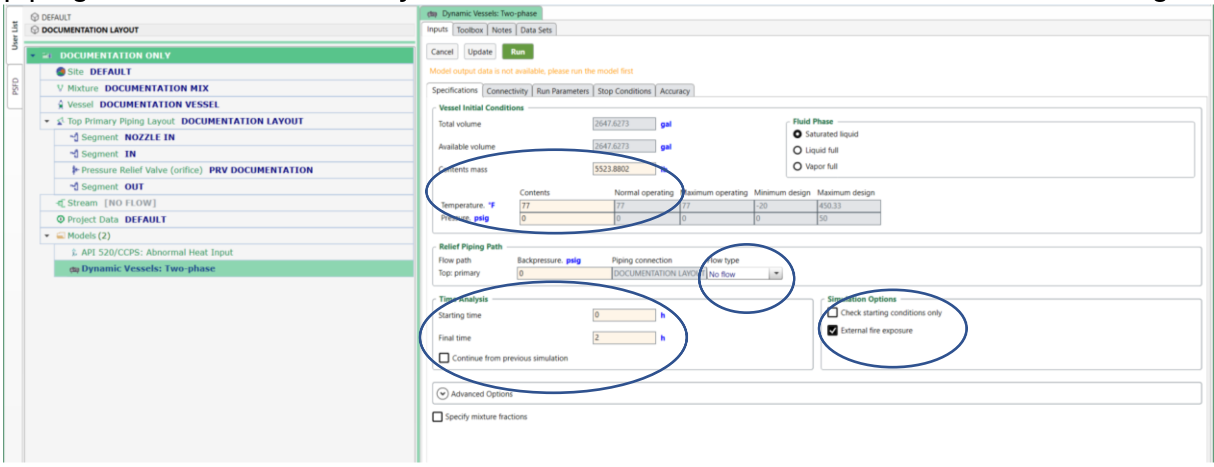


Figure 96: dynamic vessel: two-phase model

The model can now be run!
NOTE: A dynamic simulation can take up to 30 minutes and longer depending on the relief piping layout!

NOTE: Superchems returns warnings during the simulation regarding phase change and opening of the valve.

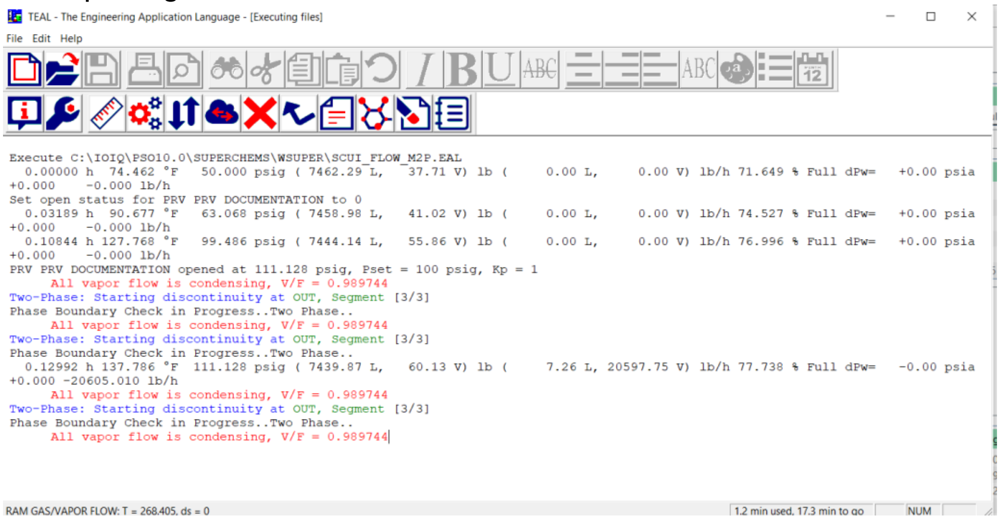


Figure 97: dynamic simulation progress

NOTE: Phase change warnings!

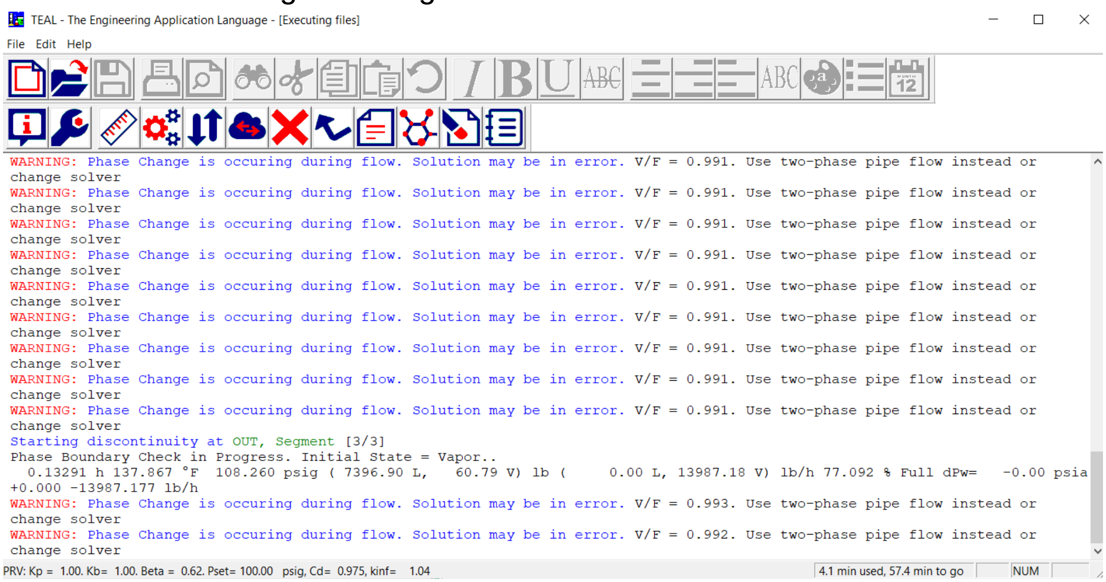


Figure 98: Phase change warnings during simulation

NOTE: SuperChems also returns output data on the initial state (in this case: vapor)!

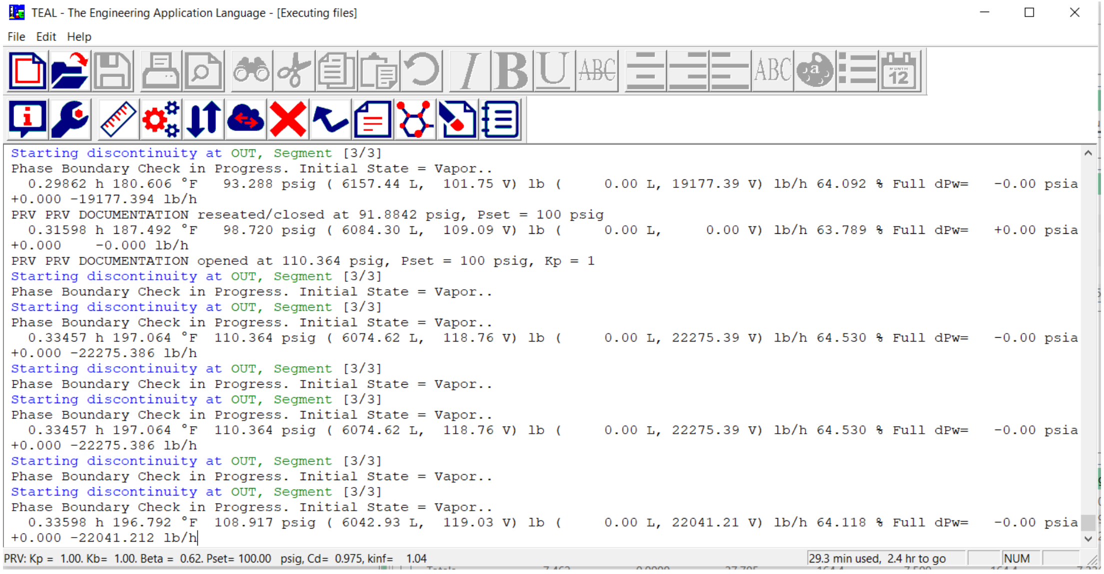


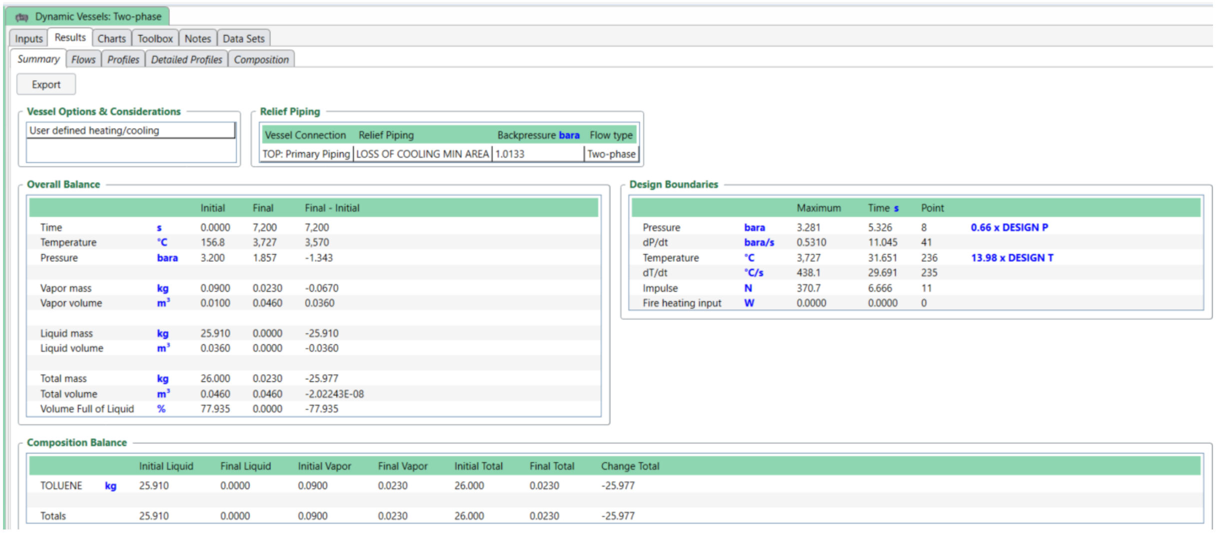
Figure 99: simulation initial state information

The result menu is equal to the one in the previous simulation.

9.1.13 Toluene relief – Combinations of different thermodynamic flow path and nozzle flow methods

The following figures show the results of four different combinations of dynamic simulations using a toluene example. The thermodynamic flow paths (isentropic or isenthalpic) and the nozzle flow methods (dH or VdP integral) have been applied in all combinations.

Figure 100 shows the results for a dynamic simulation using the isentropic thermodynamic flow path and the dH nozzle flow method.



Vessel Connection	Relief Piping	Backpressure bara	Flow type
TOP: Primary Piping	LOSS OF COOLING MIN AREA	1.0133	Two-phase

		Initial	Final	Final - Initial
Time	s	0.0000	7,200	7,200
Temperature	°C	156.8	3,727	3,570
Pressure	bara	3.200	1.857	-1.343
Vapor mass	kg	0.0900	0.0230	-0.0670
Vapor volume	m³	0.0100	0.0460	0.0360
Liquid mass	kg	25.910	0.0000	-25.910
Liquid volume	m³	0.0360	0.0000	-0.0360
Total mass	kg	26.000	0.0230	-25.977
Total volume	m³	0.0460	0.0460	-2.02243E-08
Volume Full of Liquid	%	77.935	0.0000	-77.935

		Maximum	Time s	Point	
Pressure	bara	3.281	5.326	8	0.66 x DESIGN P
dP/dt	bara/s	0.5310	11.045	41	
Temperature	°C	3,727	31.651	236	13.98 x DESIGN T
dT/dt	°C/s	438.1	29.691	235	
Impulse	N	370.7	6.666	11	
Fire heating input	W	0.0000	0.0000	0	

		Initial Liquid	Final Liquid	Initial Vapor	Final Vapor	Initial Total	Final Total	Change Total
TOLUENE	kg	25.910	0.0000	0.0900	0.0230	26.000	0.0230	-25.977
Totals		25.910	0.0000	0.0900	0.0230	26.000	0.0230	-25.977

Figure 100: Dynamic simulation results (toluene) - isentropic & dH

Figure 101 shows the results for a dynamic simulation using the isentropic thermodynamic flow path and the VdP nozzle flow method.

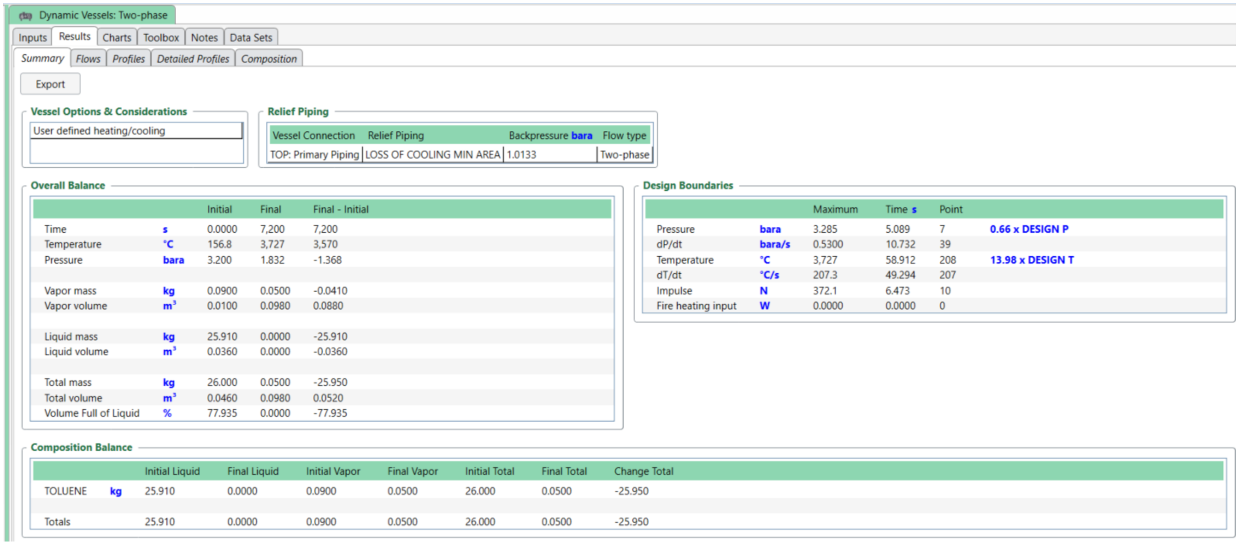


Figure 101: Dynamic simulation results (toluene) - isentropic & VdP

Figure 102 shows the results for a dynamic simulation using the isenthalpic thermodynamic flow path and the VdP nozzle flow method.

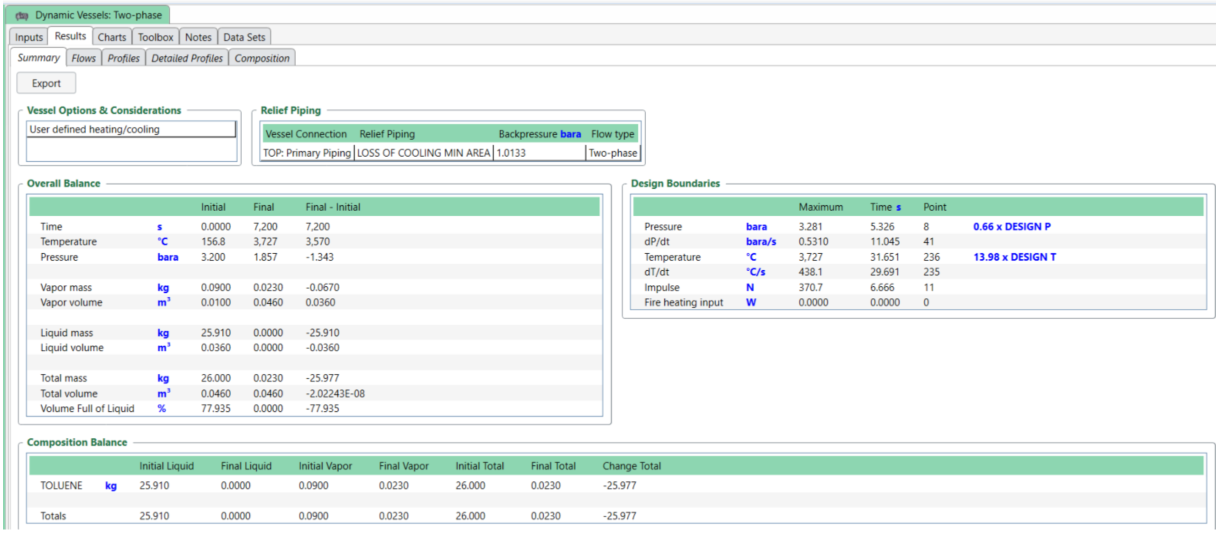
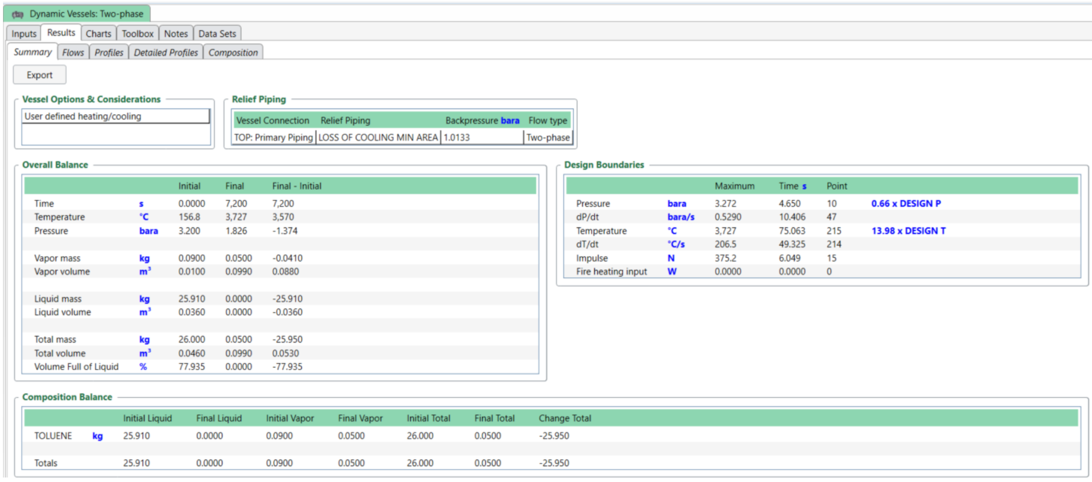


Figure 102: Dynamic simulation results (toluene) - isenthalpic & VdP

Figure 103 shows the results for a dynamic simulation using the isenthalpic thermodynamic flow path and the dH nozzle flow method.



Dynamic Vessels: Two-phase

Inputs | Results | Charts | Toolbox | Notes | Data Sets

Summary | Flows | Profiles | Detailed Profiles | Composition

Export

Vessel Options & Considerations

User defined heating/cooling

Relief Piping

Vessel Connection	Relief Piping	Backpressure bara	Flow type
TOP: Primary Piping	LOSS OF COOLING MIN AREA	1.0133	Two-phase

Overall Balance

		Initial	Final	Final - Initial
Time	s	0.0000	7,200	7,200
Temperature	°C	156.8	3,727	3,570
Pressure	bara	3.200	1.826	-1.374
Vapor mass	kg	0.0900	0.0500	-0.0410
Vapor volume	m^3	0.0100	0.0990	0.0880
Liquid mass	kg	25.910	0.0000	-25.910
Liquid volume	m^3	0.0360	0.0000	-0.0360
Total mass	kg	26.000	0.0500	-25.950
Total volume	m^3	0.0460	0.0990	0.0530
Volume Full of Liquid	%	77.935	0.0000	-77.935

Design Boundaries

		Maximum	Time s	Point	
Pressure	bara	3.272	4.650	10	0.66 x DESIGN P
dP/dt	bara/s	0.5290	10.406	47	
Temperature	°C	3,727	75.063	215	13.98 x DESIGN T
dT/dt	°C/s	206.5	49.325	214	
Impulse	N	375.2	6.049	15	
Fire heating input	W	0.0000	0.0000	0	

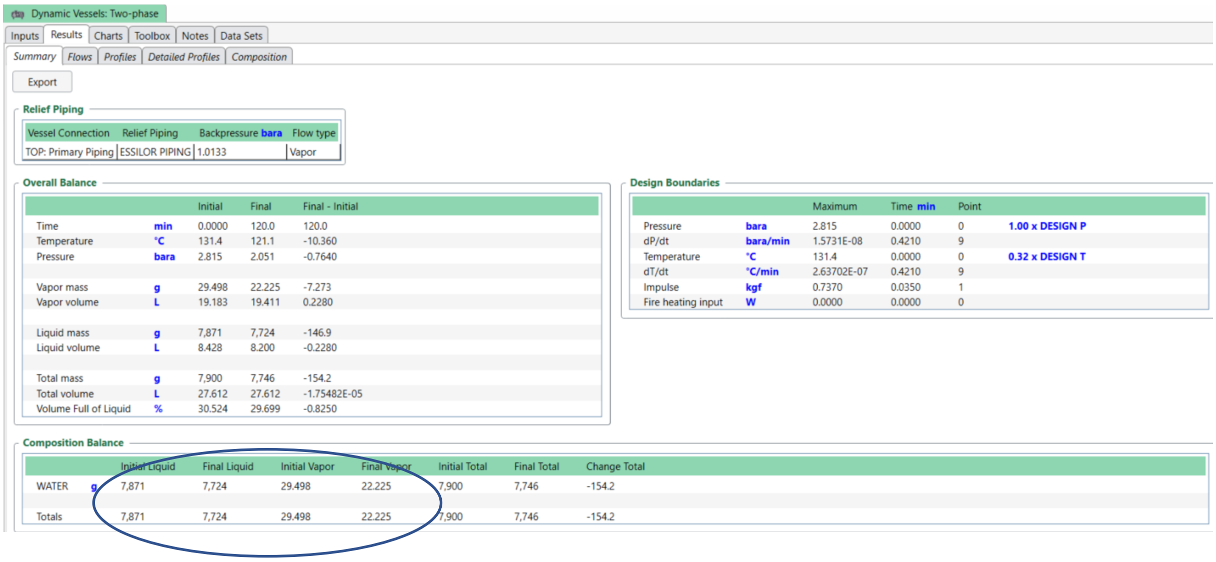
Composition Balance

		Initial Liquid	Final Liquid	Initial Vapor	Final Vapor	Initial Total	Final Total	Change Total
TOLUENE	kg	25.910	0.0000	0.0900	0.0500	26.000	0.0500	-25.950
Totals		25.910	0.0000	0.0900	0.0500	26.000	0.0500	-25.950

Figure 103: Dynamic simulation results (toluene) - isenthalpic & dH

9.1.14 SuperChems – Example for a dynamic two-phase relief

Figure 104 shows an example of the results menu for two-phase relief in SuperChems.



Dynamic Vessels: Two-phase

Inputs | Results | Charts | Toolbox | Notes | Data Sets

Summary | Flows | Profiles | Detailed Profiles | Composition

Export

Relief Piping

Vessel Connection	Relief Piping	Backpressure bara	Flow type
TOP: Primary Piping	ESSILOR PIPING	1.0133	Vapor

Overall Balance

		Initial	Final	Final - Initial
Time	min	0.0000	120.0	120.0
Temperature	°C	131.4	121.1	-10.360
Pressure	bara	2.815	2.051	-0.7640
Vapor mass	g	29.498	22.225	-7.273
Vapor volume	L	19.183	19.411	0.2280
Liquid mass	g	7,871	7,724	-146.9
Liquid volume	L	8.428	8.200	-0.2280
Total mass	g	7,900	7,746	-154.2
Total volume	L	27.612	27.612	-1.75482E-05
Volume Full of Liquid	%	30.524	29.699	-0.8250

Design Boundaries

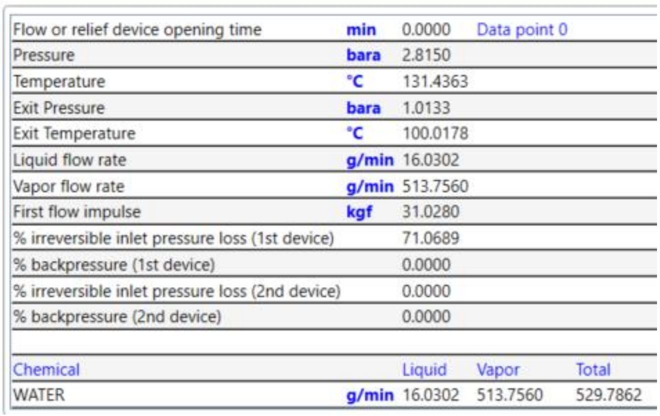
		Maximum	Time min	Point	
Pressure	bara	2.815	0.0000	0	1.00 x DESIGN P
dP/dt	bara/min	1.5731E-08	0.4210	9	
Temperature	°C	131.4	0.0000	0	0.32 x DESIGN T
dT/dt	°C/min	2.63702E-07	0.4210	9	
Impulse	kgf	0.7370	0.0350	1	
Fire heating input	W	0.0000	0.0000	0	

Composition Balance

		Initial Liquid	Final Liquid	Initial Vapor	Final Vapor	Initial Total	Final Total	Change Total
WATER	g	7,871	7,724	29.498	22.225	7,900	7,746	-154.2
Totals		7,871	7,724	29.498	22.225	7,900	7,746	-154.2

Figure 104: External fire - dyanmic two-phase relief example

Figure 105 shows the result values for a two-phase relief first flow.



Flow or relief device opening time	min	0.0000	Data point 0	
Pressure	bara	2.8150		
Temperature	°C	131.4363		
Exit Pressure	bara	1.0133		
Exit Temperature	°C	100.0178		
Liquid flow rate	g/min	16.0302		
Vapor flow rate	g/min	513.7560		
First flow impulse	kgf	31.0280		
% irreversible inlet pressure loss (1st device)		71.0689		
% backpressure (1st device)		0.0000		
% irreversible inlet pressure loss (2nd device)		0.0000		
% backpressure (2nd device)		0.0000		
Chemical		Liquid	Vapor	Total
WATER	g/min	16.0302	513.7560	529.7862

Figure 105: External fire - two-phase relief first flow composition

9.2 ChemCad – Step-by-step documentation

After opening the ChemCad program, the engineering units must be selected under the “home – engineering units” tab. A user specific profile can be created. In this case, the units were adapted to fit TÜV SÜD’s project units.

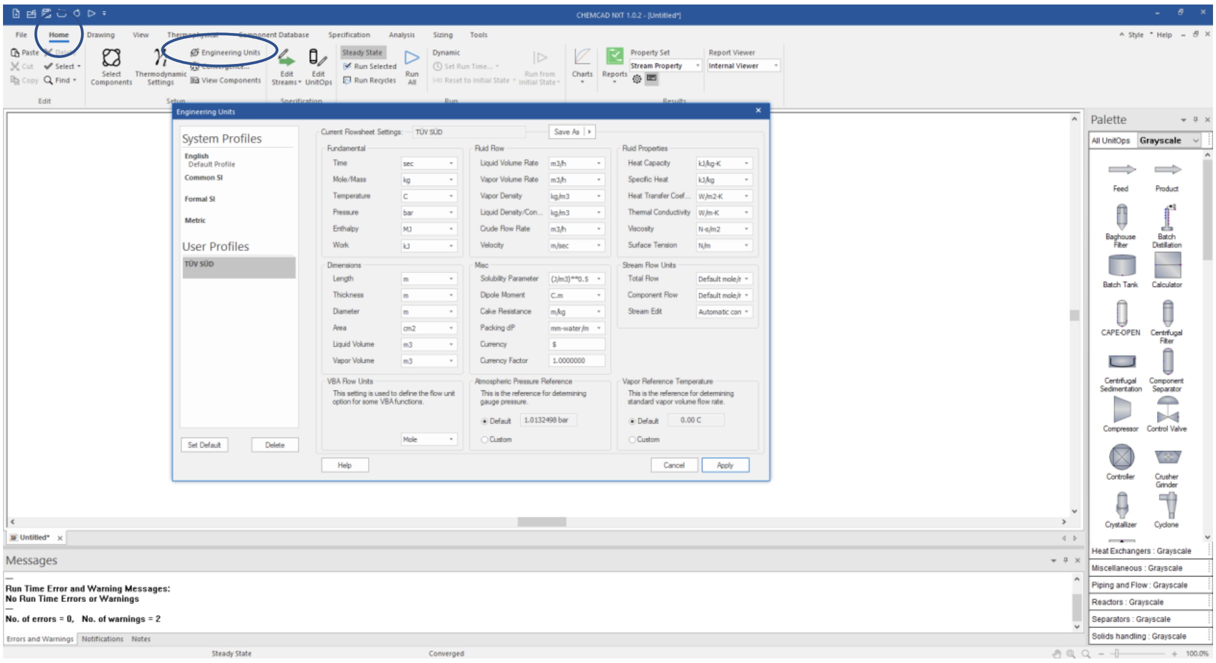


Figure 106: Selecting engineering units

9.2.1 Select components

To choose components from the ChemCad database, the “home - select components” tab is used. In this example simulation, Toluene is chosen as the only component.

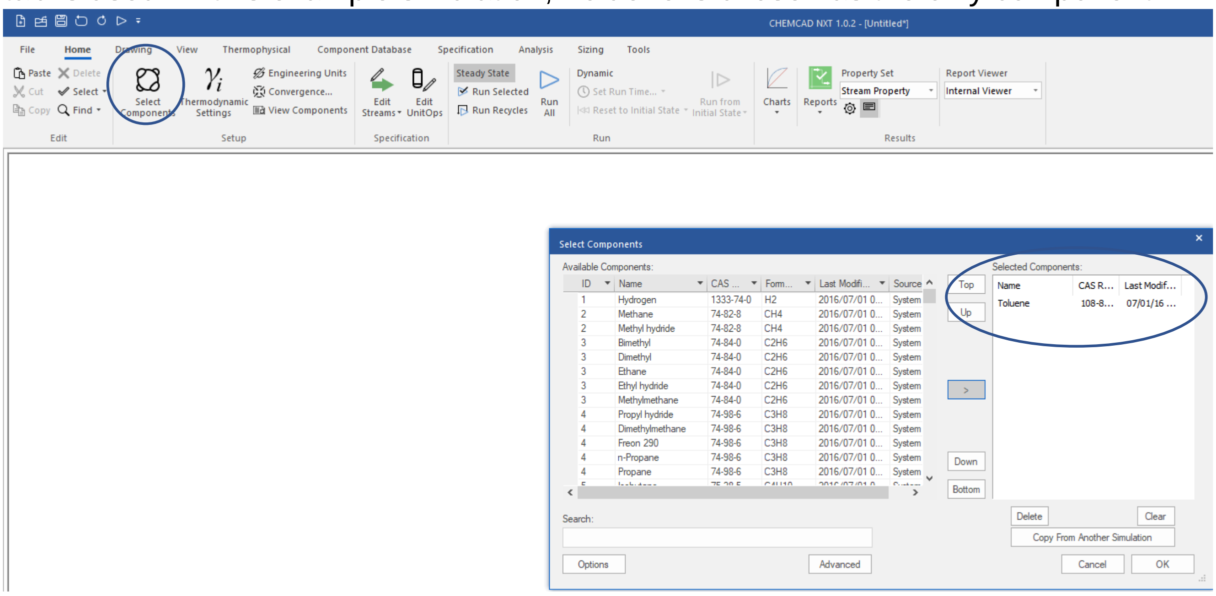


Figure 107: Selecting components

9.2.2 Select thermodynamic model

After the selection of the components, ChemCad asks for a user input regarding process temperature and pressure range to suggest thermodynamic models. The suggestions are made based on the temperature and pressure range as well on the components selected for the simulation. In this example, toluene is the only component and therefore the ideal vapor model is sufficient. If a mixture is used for the simulation, other thermodynamic models are suggested depending on the process parameters.

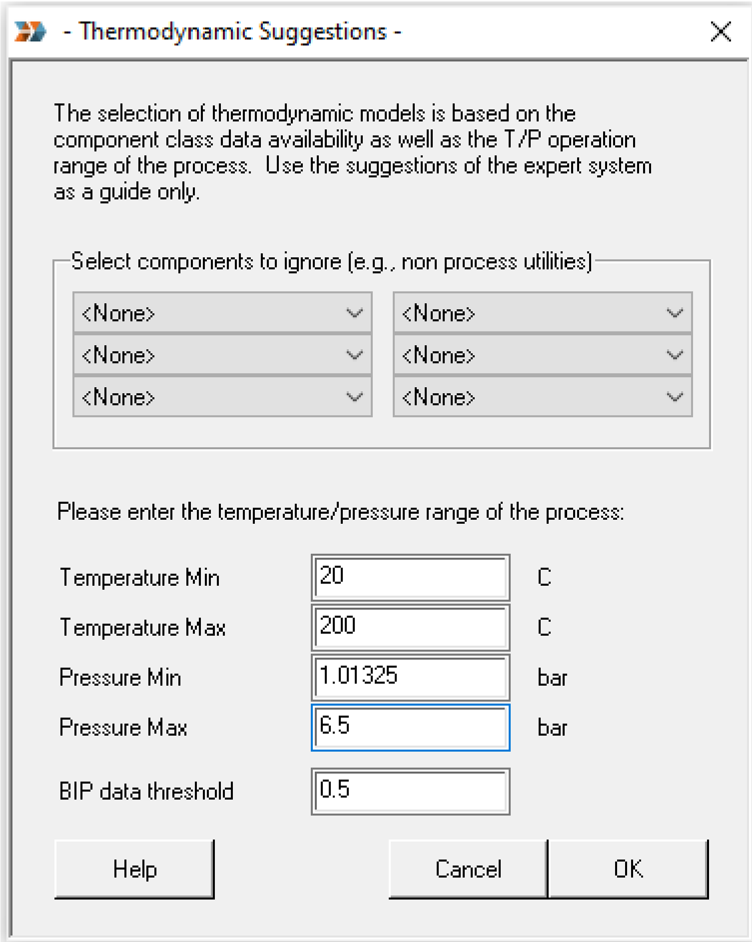


Figure 108: Thermodynamic suggestions menu

The suggested K-model is the ideal vapor pressure model, and the suggested enthalpy model is the latent heat model.

Figure 109: Thermodynamic model suggestion

The suggested models will be used for the simulations. The suggestions are being repeated for every new case.

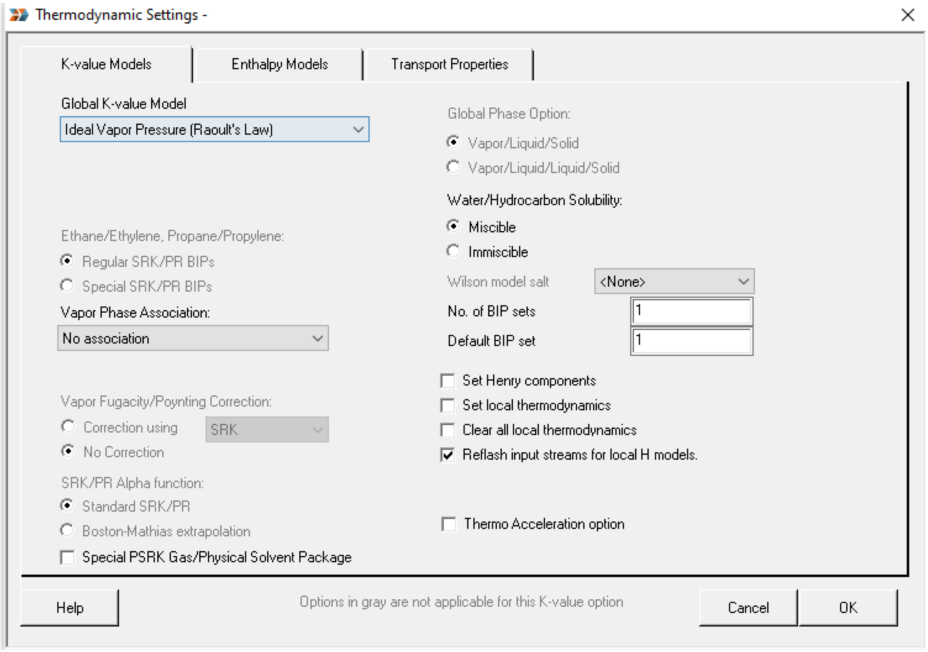


Figure 110: Thermodynamic settings menu (K-value)

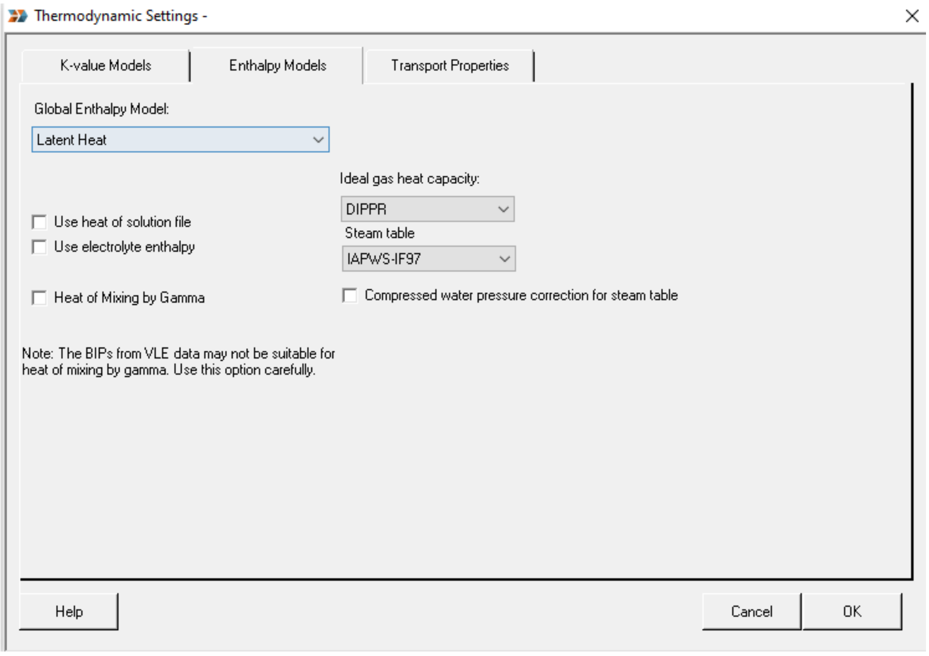


Figure 111: Thermodynamic settings menu (enthalpy)

9.2.3 Create feed and product stream

Using the drag and drop option of ChemCad, a feed and product arrows can be created on the user interface. Feed and product must be connected by clicking on the feed arrow and dragging it to the product arrow. ChemCad automatically creates a stream. In this example the created stream has the number one.

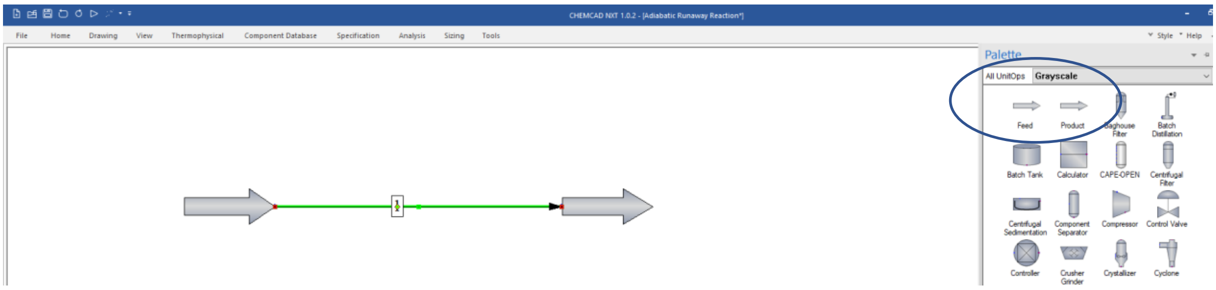


Figure 112: Feed and product arrow creation

To start the sizing calculation, the feed stream must be specified. By double-clicking on the feed arrow, the “edit streams” menu opens. Temperature, pressure and vapor fraction define a stream. Two of these three parameters must be entered for a flash calculation of the missing parameter. In this example, temperature and pressure are entered. The vapor fraction is then calculated by ChemCad. Furthermore, the stream composition must be entered. In this example toluene is the only component and is therefore set to “one”.

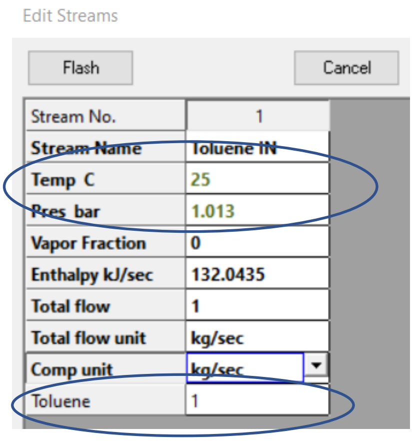


Figure 113: Inlet stream specification

9.2.4 Relief device sizing

To do a relief device sizing calculation, the "sizing – relief device" tab must be selected. A stream must be selected by clicking on the number.

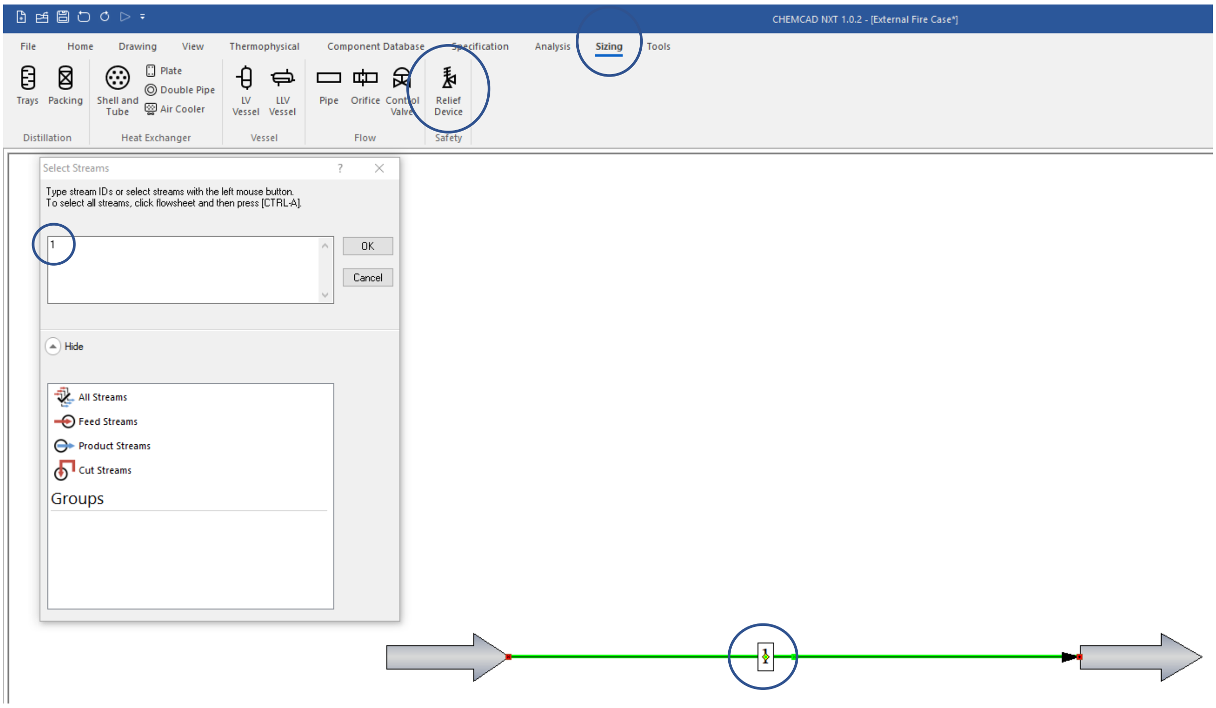
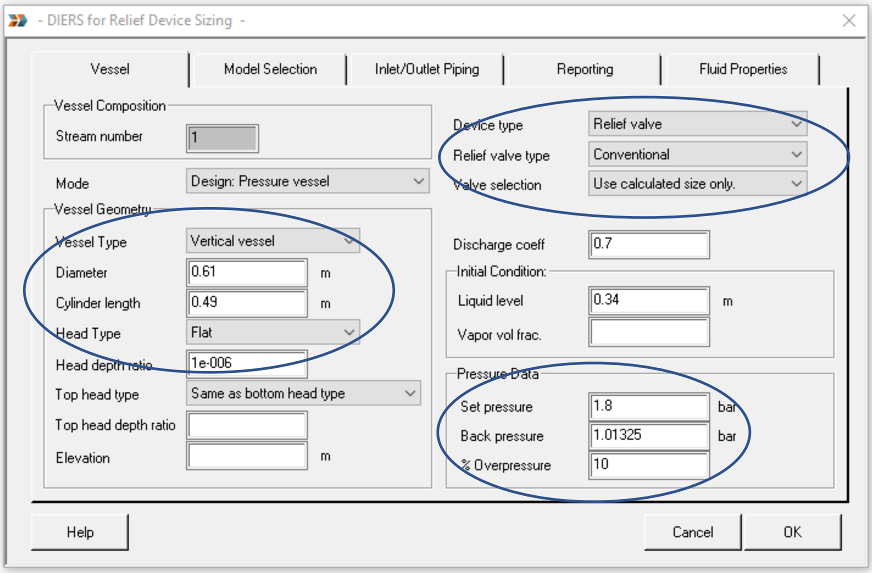


Figure 114: Basic relief device sizing – external fire case

9.2.5 Enter vessel and Relief device data

Vessel and relief data must be entered in the DIERS for Relief Device Sizing menu. In the device type section, the device type must be selected and if the relief device area will be calculated exactly or if the next best device is chosen from the API table.



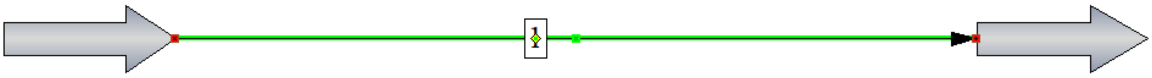


Figure 115: Basic relief device sizing menu (vessel and relief device type) – external fire case

9.2.6 Choose vessel and heat model

Under the model selection tab, the design method, latent heat option and the vessel model must be chosen. The average value latent heat option is the method used in DIERS and API. It uses the average of latent heats of vaporization for components to calculate the vent. Also, the environmental factor must be entered. If adequate fire facilities exist, the respective checkbox must be checked. Furthermore, the desired heat model must be selected. An additional heat rate can always be entered in the respective section.

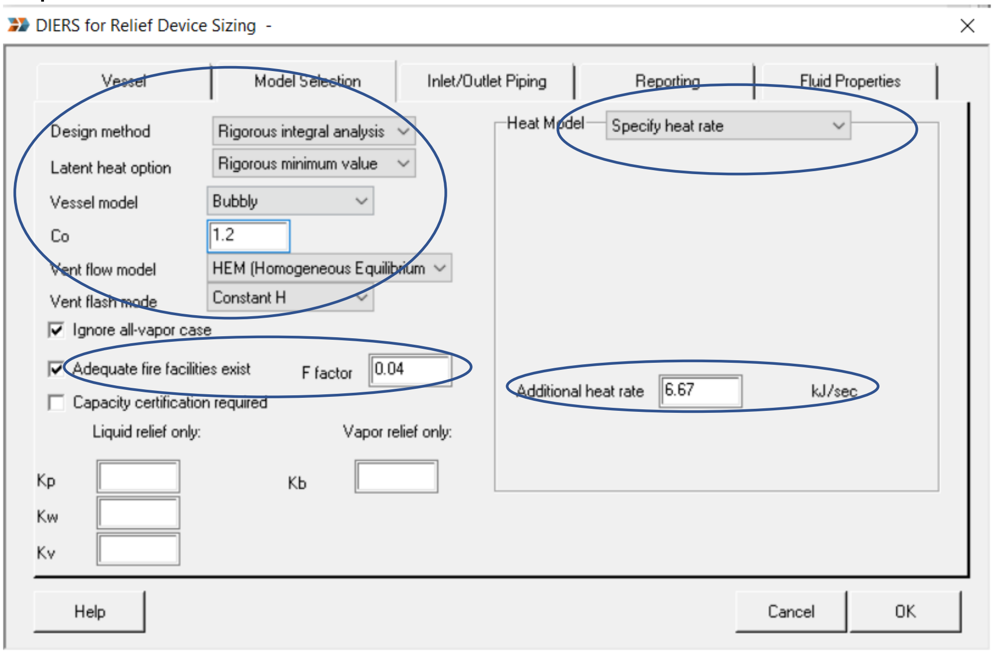


Figure 116: Basic relief device sizing menu (model selection) – external fire case

9.2.7 Specify piping

Inlet and outlet piping can be specified in the inlet/outlet piping tab. In this example, no piping was present and therefore this section is left blank.

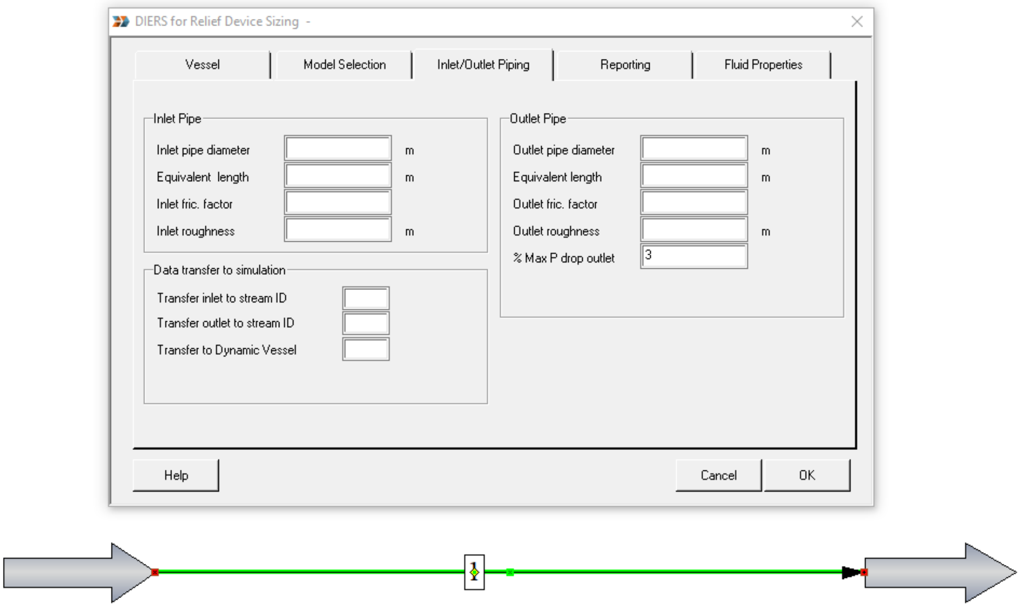


Figure 117: Basic relief device sizing menu (inlet/outlet piping) – external fire case

9.2.8 Run the simulation

The simulation can now be run by pressing the OK button.

9.2.9 Results – external fire case (steady state)

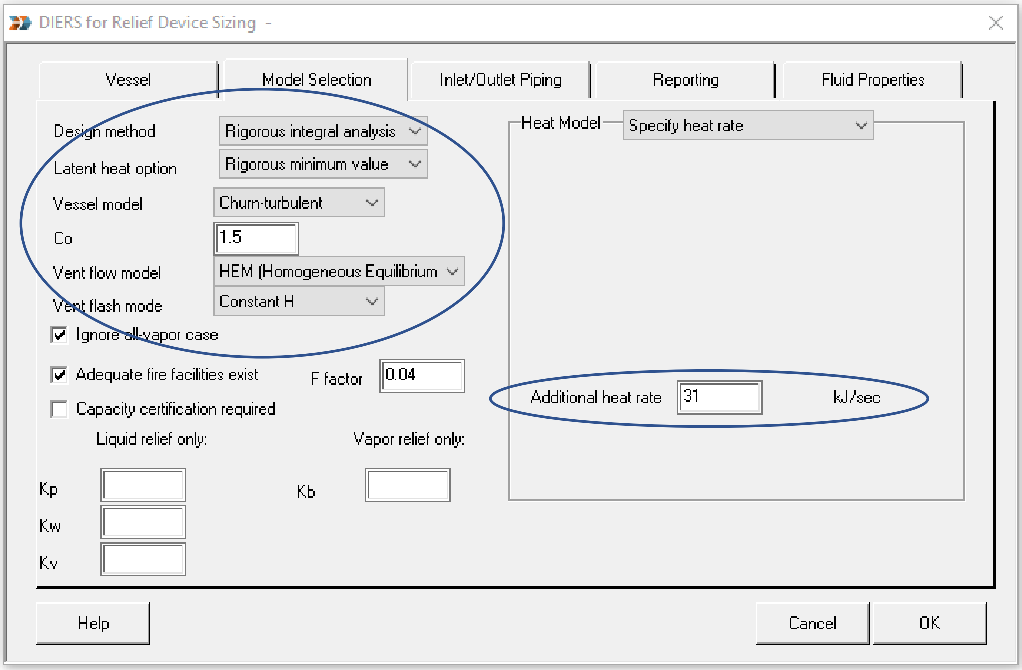
Figure 118 shows the sizing report for the external fire case. Vent rate and vent area as well as additional output information can be found in the bottom section of the report.

```
Relief Device Sizing for Stream 1

Device type: Relief valve
Valve type: Conventional valve
Vent model: HEM (Homogeneous Equilibrium Model)
Vessel model: Bubbly model
Design model: Specify heat rate
Specified heat rate:                     6.67 kJ/sec
Design, Pressure vessels.
Rigorous integral analysis used for design case.
Vertical vessel
Head type: Flat
Head K factor (dpth / R):                   0

Vessel dimensions:
Diameter:                                0.61 m
Length (T to T):                         0.49 m
Vessel volume:                         0.1432 m3
Liquid level:                            0.34 m
Initial vapor volume fraction:        0.30612
Height above ground:                        0 m

Fluid properties:
Vapor mass:                           0.23631 kg
Liquid mass:                           75.026 kg
Vapor density:                         5.3907 kg/m3
Liquid density:                        755.07 kg/m3
Surface tension:                     0.015687 N/m
Liquid viscosity:                  0.00019485 N-s/m2
Vapor Z factor:                       0.94879
Cp/Cv:                                 1.0817
Vapor MW                               92.141
Liquid heat capacity:                  2.0968 kJ/kg-K
Latent heat:                           346.26 kJ/kg

Relief device analysis:
Set pressure:                             1.8 bar
Back pressure:                         1.0132 bar
% Overpressure                             10
Temperature:                           133.91 C
Discharge coefficient:                    0.7
C0 radial distribution parameter:         1.2
* Pb/Pmax > 0.5 for conventional valve.
Kb Backpressure corr. factor:         0.99337
Heat rate:                               6.67 kJ/sec
Vent area based on all vapor vent is used.

Calculated nozzle area:               0.44033 cm2
Rate based on area:                   0.44033 cm2
Calculated vent rate                 0.019244 kg/sec
Calc critical rate                   0.019244 kg/sec
Calc critical press                    1.1057 bar
Nozzle inlet vap. mass fraction:            1
Device inlet density:                  5.3907 kg/m3
Nozzle inlet vap. vol. fraction:            1
```

Figure 118: Results report external fire case (steady state)

9.2.10 Maximum Heating case

To size the maximum heating case, another simulation stream can be created within the same project file. By repetition of the previously described steps, another stream is created. Vessel and compound specification must be repeated. The thermodynamic models will stay active for the whole simulation file and do not have to be chosen again. To account for the maximum heating case, the "sizing – relief device" tab must be clicked, and the respective stream must be selected. After the definition of the vessel geometry (same vessel as in the external fire case) the models must be chosen, and the heat rate must be specified. In this example, the heat rate for maximum heating is 31kW.



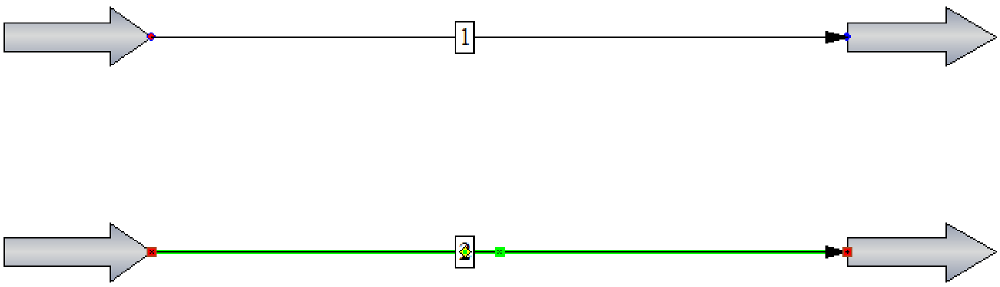


Figure 119: Basic relief device sizing menu (model selection) - maximum heating case

9.2.11 Result - maximum heating case (steady state)

Figure 120 shows the sizing report for the maximum heating case. Again, the vent area and rate can be found in the bottom section of the report.

```
Relief Device Sizing for Stream 2

Device type: Relief valve
Valve type: Conventional valve
Vent model: HEM (Homogeneous Equilibrium Model)
Vessel model: Churn turbulent model
Design model: Specify heat rate
Specified heat rate:                        31 kJ/sec
Design, Pressure vessels.
Rigorous integral analysis used for design case.
Vertical vessel
Head type: Flat
Head K factor (dpth / R):                    0

Vessel dimensions:
Diameter:                                 0.61 m
Length (T to T):                          0.49 m
Vessel volume:                          0.1432 m3
Liquid level:                             0.34 m
Initial vapor volume fraction:         0.30612
Height above ground:                         0 m

Fluid properties:
Vapor mass:                            0.23631 kg
Liquid mass:                            75.026 kg
Vapor density:                          5.3907 kg/m3
Liquid density:                         755.07 kg/m3
Surface tension:                      0.015687 N/m
Liquid viscosity:                   0.00019485 N-s/m2
Vapor Z factor:                        0.94879
Cp/Cv:                                  1.0817
Vapor MW                                92.141
Liquid heat capacity:                   2.0968 kJ/kg-K
Latent heat:                            346.26 kJ/kg

Relief device analysis:
Set pressure:                              1.8 bar
Back pressure:                          1.0132 bar
% Overpressure                              10
Temperature:                            133.91 C
Discharge coefficient:                     0.7
C0 radial distribution parameter:          1.5
* Pb/Pmax > 0.5 for conventional valve.
Kb Backpressure corr. factor:          0.99337
Heat rate:                                  31 kJ/sec
Vent area based on all vapor vent is used.

Calculated nozzle area:                 2.0465 cm2
Rate based on area:                     2.0465 cm2
Calculated vent rate                  0.089438 kg/sec
Calc critical rate                    0.089438 kg/sec
Calc critical press                     1.1057 bar
Nozzle inlet vap. mass fraction:             1
Device inlet density:                   5.3907 kg/m3
Nozzle inlet vap. vol. fraction:             1
```

Figure 120: Results report maximum heating case

Relief Device Outlet Compositions

Stream No.	10104	10105
Name	Total	Vapor
- - Overall - -		
Molar flow kmol/sec	0.0010	0.0010
Mass flow kg/sec	0.0894	0.0894
Temp C	131.6579	131.6579
Pres bar	1.0132	1.0132
Vapor mole fraction	1.000	1.000
Enth kJ/sec	61.125	61.125
Tc C	318.6400	318.6400
Pc bar	41.0800	41.0800
Std. sp gr. wtr = 1	0.872	0.872
Std. sp gr. air = 1	3.181	3.181
Degree API	30.8079	30.8079
Average mol wt	92.1410	92.1410
Actual dens kg/m3	2.8522	2.8522
Actual vol m3/h	112.8864	112.8864
Std liq m3/h	0.3693	0.3693
Std vap 0 C m3/h	78.3221	78.3221

Figure 121: Relief device outlet compositions - maximum heating case

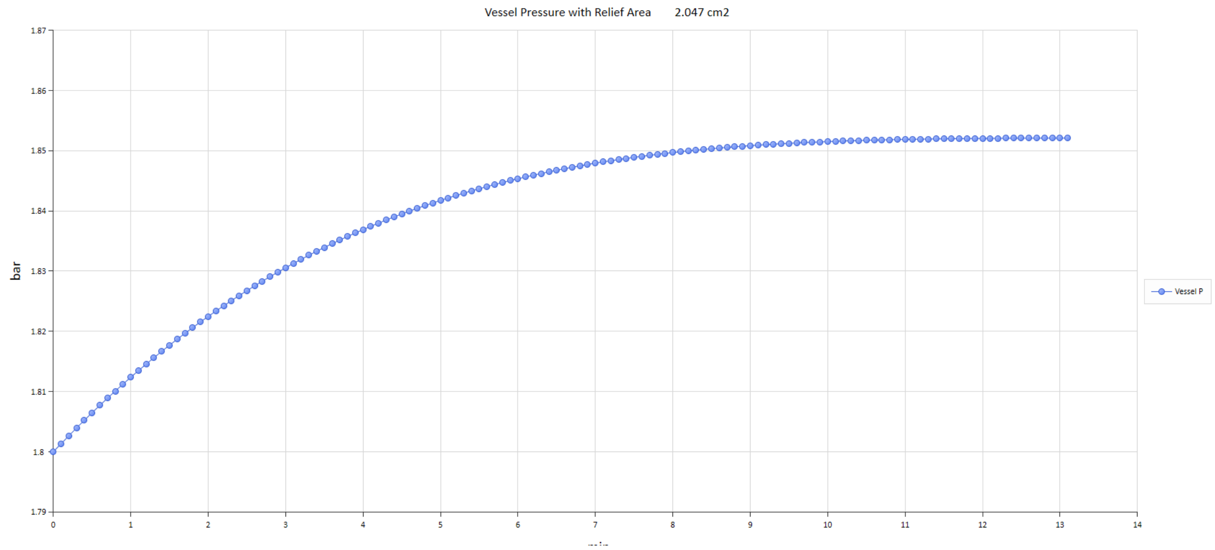


Figure 122: Vessel pressure curve - maximum heating case

9.2.12 Flowsheet creation – external fire case (dynamic method)

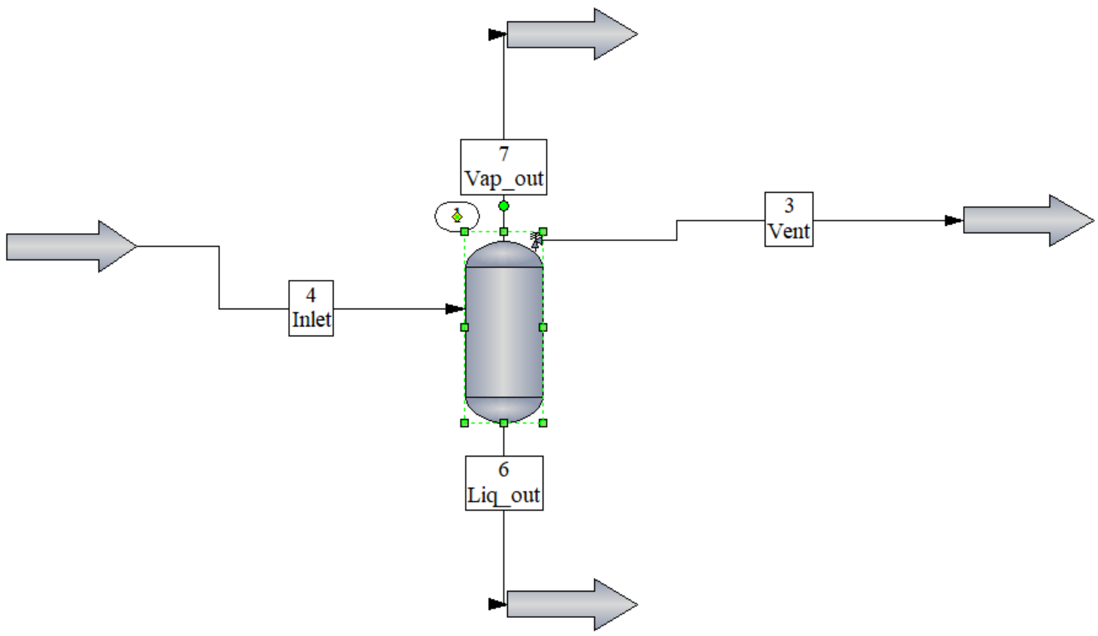


Figure 123: Flowsheet external fire case (dynamic method)

9.2.13 Stream specification

The inlet and charge streams must be defined by temperature, pressure, and vapor fraction. Two of the three must be entered for a flash calculation of the other parameter. The respective streams can be specified by clicking on them.

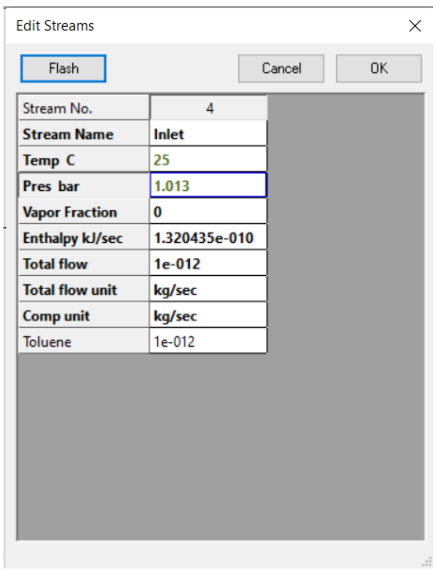


Figure 124: Inlet stream specification - external fire case (dynamic method)

Table 33 lists the stream input data for the dynamic fire case with specified heat input. The data for all vessel output streams are left blank since they will be calculated during the dynamic simulation. The inlet stream composition cannot be zero for simulation reasons (division by zero). The composition for the vessel charge is set to one since toluene is the only component (specify composition and liquid level).

Table 33: In- & outlet stream specifications - external fire case (dynamic method)

Stream	Inlet	Vapor_out	Liquid_out	Vent	Charge
Temperature [°C]	20	0	0	0	25
Pressure [bar]	1	0	0	0	1
Vapor fraction [-]	0	0	0	0	0
Composition [-]	1.00E-12	0	0	0	1

9.2.14 Dynamic mode and stream recording

To run a dynamic simulation in ChemCad, the dynamic option must be selected as Figure 125 shows. Also, the run time must be specified for the dynamic simulation. The "record streams" option can be used to record streams dynamically. ChemCad will output a dynamic chart of the chosen stream or unit operation.

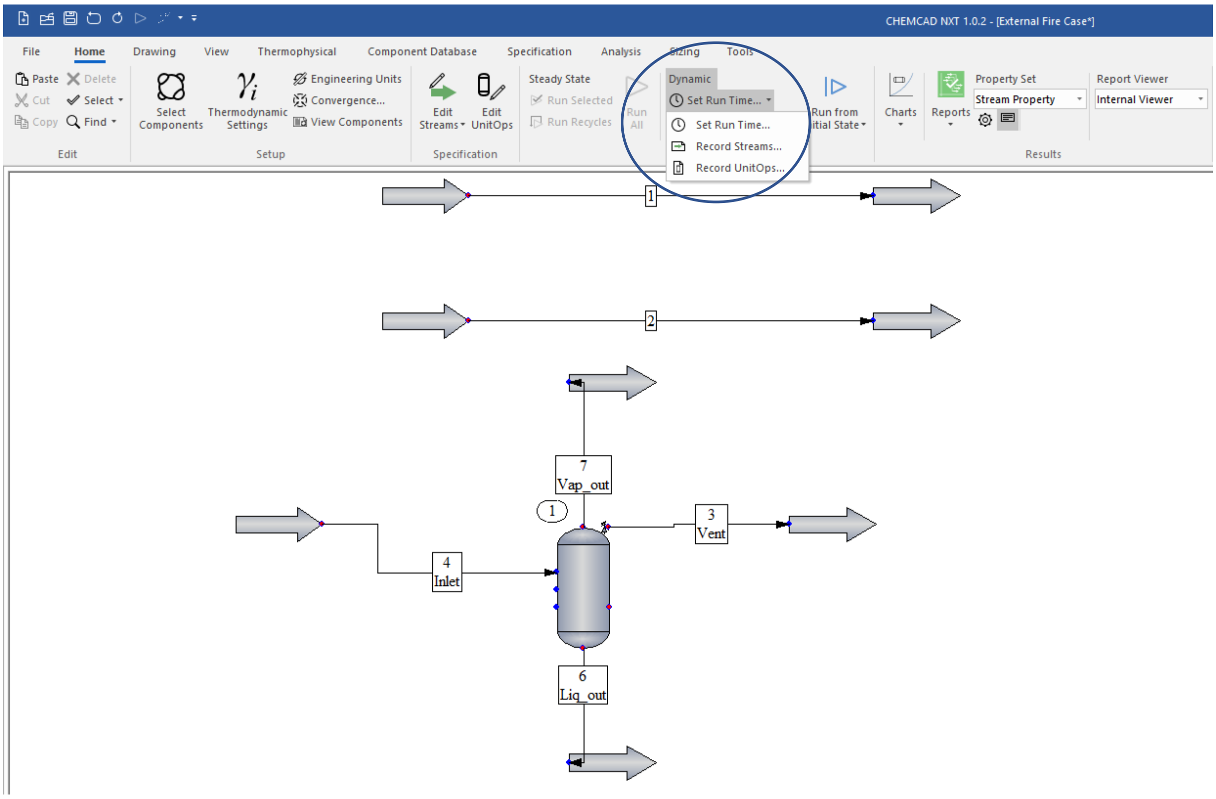


Figure 125: ChemCad dynamic mode – external fire case

To track the vessel pressure, the record unit operations tab must be selected and “unit operation one” is chosen. Also, the checkbox for “chart” is checked.

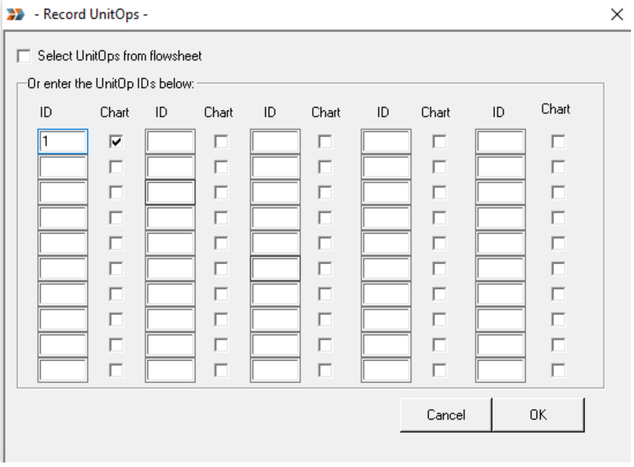


Figure 126: Equipment tracking (dynamic mode)

After clicking OK, “calculated pressure” is chosen as a variable and is acknowledged by clicking OK.

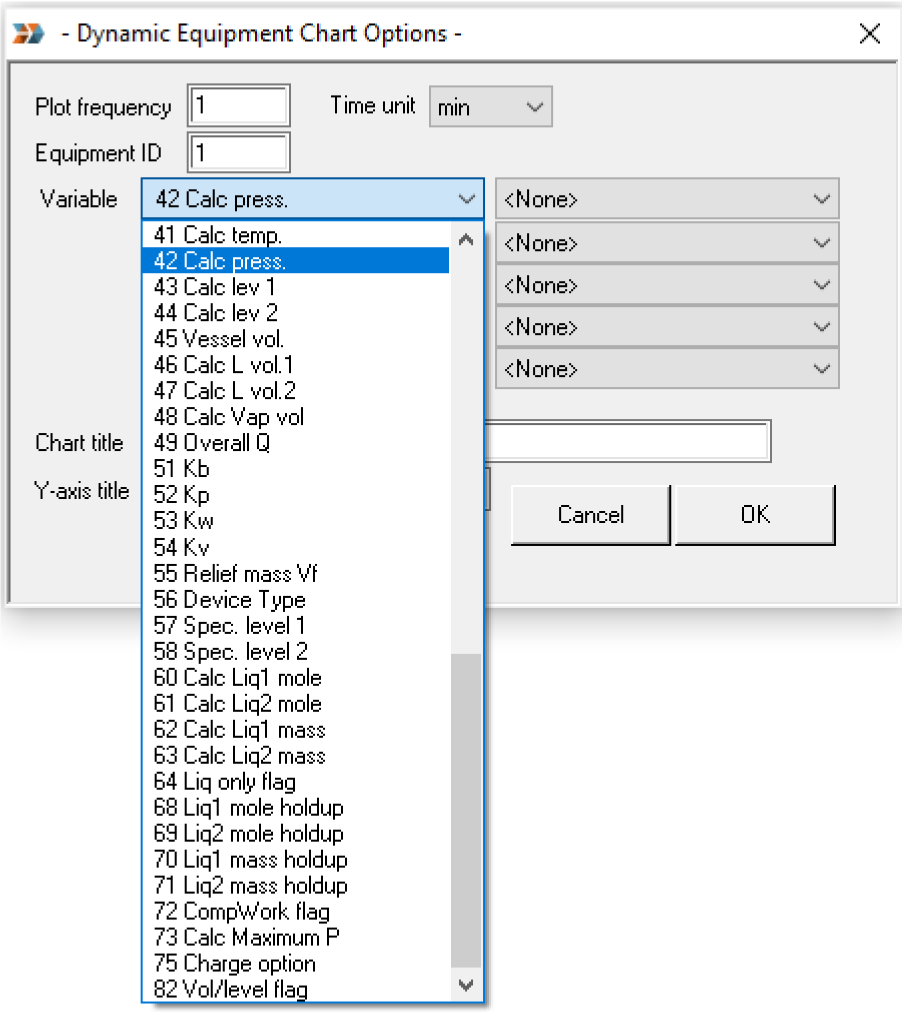


Figure 127: Plot creation for dynamic tracking

Stream must be selected for tracking during dynamic simulation for ChemCad to output the respective streams. The streams to be tracked are selected in the “dynamic – set run time – record streams” tab. The stream numbers can either be entered manually or can be selected from the flowsheet by clicking on them. To create a chart, the respective checkbox must be clicked as Figure 128 shows. In this example, the vent stream (stream number three) is being recorded.

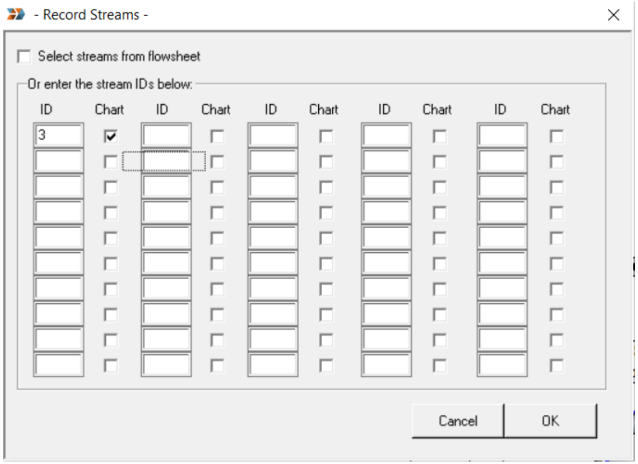


Figure 128: Stream tracking (dynamic mode)

9.2.15 Vessel and relief data input

After the specification of the streams, vessel and relief device data must be entered by double-clicking on the dynamic vessel symbol on the flowsheet. In the "general" tab in the dynamic vessel menu, the vessel geometry, the initial charge option as well as the thermal mode of the vessel is defined. In this example, the thermal mode is "flash with heat duty" and the heat input is 6.67 kW as in the steady state external fire simulation. This example uses the "specify composition and liquid level" initial charge option. Using this option, the initial liquid level and the charge composition must be defined. Since toluene is the only component in this example, the composition of the initial charge is one.

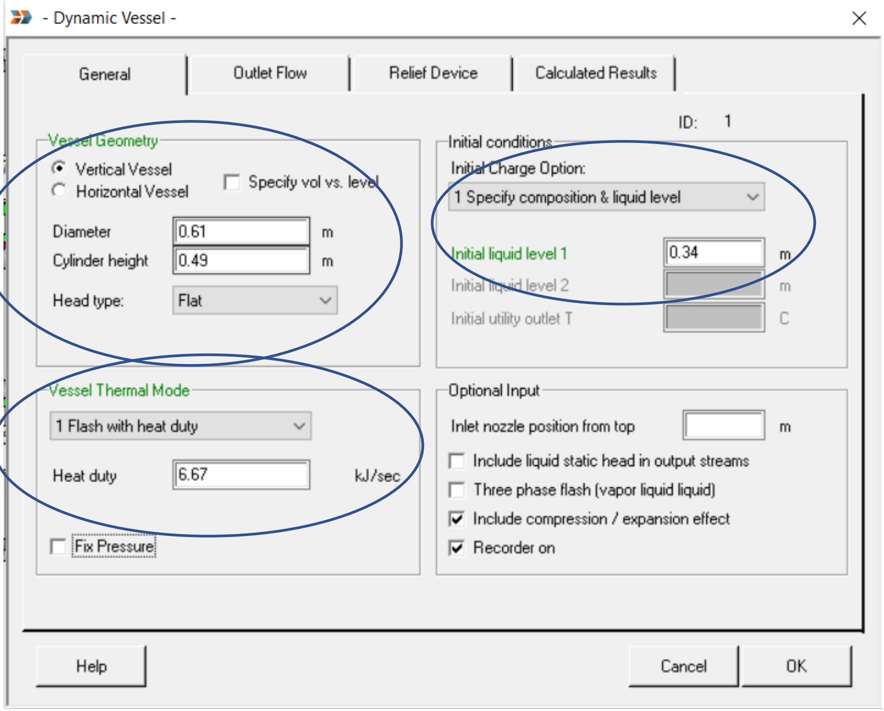


Figure 129: Dynamic vessel general menu (geometry, thermal mode & charge option) – external fire case

In the relief device section of the dynamic vessel menu the nozzle area from the steady state calculation is entered (in this case 0.4433 cm²). Also, the vessel model, the device type, relief data, vent flow model and the fire model must be entered. The “outlet flow” section is only of interest if continuous processes shall be simulated and is left blank in this example.

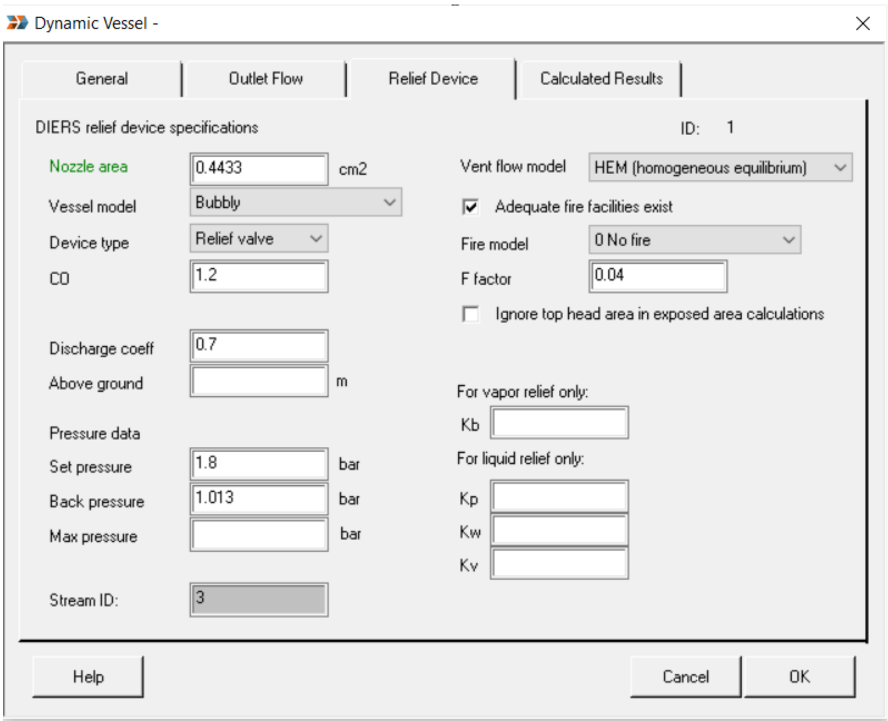


Figure 130: Dynamic vessel general menu (relief device & fire model) – external fire case

9.2.16 Vessel pressure and level – external fire case

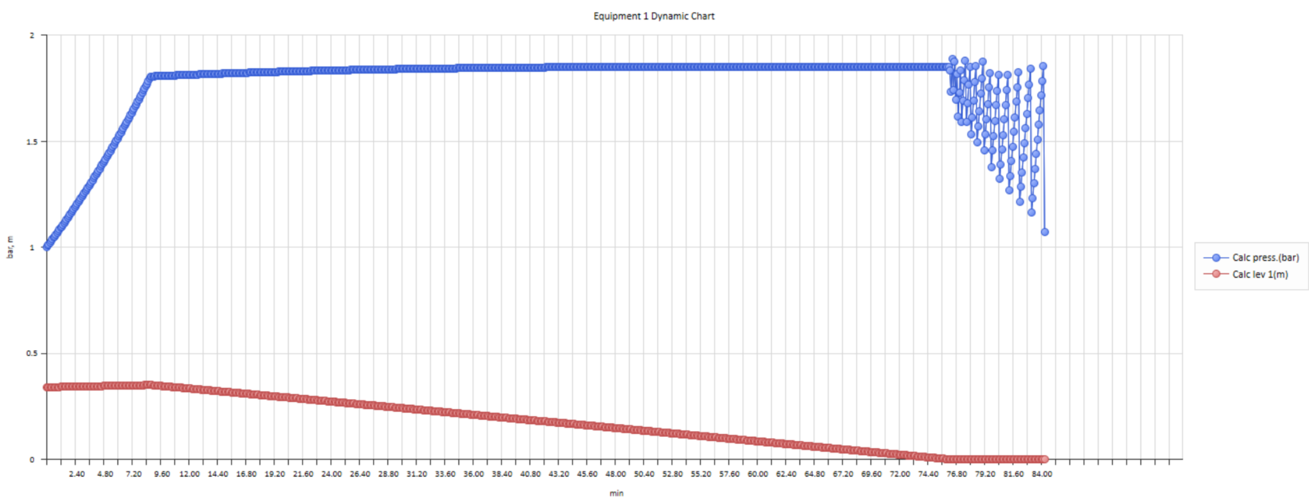


Figure 131: Vessel pressure and level (dynamic mode) – external fire case

9.2.17 Dynamic maximum heating simulation

The dynamic maximum heating case can be simulated either by specifying the heat load in the dynamic vessel general menu or by adding an additional utility stream to the simulation flow sheet as shown in Figure 132.

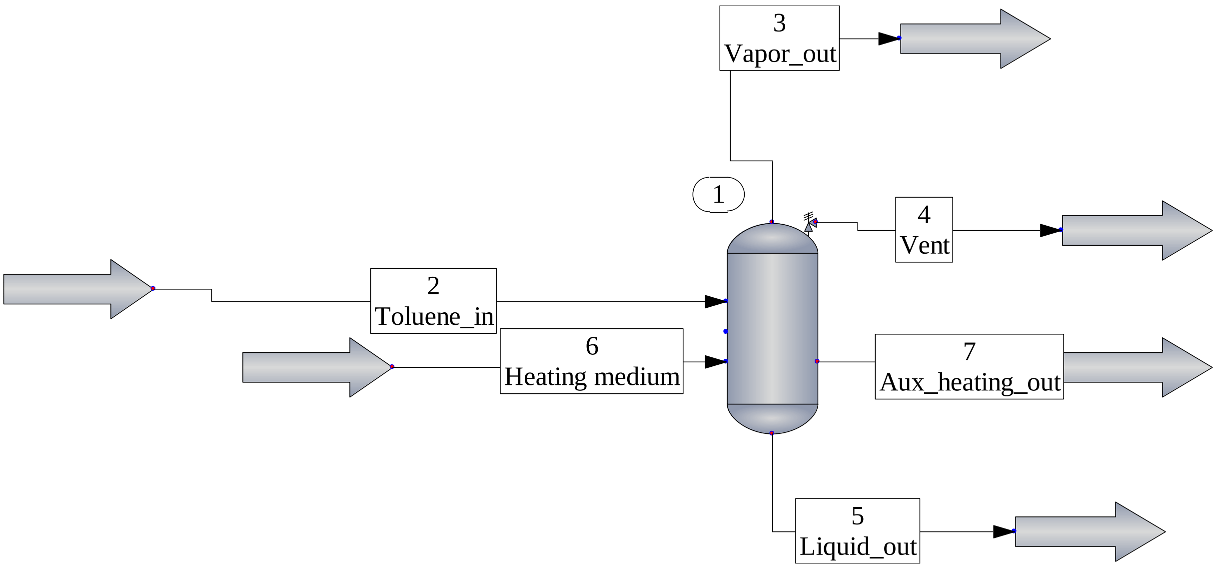


Figure 132: Flowsheet maximum heating case (dynamic method)

Table 34 lists the input and output stream as well as the vessel charge specifications. Again, the toluene inlet stream must have a very small composition for simulation reasons (division by zero).

Table 34: In- & outlet stream specifications (dynamic method) - maximum heating case

Stream	T [°C]	P [bar]	Vap. Fr. [-]	Comp. [-]	Component [-]
Toluene_in	25	1	0	1.00E-12	toluene
Heating_medium	151	5	1	1	water/steam
Vapor_out	0	0	0	0	toluene_vap
Liquid_out	0	0	0	0	toluene_liq
Vent	0	0	0	0	toluene_phase
Heating_out	0	0	0	0	water/steam
Charge	25	1	0	1	toluene

To simulate the maximum heating case, the heating medium stream must be adapted to fit the heat load. This can be done with the unit operation “heat exchanger” in combination with the unit operation “controller”. This way, the heating medium stream can be adapted to fit the heat load.

9.2.18 Heat exchanger and controller to adapt heat load

Figure 133 shows the heat exchanger and controller setup

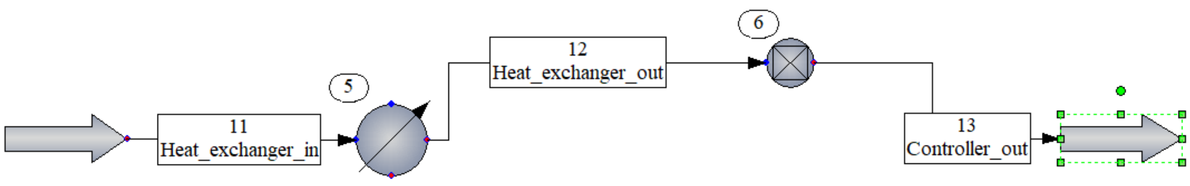
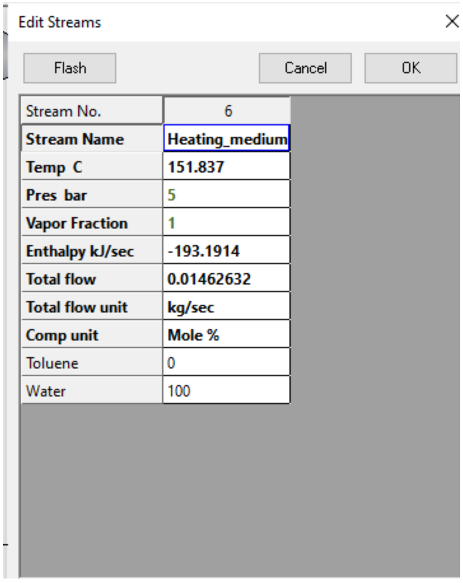


Figure 133: Heat exchanger & controller for heat load adaption - maximum heating case

Figure 134 shows the adapted heating medium stream to supply 31 kW heat load. This stream is copied and used as the heating medium inlet stream into the dynamic vessel.



Stream No.	6
Stream Name	Heating_medium
Temp C	151.837
Pres bar	5
Vapor Fraction	1
Enthalpy kJ/sec	-193.1914
Total flow	0.01462632
Total flow unit	kg/sec
Comp unit	Mole %
Toluene	0
Water	100

Figure 134: Inlet stream specification (dynamic method) - maximum heating case

Also, the dynamic vessel input information must be adapted for the “flash with UA & utility” case.

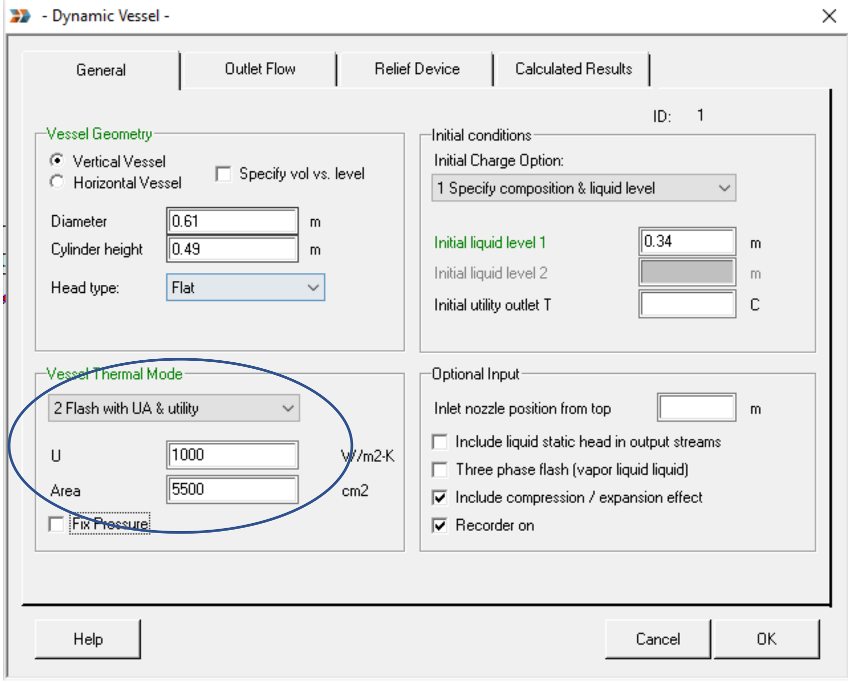


Figure 135: Dynamic vessel general menu (vessel geometry, thermal mode & charge option) - maximum heating case

The vent area must also be adapted for the maximum heating case. The vent area calculated in the steady state maximum heating case simulation must be entered.

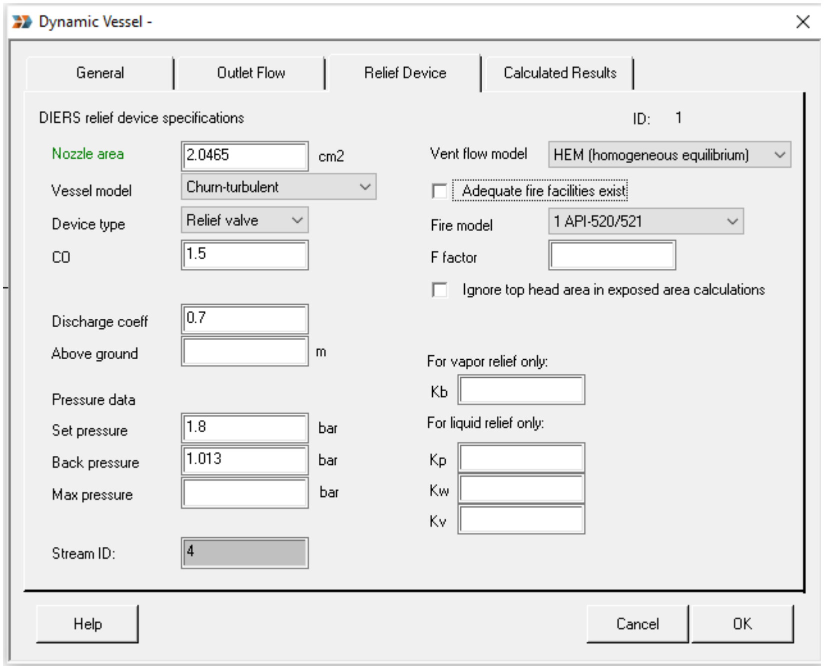


Figure 136: Dynamic vessel general menu (relief device & fire model) - maximum heating case

The simulation can now be run by clicking on the OK button.

9.2.19 Vessel pressure, level and total mass rate– maximum heating case

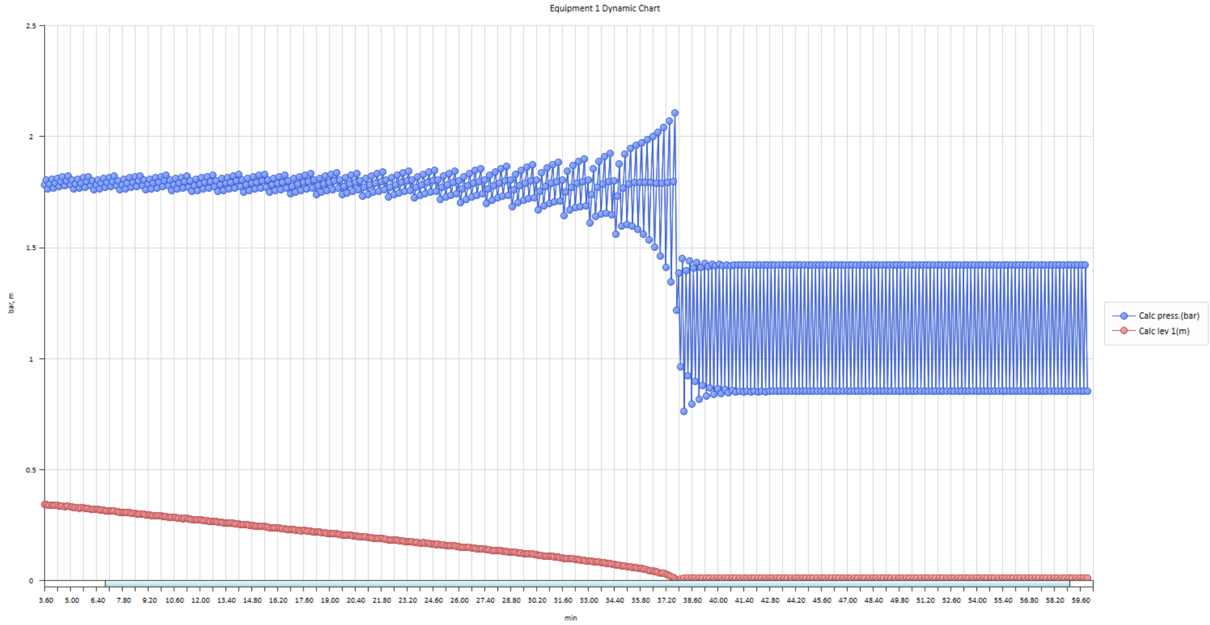


Figure 137: Vessel pressure and level - maximum heating case (dynamic method)

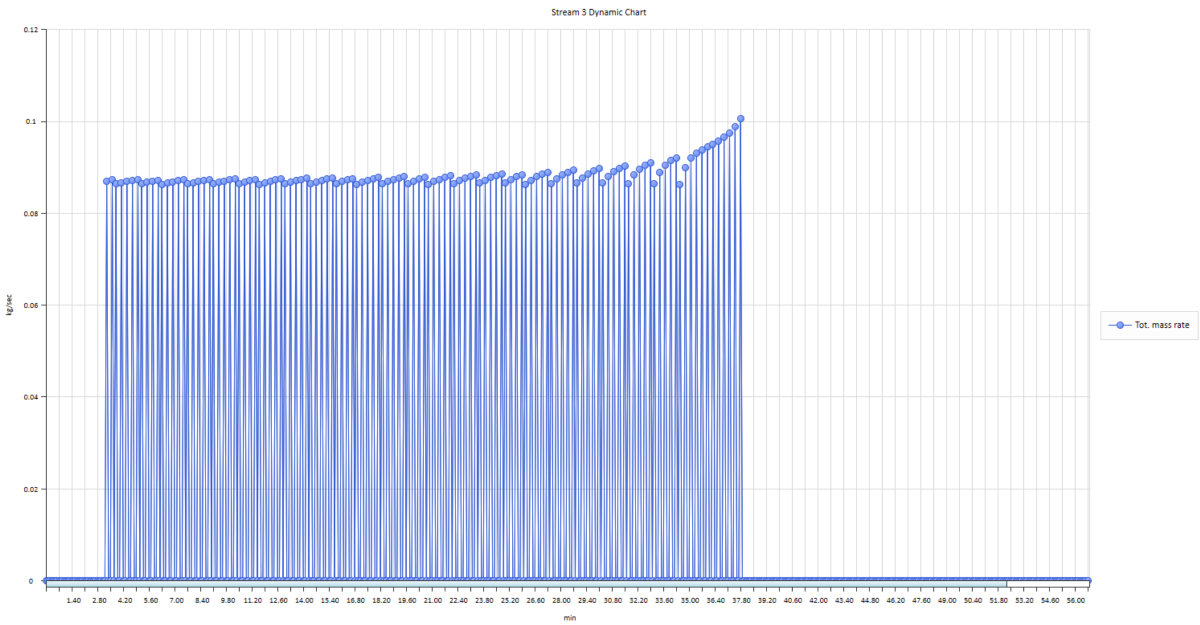


Figure 138: Total mass rate through relief valve - maximum heating case (dynamic method)

9.2.20 Maximum heating case with piping

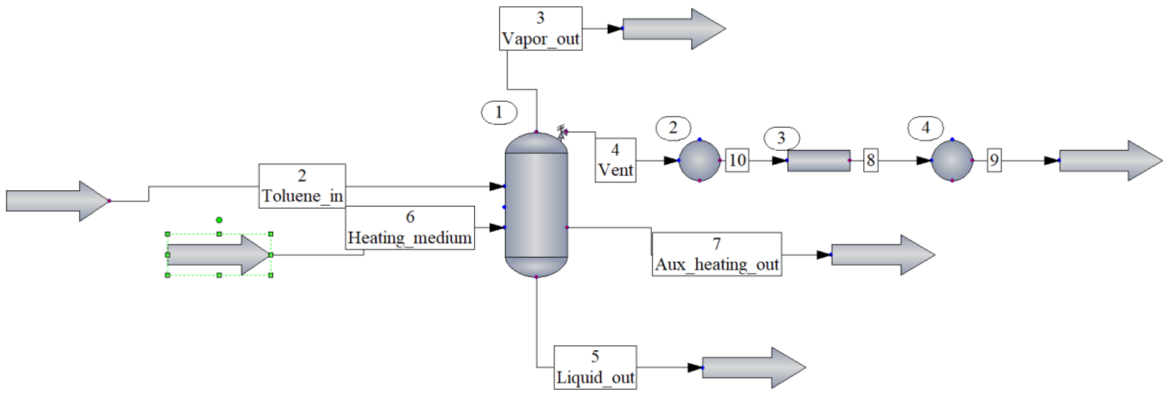


Figure 139: Flowsheet maximum heating case with piping (dynamic method)

9.2.21 Vessel pressure, level and relief piping pressure drop – maximum heating case with piping

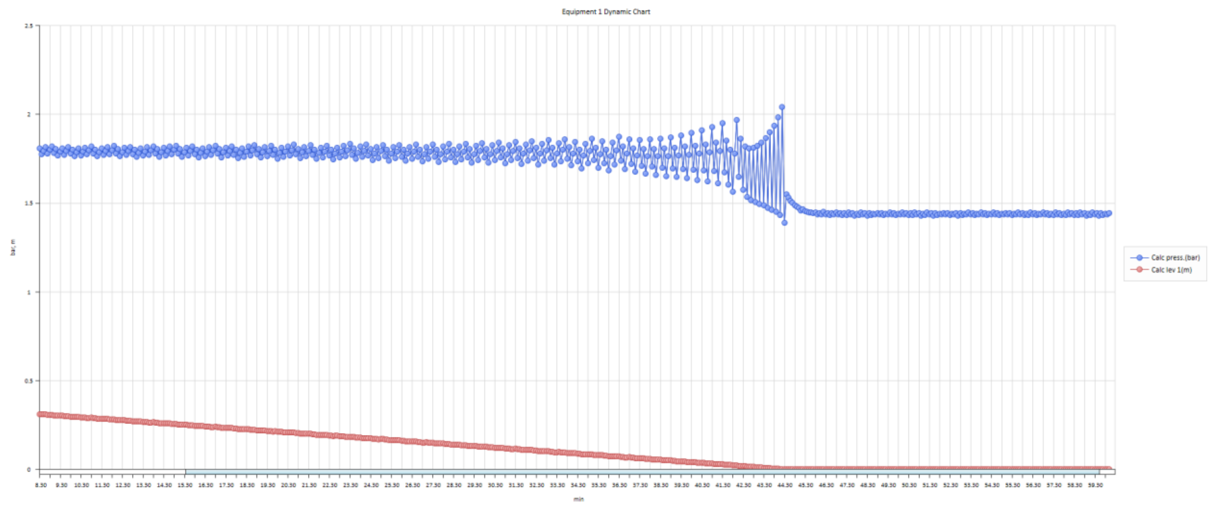


Figure 140: Vessel pressure and level - maximum heating case (dynamic method)

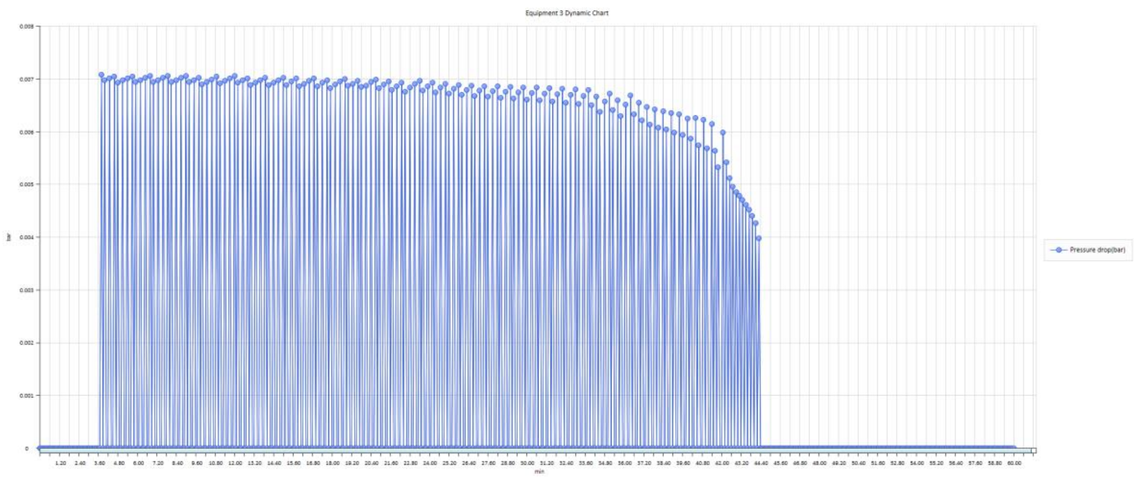


Figure 141: Relief piping path pressure drop - maximum heating case (dynamic method)

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11 Declaration of originality

I declare that I have authored this thesis independently, that I have not used other than the declared sources, and that I have explicitly marked all material which has been quoted either literally or by content from the used sources.

Basel, ……………………………….

Signature: …………………………..

Eidestattliche Erklärung

Ich erkläre an Eides statt, dass ich die vorliegende Arbeit selbstständig verfasst, andere als die angegebenen Quellen nicht benutzt, und die in den benutzten Quellen wörtlich und inhaltlich entnommenen Stellen als solche kenntlich gemacht habe.

Basel, ……………………………..

Unterschrift:……………………….

Danksagung

Ich möchte mich bei Frau Marie Sidow für die emotionale Unterstützung in dieser schwierigen Zeit bedanken, ohne welche die Arbeit deutlich mehr Energie gekostet hätte. Des Weiteren gilt mein Dank Frau Dr. Annik Nanchen für das Geben der Gewissheit, auf dem richtigen Weg zu sein und Frau Prof. Margret Bauer für die erfolgreiche Vermittlung an TÜV SÜD sowie Rückmeldungen zu meinem Fortschritt. Zudem gilt mein Dank Herrn Ingolf Gummin von DSM für die Einführung in ChemCad vor der Testlizenz und Herrn Prof. Francis Stoessel für die Erklärung thermodynamischer Modelle und Feedback zu meiner Thesis. Zusätzlich möchte ich mich bei den Supportteams von FlowNex und ChemCad für die sehr hilfreiche Unterstützung während der Testlizenzen bedanken. Zuletzt gilt mein Dank meinen Eltern für die finanzielle Unterstützung während des Studiums und das Durchsehen der Thesis.