

	Document No HLL-26-128-PRO-REP-02	Rev P1
	HLL Reactor Relief Study	

TITLE: Reactor Relief Study

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1.0 Executive Summary

Addison has undertaken a dynamic relief assessment of the proposed relief system for the HLL reactor. The purpose of the study was to determine whether the proposed DN150 reactor relief line and downstream knock-out system provide sufficient capacity to prevent the reactor pressure exceeding its Maximum Allowable Accumulated Pressure (MAAP) during the aluminium/caustic reaction.

The assessment considered the transient generation of hydrogen and reaction heat following charging of up to 16.2 kg of aluminium swarf. Reaction kinetics were represented using an Arrhenius relationship fitted to reaction-time data provided by HLL. As the available kinetic data is limited, sensitivity studies were undertaken to assess the effect of uncertainty in the fitted reaction parameters and other significant modelling assumptions.

The reactor transient was modelled using DIERS-based vessel hydrodynamics coupled with a Homogeneous Equilibrium Model (HEM) representation of the relief system. HEM was selected for the final vent-capacity assessment because the relief stream comprises water/steam together with a significant and changing concentration of non-condensable hydrogen. Under these conditions, the calculated DIERS Omega parameter may exceed the recommended range of applicability of the simplified Omega method. HEM explicitly represents the evolving multicomponent phase equilibrium and mixture properties during depressurisation and was therefore adopted as the best-estimate basis for relief-system capacity.

Alternative vessel disengagement models were considered. The bubbly-flow model was found to be the most onerous of the credible disengaging models. However, because the proposed relief connection is a side-mounted nozzle and the effect of this arrangement on the local phase composition at the relief take-off cannot be quantified with confidence, a non-disengaging foamy-flow assumption was adopted as a conservative bounding basis for the relief-stream composition. For the assessed cases, the proposed DN150 relief system provides sufficient capacity to arrest the pressure rise shortly after opening of the 4.5 barg burst disc. For the principal sensitivity cases, the maximum predicted reactor pressure was approximately 4.5 barg. A deliberately adverse bounding sensitivity was also undertaken using reduced relief-capacity factors, increased reaction kinetics and an initial reactor temperature of 140°C. This case predicted a maximum reactor pressure of 4.81barg, equivalent to approximately 73% of the 6.6barg MAAP.

The predicted reactor temperature rise during the pressure transient was less than 1°C. Consequently, for an initial reactor temperature of 140°C, the model predicts that the 145°C quench activation temperature would not be reached before the relief system arrests the pressure rise.

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The relief discharge is predicted to remain substantially two-phase for a significant part of the event. The downstream knock-out drum should therefore be capable of retaining the full reactor liquid inventory, approximately 1,400 L at ambient conditions. Allowing for vapour disengagement and freeboard, a total vessel volume of approximately 2,500L is recommended. The knock-out drum and downstream vent system should also be designed for the predicted transient backpressure, including the additional pressure drop associated with the final flame arrestor.

On the basis of the modelling assumptions and sensitivity cases assessed, the proposed DN150 reactor relief arrangement is predicted to provide sufficient capacity to prevent the reactor pressure exceeding its 6.6barg MAAP. **The conclusion remains subject to confirmation of the final relief-line geometry, knock-out drum arrangement, downstream vent-system resistance and the reaction kinetic data used as the basis of the assessment.**

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2.0 Input Data

Calculations are based on data provided by HLL. The reactor is modelled based on the supplied GA drawing and the mass balance used to set the initial reactor conditions. The 2-phase vent line from the reactor to the KO drum has been specified at DN150 with length and fittings as specified. The vapour vent line from the KO drum to atmosphere has been specified at DN100 with length and fittings as specified.

2.1 Kinetic Model

The kinetic model used in the simulation is a simple Arrhenius equation fit to 2 data points provided by HLL.

Temp [°C]	Time [m]
65	15-20
140	2-4

The quoted times represent the time required for the complete reaction of a 16.2 kg aluminium swarf charge, as defined in the project design basis. To provide a conservative kinetic representation, the lower bound of each reported time range (15 minutes and 2 minutes respectively) was used in the Arrhenius fit.

2.1.1 Model Limitations

The kinetic model is subject to the following limitations:

- The Arrhenius relationship is derived from only two experimental data points and should therefore be regarded as an engineering approximation.
- It is not known whether the reported reaction times were obtained from full-scale reactor trials or extrapolated from smaller-scale testing.
- The model does not account for any induction period associated with dissolution of the passive aluminium oxide layer by the KOH solution before significant hydrogen evolution begins.
- The reported data does not indicate whether the reaction was conducted under isothermal conditions. The model therefore assumes that the fitted Arrhenius relationship remains representative throughout the reaction.
- The reaction rate is assumed to vary only with temperature and the remaining aluminium inventory. Effects of changing particle morphology, surface area, mixing efficiency and mass transfer are not explicitly modelled.
- The reported data does not indicate whether the reaction rate remains constant throughout the reaction or decreases as the aluminium is consumed.

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3.0 Reactor Simulation

3.1 Model Inputs

The model is initiated at the operating pressure and temperature of the vessel, taken as 3.6 barg and sensitivities at 120°C, 130°C and 140°C were undertaken. From this initial state, the vapour composition is determined by assuming that the water partial pressure is equal to the saturation pressure of water at the vessel temperature, an ideal mixture, with the remaining partial pressure assigned to hydrogen, a simplifying assumption which neglects boiling-point elevation and therefore maximises the assumed water vapour partial pressure and its contribution to the total system pressure. This defines the initial vapour composition, hydrogen inventory and vapour molecular weight. Noting initially before any reaction the atmosphere would be nitrogen (i.e another non condensable gas) and water vapour.

The liquid inventory is based on the mass of the charge listed in the mass balance but is a configurable input (Default 1405kg). The corresponding liquid volume is calculated using the density of water at the vessel conditions, adjusted by a density correction factor to account for dissolved solids which is effectively an SG of the liquid. The default correction factor is 1.05. The remaining vessel volume is treated as vapour space.

The initial aluminium inventory is set at 16.2 kg, as per the charge designated by HLL, but is user configurable. The model uses an Arrhenius-style kinetic fit to determine the aluminium consumption rate, water consumption rate, hydrogen generation rate and heat release rate from the reaction. The plot uses two temperatures and corresponding reaction times to generate the Arrhenius parameters. These are configurable to investigate the effect of the kinetic model on the peak pressure. Additionally, multipliers are available to change the values of the parameters. Sensitivity was performed on the Activation Energy at +/- 10% of the calculated value.

DIERS methodology is used to determine the vessel hydrodynamics and relief-stream composition, with a selectable vessel model coupled to the HEM vent-capacity model described in Section 3.3. Until the vessel pressure reaches the burst disc pressure, the vent rate is set to zero. Once the burst disc has opened, the vent path is assumed to remain open for the remainder of the transient.

In line with API Standard 521 the calculated vent rate is multiplied by a derating factor (default 0.9) to account for calculation uncertainties. The derated vent flow is used for the inventory/pressure calculations, but the full calculated flow is used in subsequent pressure drop calculations.

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3.2 Vessel Model Selection

Four vessel hydrodynamic methodologies were considered to represent the potential behaviour of the reacting aluminium/caustic system during relief. The models are described in more detail in the DIERS Manual but a brief summary is included here. The non-boiling height methodology was discounted as non-representative, leaving three vessel models for further consideration.

Bubbly Flow Model

The bubbly flow model assumes that gas generated within the liquid phase forms discrete bubbles which are able to rise and disengage from the liquid surface. The vapour space therefore contains a higher proportion of gas than the bulk vessel inventory and the vent quality is determined from the calculated void fraction and disengagement behaviour. This model is generally considered appropriate for low viscosity systems where gas bubbles can readily separate from the liquid. For the present aluminium/caustic reaction, the use of a silicone-based defoamer specifically intended to promote bubble release provides supporting evidence that significant gas disengagement occurs.

Churn-Turbulent Flow Model

The churn-turbulent model assumes a more vigorous gas-liquid interaction with substantial mixing and liquid entrainment. Gas disengagement is significant and the vent stream typically contains a higher vapour fraction than predicted by the bubbly model due to the increased gas throughput and turbulence. As a result, relief capacity is generally increased and vessel pressures tend to reduce more rapidly once relief commences. This model may be representative of conditions at elevated reaction rates where hydrogen evolution is sufficiently intense to disrupt orderly bubble rise and create large-scale circulation within the vessel.

Foamy (Non-Disengaging) Flow Model

The foamy model assumes little or no separation between the gas and liquid phases within the vessel. Gas generated by the reaction remains entrained within the liquid inventory and the vent quality is assumed to be equal to the bulk vessel quality. This produces the lowest vapour fraction at the relief device and consequently the lowest predicted relief capacity. The model therefore represents a conservative bounding case for systems capable of forming stable foams. For the present aluminium/caustic system, the routine addition of silicone-based defoamer and the process objective of promoting bubble disengagement suggest that persistent non-disengaging foam behaviour is unlikely.

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Non-boiling height model

The non-boiling height methodology assumes that vapour generation occurs primarily at the liquid surface, allowing a relatively quiescent liquid region to exist below the boiling interface. This assumption was considered inappropriate for the present system as hydrogen is generated directly by the aluminium/caustic reaction throughout the wetted reaction zone, including the lower regions of the vessel. Gas generation within the bulk liquid promotes mixing, bubble formation and gas holdup throughout the vessel inventory, making the assumption of a distinct non-boiling liquid region non-representative. Consequently, vessel models incorporating bulk gas generation and gas-liquid interaction were considered more appropriate for this assessment.

DIERS correlating parameter, C_0

The DIERS correlating parameter C_0 is used within the vessel disengagement/void fraction methodology to characterise slip between the gas and liquid phases. It influences the calculated vessel void fraction, gas holdup and the quality of material presented to the relief device. Lower values of C_0 , approaching unity, represent poorer gas-liquid slip or more conservative disengagement behaviour, leading to greater liquid carryover and a more onerous relief duty. Higher values, typically around 1.5, represent improved gas-liquid disengagement, greater vapour enrichment at the vent and increased relief effectiveness.

The modelling showed that the behaviour of the system is strongly influenced by the presence of hydrogen as a non-condensable gas within the vapour space. The accumulation of hydrogen increases the total vessel pressure without requiring bulk boiling of the liquid inventory. Consequently, vessel pressure is governed primarily by the hydrogen inventory and its net change over each timestep, with a secondary contribution from changes in water vapour pressure as the vessel temperature changes. Models that predict lower vapour disengagement and consequently lower discharge of the generated hydrogen therefore tend to predict higher peak vessel pressures.

The proposed relief connection is a side-mounted nozzle, with the normal bulk liquid level only slightly below the nozzle centreline. The DIERS vessel disengagement models are principally formulated for top venting and therefore do not explicitly account for the effect of a side take-off on the local phase composition presented to the relief line. Although the nozzle is above the bulk liquid level and some vapour disengagement is therefore expected, the proximity of the nozzle to the swollen and highly aerated liquid region may increase liquid entrainment relative to an equivalent top-mounted vent.

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The effect of the side-mounted relief connection cannot be quantified with sufficient confidence using the available vessel models. The foamy, non-disengaging model was therefore adopted as a conservative bounding basis for determining the relief-stream composition and vent capacity. This should not be interpreted as an assumption that persistent stable foaming is expected within the reactor; rather, it provides a conservative representation of reduced phase disengagement and increased liquid carryover at the side-mounted relief connection.

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3.3 Vent Model Selection

The vent model used in the final version of the calculation is HEM. The DIERS Omega method was initially selected as it represents a shortcut method that is suitable for repeated calculations of the parameters in a multi-step time calculation. However, after review of 'Boicourt's 1995 paper ERS Design: An integrated approach using DIERS Methodology', the statement is made "In multicomponent systems where the components show widely differing boiling points the mass fluxes calculated using the simplified "omega" method yield conservative results in that the relief devices will be excessively large. It goes on to say that the DIERS Omega method should not be used for values of Omega less than 1 or greater than 100. It was noted that as the relief progressed and greater proportions of hydrogen accumulated in the vessel the Omega parameter increased significantly and exceeded 100. It was noted that this typically occurred beyond the region of interest i.e. after turnaround but in some cases such as very low mass quality cases the value of Omega calculated was greater than 100 i.e. when the foamy model was selected. In this system the presence of the non-condensable gas hydrogen represents an extreme case of widely different boiling points. This results in substantially lower predicted relief capacities and, in some cases, predicted vessel pressures exceeding MAAP under conditions for which the applicability of the simplified Omega method is questionable.

In this system the change in specific volume is primarily governed by the expansion of hydrogen along the flow path until the pressure in the vent line has reduced to the saturation pressure of water at the relief temperature. At this point the change in specific volume is additionally governed by the flash of water to steam and its subsequent expansion. DIERS Omega would tend to overpredict the flash and its onset leading to lower calculated vent capacities.

The HEM model was therefore selected as the best-estimate model because it explicitly resolves the evolving multicomponent phase equilibrium and mixture properties throughout the depressurisation path.

3.4 HEM Implementation

HEM was implemented by using The Process Simulation Software DWSim. The pipelines between the reactor and the KO Drum and the KO Drum to atmosphere were explicitly modelled as pipes of equivalent length. The mass flow was adjusted at the specified inlet conditions until a final exit pressure of approximately atmospheric pressure was achieved.

The relief line was modelled as a Sch 10S DN150 line of equivalent length 61m. The total height rise is estimated at 0.8m. The line was split into 5 sections as detailed below for ease and speed

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of calculation. Allowing extra fidelity in the sections of the pipe where the flashing was found to occur.

Section	Length	Elevation	Steps
1	40	0.65	10
2	10	0.2	25
3	6	0.1	25
4	3	0.05	50
5	2	-0.2	100
Totals	61	0.8	

The vent line was modelled as a Sch 10S DN100 line of equivalent length 54.5m with a change in height of 6m. The line is vapour only so 10 calculation steps were used.

Under the HEM Model the mass flow is effectively a function of 3 main parameters.

$$\dot{m} = f(P, \alpha, T)$$

However, as the modelling has shown the initial pressure rise from operating to relief is near isothermal with temperature increases less than 1°C. Therefore, at the region of interest (the onset of relief) the temperature may reasonably be assumed to be constant and equal to the initial temperature of the vessel. Therefore, the following simplification is applied.

$$\dot{m} \approx f(P, \alpha)|_{T=T_{Op}}$$

This reduces the vent capacity to a function of two variables and allows a grid of $\dot{m}$ vs P and α to be constructed. The vent flow at any point is then determined by interpolation from the grid. The pressure range 4bara to 6.5bara and void fraction range 0.25 to 0.6 was used to generate the grid.

For this system the impact of temperature on the HEM result is expected to be that at lower temperatures the saturation pressure is lower and therefore the vent capacity will be increased as the onset of water flash and its magnitude are inhibited. Conversely an increase in temperature results in increased flash and a reduction in capacity.

The effect of temperature was investigated at the burst pressure and a void fraction of 0.35 and found to result in a 20% reduction in vent capacity at 140°C. Therefore, a temperature derating factor of 0.8 can be applied to initial reactor temperature cases above 130°C to account for the reduction in vent capacity.

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3.5 Mass and Energy Balances

3.5.1 Energy Balance

The energy balance for the vessel may be written as follows

$$\frac{dU}{dt} = Q_{rxn} + \dot{m}_{in}h_{in} - \dot{m}_{out}h_{out} - Q_{loss} - W$$

$\frac{dU}{dt}$ Represents the change in internal energy of the system over time

Q_{rxn} Represents the heat generated by the reaction

$\dot{m}_{in}h_{in}$ Represents the enthalpy flow into the vessel. This is zero as there is no flow into the vessel.

$\dot{m}_{out}h_{out}$ Represents the enthalpy flow out of the vessel. This is the energy carried away by the vent line once the burst disc is opened.

Q_{loss} Represents the heat loss to the surroundings. This is assumed to be zero as cooling is assumed to have failed and the duration of the transient is sufficiently short that the heat loss from the vessel is small compared to the internal heat generation.

W Represents the work done by the fluid. This is assumed to be zero.

Thus the energy balance simplifies to:

$$\frac{dU}{dt} = Q_{rxn} - \dot{m}_{out}h_{out}$$

The change in internal energy goes to heating the bulk vessel contents with an additional contribution to the net change in the steam composition over the timestep. Interphase water transfer is not explicitly included as a separate latent-heat term in the transient energy balance. This approximation is considered acceptable for the present assessment because the predicted temperature excursion is less than 1°C and the pressure transient is dominated by the changing non-condensable hydrogen inventory and relief discharge.

Therefore,

$$\Delta U \approx m_l C_{p,l} \Delta T$$

Combining these equations gives the overall energy balance equation used in the simulation.

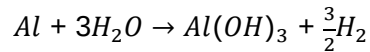
$$m_l C_{p,l} \frac{\Delta T}{\Delta t} \approx Q_{rxn} - \dot{m}_{out}h_{out}$$

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3.5.2 Mass Balance

At each step the aluminium consumption rate is determined using the kinetic equation developed. This is used to track the aluminium inventory across the model.



The overall reaction equation above is used to determine the water consumed and hydrogen generated at each time step.

Hydrogen balance considers the hydrogen evolved at each time step and the hydrogen vented.

$$\Delta m = m_{rxn} - m_{vent}$$

The updated hydrogen inventory is used to determine the partial pressure of hydrogen in the vapour space.

The water balance considers the amount of water consumed in the reaction and both the steam and liquid water vented.

$$\Delta m = -m_{rxn} - m_{vent,v} - m_{vent,l}$$

The updated water inventory is used to determine the remaining liquid volume within the vessel.

It is assumed that the liquid and vapour phases remain in equilibrium with respect to water throughout the transient. This is considered reasonable because the pressure rise occurs over tens of seconds, the reactor is stirred, and the vessel cross-sectional area to volume ratio provides sufficient phase contact for water vapour equilibrium to be a credible engineering assumption.

The timestep is sufficiently small that the mass transferred between the liquid and vapour phases by evaporation or condensation is small compared with the bulk liquid inventory and the relief discharge over a single timestep. This interphase transfer is therefore neglected in the transient mass balance.

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4.0 Modelling Results

4.1 General Factors

4.1.1 Vessel/Vent Model

The final selection of a foamy vessel model and HEM for the vent line flow are discussed in previous sections.

4.1.2 Pressure Turnaround

Considering the ideal gas law

$$PV = nRT$$

It follows that

$$P \propto \frac{nT}{V}$$

The vessel pressure begins to decrease once the quantity nT/V begins to decrease. Once relief is initiated, the vapour space volume (V) increases as liquid is discharged from the vessel. If sufficient enthalpy is removed by the relief stream, the vessel energy balance becomes negative and the vessel temperature (T) decreases.

The vapour inventory (n) is governed by:

- Hydrogen generation by the reaction.
- Hydrogen discharge through the relief system.
- Steam discharge through the relief system.
- Condensation of steam from the vapour phase to the liquid phase as the vessel cools.

Therefore, pressure turnaround is governed by the combined effects of changes in vapour inventory, vapour temperature and vapour space volume. Consequently, vessel pressure may begin to decrease even if hydrogen continues to accumulate within the vessel, provided that the combined effects of cooling, steam condensation and increasing vapour space volume outweigh the increase in hydrogen inventory. Conversely, if hydrogen generation is sufficiently high that the increase in vapour inventory exceeds the combined reductions associated with temperature, condensation and increasing vapour space volume over a timestep, vessel pressure will continue to rise.

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4.2 Sensitivities Testing and Results

Copies of the results for each model run using HLL-26-128-PRO-CAL-01 are summarised in appendix A.

4.2.1 Temperature Rise

The effect of initial temperature on the temperature rise.

Reactor Start Temperature	120	130	140	[°C]
Temperature Derating Factor	1	1	0.8	[-]
Reactor Max Pressure	4.52	4.52	4.51	[barg]
% MAAP	68.5	68.5	68.3	[%]
Reactor Max Temperature	120.76	130.72	140.67	[°C]
Max Delta T	0.76	0.72	0.67	[°C]
Time of Peak	3.6	2.7	2.0	[s]
Max KO Drum Pressure	1.45	1.45	1.45	[barg]
Max KO Drum Vapour Rate	1.68	1.68	1.67	[kg/s]

The temperature rise within the vessel prior to effective relief is governed by the net accumulation of reaction energy before the burst disc opens and the relief system becomes established. For the DN150 vent, pressure turnaround occurs essentially at burst disc opening, with the vessel pressure reducing immediately following relief initiation. Consequently, the predicted temperature rise is negligible (<1°C), as only a small quantity of reaction energy is accumulated whilst the vessel pressure increases from the operating pressure of 3.6barg to the burst disc opening pressure of 4.5barg. It is therefore concluded that, with an initial vessel temperature of 140°C, the quench activation temperature of 145°C is not reached.

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4.2.2 Activation Energy

The effect of activation energy on the predicted results:

Activation Energy Multiplier	0.9	1	1.1	
Activation Energy	28084	31205	34325	[J/mol]
Reactor Max Pressure	4.55	4.52	4.51	[barg]
% MAAP	69.0	68.5	68.3	[%]
Reactor Max Temperature	130.75	130.72	130.71	[°C]
Max Delta T	0.75	0.72	0.71	[°C]
Time of Peak	1.1	2.7	6.8	[s]
Max KO Drum Pressure	1.45	1.45	1.45	[barg]
Max KO Drum Vapour Rate	1.68	1.68	1.68	[kg/s]

A 10% reduction in the activation energy corresponding to 28,084J/mol still results in a turnaround at vent opening. HLL advised that a widely reported literature value for the reaction was ~28.3kJ/mol

4.3 KO Drum Sizing (For Guidance Only)

Although the foamy model was adopted as the conservative basis for reactor pressure assessment, the bubbly model was used to assess vessel swelling and demonstrates that substantial two-phase carryover is predicted even where vapour disengagement is permitted. The bubbly vessel model predicts a swollen liquid void fraction of approximately 0.990–0.991 throughout the relief event. This indicates that the vessel contents remain highly aerated, with the high superficial vapour velocity associated with the DN150 relief nozzle in a relatively small vessel providing insufficient residence time for significant vapour disengagement. Consequently, the discharge is predicted to remain effectively two-phase until the vessel is almost completely de-inventoried. On this basis, the downstream knock-out vessel should be sized to retain the full reactor liquid inventory at ambient conditions (approximately 1,400 L). Allowing for vapour disengagement space and freeboard suggests a total knock-out vessel volume of approximately 2,500 L.

The maximum KO drum backpressure predicted is ~2barg at 140°C initial reactor temperature. **No allowance has currently been included for the end-of-line flame arrestor; however, an additional allowance of up to 0.5bar is considered appropriate for the high vent flow during relief. On this basis, the KO drum should be rated for at least 3barg.**

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4.4 Default Model Run and Results

A model run again using HLL-26-128-PRO-CAL-01 was completed at the default values listed in the previous sections.

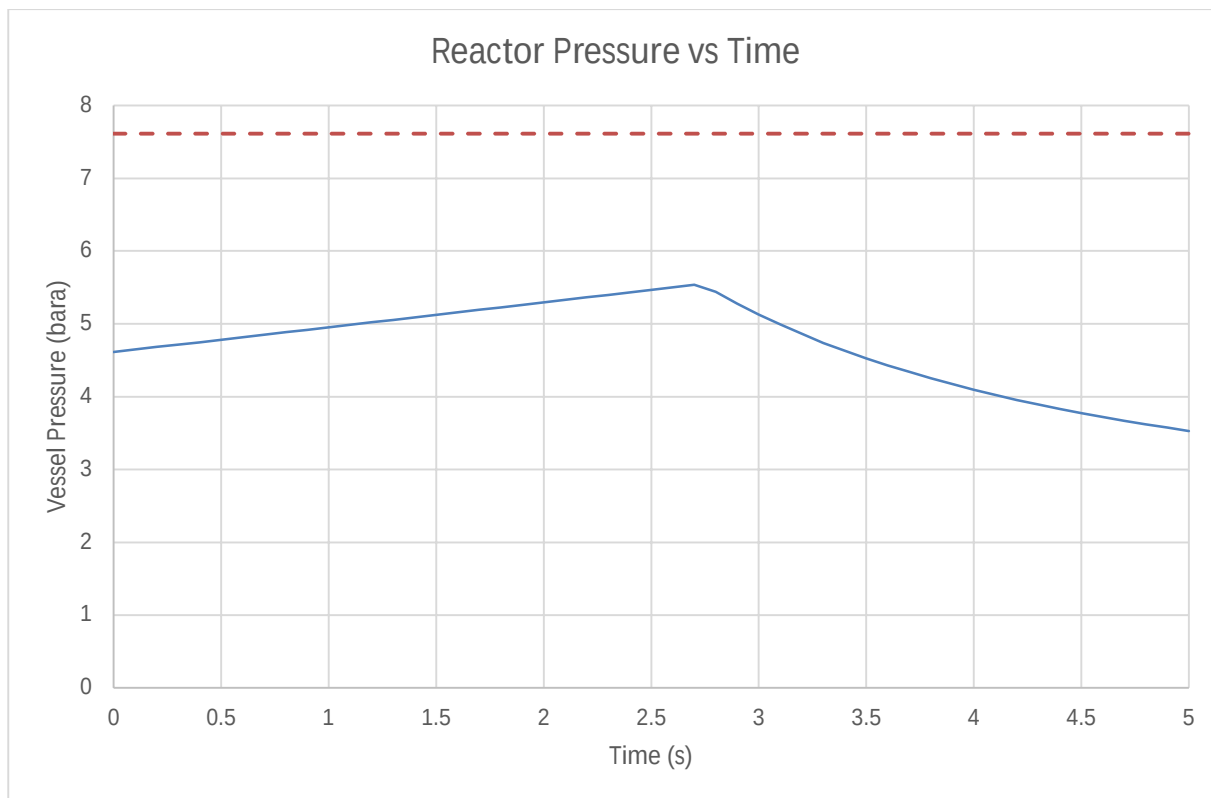
Inputs

Parameter	Value	
Initial Temperature	130	[°C]
Liquid Density Factor	1.05	[-]
Specific Heat Capacity Factor	1.05	[-]
Derating Factor	0.9	[-]
Temperature Derating Factor	1	[-]
Activation Energy Multiplier	1	[-]
Activation Energy	31204.7	[J/mol]
Pre Rate Contant Multiplier	1	[-]
Timestep	0.1	[s]

Results

Parameter	Value	
Reactor Max Pressure	4.52	[barg]
% MAAP	68.5	[%]
Reactor Max Temperature	130.72	[°C]
Max Delta T	0.72	[°C]
Time of Peak	2.7	[s]
Max KO Drum Pressure	1.45	[barg]
Max KO Drum Vapour Rate	1.68	[kg/s]

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Note: The dashed line is the Maximum Allowable Accumulated Pressure

4.5 Worst Case Sensitivities and Results

A deliberately adverse combination of modelling assumptions was evaluated to provide a conservative bounding sensitivity. All the fluid properties were returned to that of water. The standard relief derating factor was reduced to 0.8, the initial reactor temperature was set to 140°C, and the temperature derating factor was reduced to 0.75.

The reaction kinetics were adjusted to use a 15% reduction in activation energy and a 15% increase in pre-rate constant in order to increase the reaction rate towards a maximum value.

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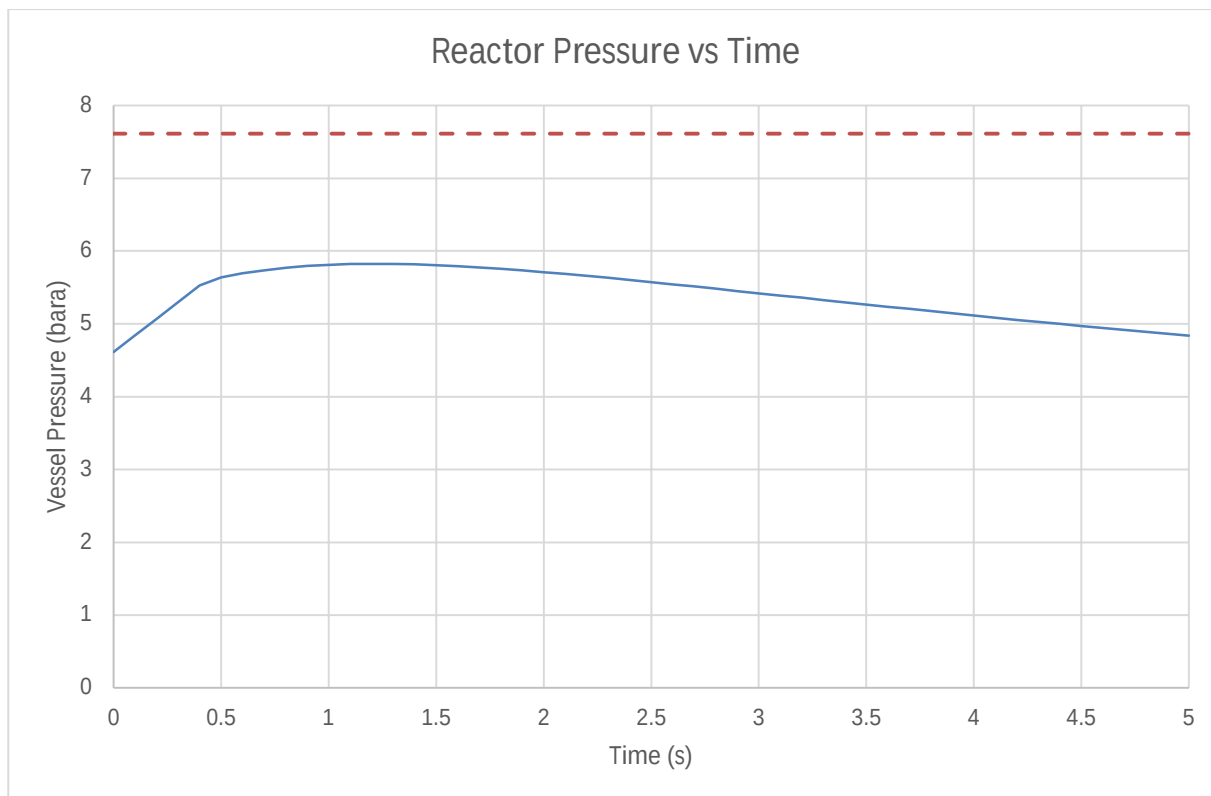
Inputs

Parameter	Value	
Initial Temperature	140	[°C]
Liquid Density Factor	1	[-]
Specific Heat Capacity Factor	1	[-]
Derating Factor	0.8	[-]
Temperature Derating Factor	0.75	[-]
Activation Energy Multiplier	0.85	[-]
Activation Energy	26524	[J/mol]
Pre Rate Contant Multiplier	1.15	[-]
Timestep	0.1	[s]

Results

Parameter	Value	
Reactor Max Pressure	4.81	[barg]
% MAAP	72.9	[%]
Reactor Max Temperature	140.63	[°C]
Max Delta T	0.63	[°C]
Time of Peak	1.2	[s]
Max KO Drum Pressure	1.48	[barg]
Max KO Drum Vapour Rate	1.69	[kg/s]

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Note: The dashed line is the Maximum Allowable Accumulated Pressure

Even when pushed to the extremes it may be concluded that the proposed DN150 vent arrangement has sufficient capacity to prevent overpressure of the vessel.

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5.0 Appendix A

Sensitivity Parameters

Initial Temperature	120	[°C]
Liquid Density Factor	1.05	[-]
Specific Heat Capacity Factor	1.05	[-]
Derating Factor	0.9	[-]
Temperature Derating Factor	1	[-]
Activation Energy Multiplier	1	[-]
Activation Energy	31205	[J/mol]
Pre Rate Constant Multiplier	1	[-]
Timestep	0.1	[s]

Calculation Results

Reactor Max Pressure	4.519	[barg]
% MAAP	68.5	[%]
Reactor Max Temperature	120.76	[°C]
Max Delta T	0.76	[°C]
Time of Peak	3.6	[s]
Max KO Drum Pressure	1.450	[barg]
Max KO Drum Vapour Rate	1.677	[kg/s]

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Sensitivity Parameters

Initial Temperature	130	[°C]
Liquid Density Factor	1.05	[-]
Specific Heat Capacity Factor	1.05	[-]
Derating Factor	0.9	[-]
Temperature Derating Factor	1	[-]
Activation Energy Multiplier	1	[-]
Activation Energy	31205	[J/mol]
Pre Rate Contant Multiplier	1	[-]
Timestep	0.1	[s]

Calculation Results

Reactor Max Pressure	4.522	[barg]
% MAAP	68.5	[%]
Reactor Max Temperature	130.72	[°C]
Max Delta T	0.72	[°C]
Time of Peak	2.7	[s]
Max KO Drum Pressure	1.450	[barg]
Max KO Drum Vapour Rate	1.676	[kg/s]

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Sensitivity Parameters

Initial Temperature	140	[°C]
Liquid Density Factor	1.05	[-]
Specific Heat Capacity Factor	1.05	[-]
Derating Factor	0.9	[-]
Temperature Derating Factor	0.8	[-]
Activation Energy Multiplier	1	[-]
Activation Energy	31205	[J/mol]
Pre Rate Constant Multiplier	1	[-]
Timestep	0.1	[s]

Calculation Results

Reactor Max Pressure	4.505	[barg]
% MAAP	68.3	[%]
Reactor Max Temperature	140.67	[°C]
Max Delta T	0.67	[°C]
Time of Peak	2	[s]
Max KO Drum Pressure	1.449	[barg]
Max KO Drum Vapour Rate	1.675	[kg/s]

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Sensitivity Parameters

Initial Temperature	130	[°C]
Liquid Density Factor	1.05	[-]
Specific Heat Capacity Factor	1.05	[-]
Derating Factor	0.9	[-]
Temperature Derating Factor	1	[-]
Activation Energy Multiplier	0.9	[-]
Activation Energy	28084	[J/mol]
Pre Rate Constant Multiplier	1	[-]
Timestep	0.1	[s]

Calculation Results

Reactor Max Pressure	4.552	[barg]
% MAAP	69.0	[%]
Reactor Max Temperature	130.75	[°C]
Max Delta T	0.75	[°C]
Time of Peak	1.1	[s]
Max KO Drum Pressure	1.453	[barg]
Max KO Drum Vapour Rate	1.677	[kg/s]

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Sensitivity Parameters

Initial Temperature	130	[°C]
Liquid Density Factor	1.05	[-]
Specific Heat Capacity Factor	1.05	[-]
Derating Factor	0.9	[-]
Temperature Derating Factor	1	[-]
Activation Energy Multiplier	1	[-]
Activation Energy	31205	[J/mol]
Pre Rate Contant Multiplier	1	[-]
Timestep	0.1	[s]

Calculation Results

Reactor Max Pressure	4.522	[barg]
% MAAP	68.5	[%]
Reactor Max Temperature	130.72	[°C]
Max Delta T	0.72	[°C]
Time of Peak	2.7	[s]
Max KO Drum Pressure	1.450	[barg]
Max KO Drum Vapour Rate	1.676	[kg/s]

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Sensitivity Parameters

Initial Temperature	130	[°C]
Liquid Density Factor	1.05	[-]
Specific Heat Capacity Factor	1.05	[-]
Derating Factor	0.9	[-]
Temperature Derating Factor	1	[-]
Activation Energy Multiplier	1.1	[-]
Activation Energy	34325	[J/mol]
Pre Rate Constant Multiplier	1	[-]
Timestep	0.15	[s]

Calculation Results

Reactor Max Pressure	4.509	[barg]
% MAAP	68.3	[%]
Reactor Max Temperature	130.71	[°C]
Max Delta T	0.71	[°C]
Time of Peak	6.8	[s]
Max KO Drum Pressure	1.449	[barg]
Max KO Drum Vapour Rate	1.676	[kg/s]

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Sensitivity Parameters

Initial Temperature	130	[°C]
Liquid Density Factor	1.05	[-]
Specific Heat Capacity Factor	1.05	[-]
Derating Factor	0.9	[-]
Temperature Derating Factor	1	[-]
Activation Energy Multiplier	1	[-]
Activation Energy	31205	[J/mol]
Pre Rate Constant Multiplier	1	[-]
Timestep	0.1	[s]

Calculation Results

Reactor Max Pressure	4.522	[barg]
% MAAP	68.5	[%]
Reactor Max Temperature	130.72	[°C]
Max Delta T	0.72	[°C]
Time of Peak	2.7	[s]
Max KO Drum Pressure	1.450	[barg]
Max KO Drum Vapour Rate	1.676	[kg/s]

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Sensitivity Parameters

Initial Temperature	140	[°C]
Liquid Density Factor	1	[-]
Specific Heat Capacity Factor	1	[-]
Derating Factor	0.8	[-]
Temperature Derating Factor	0.75	[-]
Activation Energy Multiplier	0.85	[-]
Activation Energy	26524	[J/mol]
Pre Rate Contant Multiplier	1.15	[-]
Timestep	0.1	[s]

Calculation Results

Reactor Max Pressure	4.812	[barg]
% MAAP	72.9	[%]
Reactor Max Temperature	140.63	[°C]
Max Delta T	0.63	[°C]
Time of Peak	1.2	[s]
Max KO Drum Pressure	1.475	[barg]
Max KO Drum Vapour Rate	1.692	[kg/s]

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