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### Abstract

API Standard 521 is open to the application of dynamic simulations when considering pressure relief system calculations. Some overpressure scenarios are very dynamic in their nature, such as external fire exposure, abnormal heat input, vapor breakthrough and runaway reaction, to name a few.

Modeling overpressure scenarios dynamically can allow for a more accurate, less conservative, representation of the affected system; often resulting in a lower relief requirement, as well as an understanding of how the system pressure and temperature changes over time.

This paper compares an external fire overpressure scenario which is modeled using steady state calculations versus the same system modeled dynamically. It is intended to give the user a better understanding of the differences in the two approaches, as well as the benefits of applying dynamic simulation for specific scenarios.

### **1** Introduction

Traditional pressure relief sizing calculations have typically used steady state equations to determine both the required relief rate and the pressure relief system capacity, for every applicable overpressure scenario. These equations are well accepted and understood and are available in API Standards 520 and 521.

API Standard 521 is open to the application of dynamic simulations when considering pressure relief system calculations. Some overpressure scenarios are very dynamic in their nature, such as external fire exposure, abnormal heat input, vapor breakthrough and runaway reaction, to name a few.

Modeling overpressure scenarios dynamically can allow for a more accurate, less conservative, representation of the affected system; often resulting in a lower relief requirement as well as an understanding how the system pressure and temperature changes over time.

This paper compares an external fire overpressure scenario which is modeled using steady state calculations versus the same system modeled dynamically. It is intended to give the user a better understanding of the differences in the two approaches, as well as the benefits of applying dynamic simulation for specific scenarios.

### 2 Overpressure Scenarios

Some overpressure scenarios are very dynamic in their nature, such as external fire exposure, abnormal heat input, vapor breakthrough, transient analysis of a tube rupture, and runaway reaction. In cases such as these, it can be advantageous to utilize dynamic modeling.

#### **External** Fire

Pressure vessels, other pressure-containing equipment, or storage tanks may be exposed to fire at some time in the life of an operating plant that handles or processes flammable liquids or gases. Unless external fire can be specifically excluded, the ASME Boiler and Pressure Vessel Code and NFPA 30 require consideration of a fire scenario for such equipment.

For pressure vessels in process areas, the maximum fire height is usually taken as 25 feet above a height where liquids can pool. API Standard 521 heat flux calculations for process vessels typically specify a wetted area based on liquid level, plus an extra allowance for process piping and instrumentation exposed to fire.

As the fire burns, heat is transferred to the vessel wall. Where the vessel wall is in contact with the liquid contents, the heat is transferred directly to the liquid inside the vessel. In the case where the vessel wall is in contact with the vapor contents, the heat is transferred to the metal wall, resulting in a significant temperature rise of the metal wall.

Dynamic modeling of such an event allows the following phenomena to be analyzed:

- Temperature and pressure rise of vessel contents over time
- Vessel contents composition changes over time
- Liquid level changes over time, resulting in a change to the wetted area
- Pressure relief valve venting time, and duration
- Vessel wall temperature effects

#### Abnormal Heat Input

Abnormal heat input is an overpressure scenario where excess vapor volume is generated as a result of unexpected high process heat input. This scenario is typically considered as a case for reboilers in the event of temperature control valve failure. Vapor generation can exceed the system's ability to condense or otherwise absorb the build-up of pressure, which may include non-condensables caused by overheating.

Abnormal heat input may occur as a result of numerous initiating events such as: failure of automatic controls, power failure, inadvertent opening of normally closed valves, or general operator error.

The relief requirement for abnormal heat input is typically based on the amount of material that can be vaporized due to the additional heat load. For fired heaters, when evaluating the fuel control valve fails wide-open case, the duty can be expected to increase to 150% of normal value unless manufacturer data dictates otherwise. For heat exchangers, the duty can be expected to increase to no more than 200% of design duty.

Similar to an external fire scenario, dynamic modeling of such an event allows the following phenomena to be analyzed:

- Temperature and pressure rise of vessel contents over time
- Vessel contents composition changes over time
- Liquid level changes over time
- Pressure relief valve venting time, and duration

#### Vapor Breakthrough

Vapor breakthrough, also known as gas blow-by, can result from the failure open of a liquid outlet level control valve that flows to a downstream system with a design pressure less than the upstream maximum normal operating pressure.

The vapor breakthrough case relief load could be based on the maximum flow through a control valve and bypass valve simultaneously wide open, or either separately. When modeling such a scenario dynamically, consideration can be given to the relative liquid volumes of the two vessels to determine if a liquid release may occur in the downstream vessel. The dynamic simulation will determine if the downstream vessel can be hydraulically filled, and the relief device sizing calculation then evaluated for liquid displacement for gas blow-by.

The dynamic mode can also determine if the downstream vessel can be filled to a level that is higher than the height of the inlet nozzle at the start of the gas blow-by scenario. If so, two phase flow would be evaluated.

Dynamic modeling of such an event allows the following phenomena to be analyzed:

- Temperature and pressure rise of vessel contents over time
- Phase, liquid level and volume changes over time
- Pressure relief valve venting time, and duration

#### **Runaway Reaction**

Runaway chemical reactions may result in overpressure due to the rapid increase in pressure developed during an exothermic reaction.

Such an overpressure scenario really lends itself to dynamic modeling.

The reaction chemistry should first be qualified using small scale experiments. This data can then be coupled with fluid dynamics to design the emergency relief system. In addition to vent sizing information, the dynamic modeling approach can provide insights into process modification and refinement as well as the establishment of a safe operating envelope.

Modeling the runaway reaction dynamically can account for vessel insulation, a glass lining, jacketing or protection by water spray.

For dynamically modeled reactive systems, essential parameters that can be evaluated include:

- System Thermal Stability, i.e. nature and relative magnitude of any exothermic (or endothermic) effects. These include primary thermal runaway and any subsequent secondary decomposition reactions.
- Total Heat Released, characterized by the specific reaction heat release per (mass or molar) unit of reacting material.
- Rate of Heat Release, characterized by global kinetic parameters describing heat generation as a function of temperature and residual reactant concentration.
- Rate of Gas Generation, due to volatilization of liquid components and vapor expansion effects with increasing reaction temperature or generation of additional gaseous reaction or decomposition products.
- Scale-Up or Loading Factors, including credible heat influx from external fire events and physical characteristics of a full-scale containment vessel.
- Vent Flow Characteristics, including multiphase/multicomponent system properties and effects of continuing chemical reaction.

#### **Tube Rupture Transient Analysis**

A heat exchanger single tube failure may be considered when the high-pressure side maximum operating pressure exceeds the low-pressure side corrected hydrostatic test pressure.

The required relieving rate should be calculated to consider displacement of the pre-existing fluid, any mixing of high-pressure side and low-pressure side fluids, including flashing; and high-pressure side fluids after displacement has been completed.

API Standard 521 discusses the benefits of a dynamic analysis for a tube rupture scenario; and also acknowledges that in some cases where there is a wide difference in design pressure between the two exchanger sides, then transient conditions can produce overpressure above the test pressure. A dynamic pressure relief analysis gives the user an understanding of the pressure rise rate, and whether a pressure relief device can act fast enough to provide sufficient overpressure protection for this scenario.

# 3 Example Case – External Fire Comparison Between Steady State and Dynamic Models

In order to examine the differences between a steady state and a dynamic model for an external fire exposure scenario, the following system was studied:

A vertical vessel with a straight side length of 30 feet (tangent to tangent) and inner diameter of 10 feet, at 8 feet above grade level, was modeled being exposed to a three-hour external fire. The vessel was initially 45% liquid full with a hydrocarbon mixture, with an additional 10% wetted area added to account for interconnected piping. Adequate drainage and firefighting consideration was applied to both the dynamic and steady state models. The design pressure of the vessel is 250 psig, initially operating at 100 psig and 97 °F.

Calculations were based on an allowable accumulation of 21% for an external fire exposure scenario. API discharge coefficients were used for sizing the required relief area. The relief fluid for the steady state model is based on a 5 mol% vaporization, while the relief fluid for the dynamic model was determined with respect to time, heat input, and vaporization of the residing fluid. Table 3 provides a summary of the inputs used in this calculation.



#### Figure 1: Vessel layout

The dynamic model also takes the currently installed relief system into account during an overpressure event. For this example, a simple relief system installation was used. The relief device modeled in the dynamic calculation was a 2" H 3" bellows relief device certified for vapor service, with 1.25' of 2" Nominal Pipe Size (NPS) Schedule 40 vertical inlet piping and 1' of 3" NPS Schedule 40 horizontal outlet piping discharging to the atmosphere. The lift versus overpressure and lift versus backpressure curves used, are the API curves for a standard API 526 valve with vapor trim (a relief device certified for vapor service).

The use of a simple layout means that there are no fitting losses due to any bends, elbows, or manual valves. The relief device has a set pressure of 250 psig, and a reseat pressure of 241.8 psig which corresponds to a 7% blowdown. API discharge coefficients were used for the relief device, to match the API discharge coefficients used in the relief requirement calculations (both steady state and dynamic models).



Figure 2: Pressure relief system layout

| Component     | Chemical<br>Formula | Mole<br>Fraction | Molecular<br>Weight |
|---------------|---------------------|------------------|---------------------|
| Propylene     | С3Н6                | 0.2358           | 42.08               |
| Propane       | С3Н8                | 0.2147           | 44.10               |
| 1-Butene      | C4H8                | 0.1768           | 56.11               |
| 1,3-Butadiene | C4H6                | 0.1902           | 54.09               |
| n-Butane      | C4H10               | 0.1236           | 58.12               |
| 1-Hexene      | C6H12               | 0.0589           | 84.16               |

Table 1: Initial Vessel Liquid Inventory

### **External Fire Heat Input Equations**

Fire exposure on process equipment can result in overpressure due to the vapor generation from boiling of the liquid mixture. In this example case, the external fire is based on an open pool fire - both API 521 and API 2000 are based on open pool fires, with a heat flux comparable to a heavy hydrocarbon, as the basis for sizing pressure relief devices for fire cases.

In the case of an external fire, it is necessary to determine the portion of the vessel that is wetted by its internal liquid level up to 25 ft above the source of the flame, meaning any wetted area above the 25 ft fire limit is not considered with respect to heat input from external fire exposure.

The wetted area for the vertical vessel can be calculated with the following equations:

$$A_{cylinder} = \pi * z * D$$

$$A_{Elliptical\ head} = \pi * b^{2} + \pi * \frac{a^{2}}{2 * \epsilon} * \ln(\frac{1 + \epsilon}{1 - \epsilon})$$
$$\epsilon = \sqrt{1 - \frac{a^{2}}{b^{2}}}$$

Z is the liquid height from the tangent line of the vessel

D is the inside diameter of the vessel

a is the minor semi-axis

b is the major semi-axis

The wetted area would include the areas exposed to the liquid contained within the vessel, up to 25 ft. This would include the cylinder area up to the liquid level (z) plus the bottom head, as they are within the height limit.

It is common practice to assume the vessel to be isolated to simplify the analysis. This assumption is based on rotating equipment being stopped; and emergency procedures being implemented, which would include closing appropriate manual valves.

The heat input rate caused by an external fire is calculated with the following equation if there are prompt firefighting efforts and drainage of flammable materials away from the vessels. API Standard 521,  $6^{th}$  edition, Section 4.4.13.2.4.2.

$$Q = C * F * A^{0.82}$$

Q is the total heat absorption to the wetted surface (Btu/h)

C is a constant 21,000 in USC units (or C can be 34,500 if adequate drainage and firefighting are not present)

F is an environmental factor; F=1 for vessels without insulation credit (Table 5 of API Std 521 provides examples based on different insulation thermal conductivity)

A<sub>s</sub> is the total wetted surface (ft2)

The fire relief rate is equal to the fire heat input rate divided by the latent heat of vaporization of the relief vapors.

$$W = Q/\lambda$$

W is the rate of vapor generation (lb/h)

Q is the total heat absorption to the wetted surface (Btu/h)

 $\lambda$  is the latent heat of vaporization at relieving conditions (BTU/lb)

In order to establish the vapor relief requirement for a mixture under external fire exposure, the latent heat of vaporization is required. For pure liquid mixtures it is relatively simple to establish the latent heat, as data for single components can be obtained from literature (see Figure A.6 in API 521). However, in the case of our example, a vessel containing multicomponent liquid mixture, calculating the latent heat contains many pitfalls. In the absence of advanced tools such as SuperChems Expert, calculating the heat of vaporization of the mixture presents various challenges. The latent heat for mixtures of components with a wide range of boiling points will require a more complex calculation due to the constantly changing composition, temperature, and heat of vaporization as the mixture changes over time. This calculation is best modeled using a dynamic analysis as noted by API 521 section 4.4.13.2.5.2.

"For these and other multicomponent mixtures that have a wide boiling range, it might be necessary to develop a time dependent model where the total heat input to the vessel not only causes vaporization but also raises the temperature of the remaining liquid, keeping it at its boiling point."

In this paper, results using an integral isobaric latent heat established at the first 5 mol% of the liquid vaporized at maximum allowable venting pressure is compared against a dynamic solution using the SuperChems software. Note that the integral isobaric latent heat calculation will result in a relief fluid biased toward the light ends of the mixture. One potential flaw is that the maximum relief requirement may not be established until after the light ends are vaporized.

Note that in our steady state calculation the relief requirement is adjusted by accounting for the density correction factor. Calculating the required rate by dividing the rate of heat absorption by the latent heat of vaporization becomes overly conservative near the critical point where the latent heat goes to zero. In order to calculate a more accurate requirement, the relief requirement can be adjusted by the specific volume.

$$W_r = W * (\frac{\rho_l - \rho_v}{\rho_l})$$

Wr is mass relief rate (lb/h)

ρl is liquid density (lb/ft3)

ρv is vapor density (lb/ft3)

The steady state assumption previously discussed may be deemed inappropriate, and hence more rigorous methods of calculations may be used, such as dynamic analysis.

## 4 **Results Comparison**

Running the same external fire calculation both at steady state and dynamically yields results, as follows:

 Table 2: External Fire Results Comparison

|                            | Relief Requirement | Pressure Relief Capacity |
|----------------------------|--------------------|--------------------------|
| Steady State External Fire | 27,583 lb/hr       | 24,298 lb/hr             |
| Dynamic External Fire      | 24,007 lb/hr       | 24,298 lb/hr             |

As can be observed, the dynamic calculation results in a lower relief requirement (by approximately 13 % less) than the steady state calculation. In both cases, the pressure relief capacities are the same, as this is based on the steady state system rated capacity at 21% overpressure.

The following tables summarize calculation inputs and outputs for an external fire calculation, modeled both steady state and dynamically.

Table 3 shows steady state detailed calculation results for the external fire scenario.

Table 4 shows dynamic simulation calculation results for the external fire scenario.

Table 5 shows the steady state pressure relief system capacity results for the external fire scenario.

**Table 3: External Fire Steady State Detailed Calculation Results** 

| GAS/VAPOR RELIEF UNDER FIRE/USER HEATING USING CCPS/API 520 (SUPPORT) INFORMATION |                           |
|---|---------------------------|
| Inputs  |                           |
| Vessel wetted surface area  | 75,927.97 in <sup>2</sup> |
| Additional wetted surface area  | 7,592.80 in <sup>2</sup>  |
| Heating rate  | 3,877,954.29 BTU/hr       |
| Set pressure  | 250.00 psig               |
| Back pressure   | 0.00 psig                 |
| Percent overpressure  | 21.00 %                   |
| Discharge coefficient   | 0.975                     |
| Outputs   |                           |
| Temperature at maximum pressure   | 187.37 °F                 |
| Compressibility factor  | 0.70                      |
| Density   | 3.16 lb/ft <sup>3</sup>   |
| Heat of vaporization  | 124.28 BTU/lb             |
| Average Molecular Weight  | 48.14                     |
| Specific Volume Correction Factor   | 0.88                      |
| Correction factor vapor density   | 3.16 lb/ft <sup>3</sup>   |
| Correction factor liquid density  | 27.20 lb/ft <sup>3</sup>  |
| Back pressure correction factor (Kb)  | 1.00                      |
| Flow is critical (choked)   | Yes                       |
| Evaporation/relief rate   | 27,582.44 lb/h            |
| Volumetric flow rate  | 212,817.51 SCFH           |
| Required relief device orifice area   | 0.834 in <sup>2</sup>     |

# Table 4: External Fire Dynamic Simulation Calculation Results

| VESSELS CONTAINING TWO PHASES (DYNAMIC) (SUPPORT) INFORMATION |                        |
|---|------------------------|
| Inputs  |                        |
| Initial total mass  | 41,474.24 lb           |
| Volume full of liquid   | 45.00 %                |
| Temperature   | 97.27 °F               |
| Pressure  | 100.00 psig            |
| User defined top flow type                                    | Vapor                  |
| Top flow user specified backpressure                          | 0.00 psig              |
| User defined bottom flow type                                 | No flow                |
| Bottom flow user specified backpressure                       | 0.00 psig              |
| Consider external fire exposure                               | YES                    |
| Set pressure  | 250.00 psig            |
| Discharge coefficient   | 0.975                  |
| Outputs   |                        |
| Top: First Flow   |                        |
| Time  | 0.608 h                |
| Temperature   | 172.77 °F              |
| Pressure  | 257.85 psig            |
| Liquid flow rate  | 0.00 lb/h              |
| Vapor flow rate   | 13,502.89 lb/h         |
| Total flow rate   | 13,502.89 lb/h         |
| Top: Flow at Maximum Pressure Data                            |                        |
| Time  | 1.874 h                |
| Temperature   | 234.18 °F              |
| Pressure  | 301.41 psig            |
| Liquid flow rate  | 0.00 lb/h              |
| Vapor flow rate   | 24,007.01 lb/h         |
| Total flow rate   | 24,007.01 lb/h         |
| Required relief device orifice area                           | 0.7850 in <sup>2</sup> |

# Table 5: External Fire Pressure Relief System Capacity Results

| RELIEF CAPACITY - PSV-100 LAYOUT - 250 PSIG               |                        |  |  |
|---|------------------------|--|--|
| Relief Conditions:  |                        |  |  |
| Temperature   | 187.37 °F              |  |  |
| Pressure  | 302.50 psig            |  |  |
| Superimposed backpressure                                 | 0.00 psig              |  |  |
| Exit Conditions:  |                        |  |  |
| Exit Temperature  | 104.82 °F              |  |  |
| Exit Pressure   | 6.50 psig              |  |  |
| Exit Mach Number  | 0.96                   |  |  |
| Kb correction   | 1.00                   |  |  |
| Kp correction   | 1.00                   |  |  |
| Pressure at device inlet                                  | 302.07 psig            |  |  |
| Irreversible inlet pressure drop                          | 0.40 psi               |  |  |
| Backpressure  | 10.14 psig             |  |  |
| % Irrev. inlet pressure drop relative to actual set point | 0.16 %                 |  |  |
| % back pressure relative to actual set point              | 4.05 %                 |  |  |
| Vapor Mass Flow Rate                                      | 24,312.05 lb/h         |  |  |
| Volumetric Flow Rate                                      | 187,582.21 SCFH        |  |  |
| Relief Device Flow Area                                   | 0.7850 in <sup>2</sup> |  |  |

Significantly, in the case of the steady state calculation, the pressure relief valve would be considered undersized and to provide inadequate pressure relief flow capacity; whereas with the dynamic calculation would result in the pressure relief system being considered adequately sized.

This of course could result in unnecessary discussion list items which could in turn result in unnecessary mitigation actions and unnecessary capital expenditure.

The following figures provide additional understanding of conditions inside the affected process equipment during an external fire scenario modeled dynamically.

Figure 3 shows a dynamic graph of vessel pressure versus time for the external fire scenario; and demonstrates pressure rise rate until the pressure relief device opens after approximately 0.6 hours. The pressure continues to build even as the pressure relief device opens and continues to vent vapor until the vessel empties.

Figure 4 shows a dynamic graph of vessel contents temperature versus time for the external fire scenario. After two hours of fire exposure, the vessel is vapor-full and the vessel wall temperature rises more rapidly.

Figure 5 shows the dynamic graph of liquid height versus time for the external fire scenario, showing that after approximately two hours there is no liquid left in the vessel.



Figure 3: Dynamic graph of vessel pressure versus time



Figure 4: Dynamic graph of vessel contents temperature versus time



Figure 5: Dynamic graph of liquid height versus time

Additionally, external fire calculations can also be used to consider the effects of fire impinging on the vessel metal wall. From this, it can be determined if, or when, the vessel may be likely to fail due to increased temperature rather than pressure. Figure 6 illustrates an example of dynamic simulation to predict vessel wall failure due to fire exposure.

Various parts of the vessel can be represented by "segments" which have differing levels of heat flux exposure due to changing liquid levels in the vessel. The vessel stress due to internal pressure and temperature can be predicted for each segment.



At the point where the wall failure stresses are less than the vessel stress caused by internal pressure (approximately 34 minutes), failure of the vessel could be expected.

Figure 6: Dynamic graph of metal wall temperature and vessel stress versus time

## 5 Conclusions

Modeling overpressure scenarios dynamically can allow for a more accurate, less conservative, representation of the affected system; often resulting in a lower relief requirement as well as an understanding how the system pressure and temperature changes over time.

The availability of dynamic simulation software tools allows the relief systems analyst a broad range of options for performing pressure relief sizing calculations.

The option of dynamic pressure relief calculations can ensure that excessive design conservatism is removed, and that any unnecessary capital expenditure changes can be avoided.

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