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Use dynamic models when designing high-pressure vessels

By definition, a pressure vessel is a closed container that is designed to hold gases and/or liquids at pressures substantially different from ambient conditions. They are used in many applications such as oil and gas production, crude oil refineries and petrochemical plants. Pressure vessels are used as part of the process or as storage vessels for gases such as ammonia, chlorine, propane, butane and liquefied petroleum gas. More importantly, pressure vessels must operate safely within a set of process conditions as defined by the "design pressure" and "design temperature." A pressure vessel that is inadequately designed to handle a high pressure constitutes a significant safety hazard.

Accidents and failures. Disturbances, accidents and malfunctions can cause deviations in operating conditions for a pressure vessel that are outside the safe operating window. For example, high pressures and temperatures can result from exposure to a fire. Since their invention during the industrial revolution, many fatal accidents have been attributed to pressure vessels. Consequently, pressure vessel design, manufacture and operation are regulated by engineering authorities and backed by legislation.

PROTECTION SYSTEMS

A common method of protecting process equipment against excessively high pressure or temperature is emergency depressurization (also known as a blowdown) by means of relief devices such as relief valves and orifices, rupture disks and safety valves. Emergency depressuring removes the potentially dangerous contents of process equipment, such as separation vessels, heat exchangers, distillation columns and compressors, and transfers them to a safe and lower-pressure location. It also decreases the force exerted by the fluid on the walls of equipment by reducing the pressure quickly and diminishes the risk of event escalation due to a fire or a leak of an explosive or toxic gas.

During depressurization in a typical two-phase separator, the vessel's inlets and outlets (both gas and liquid) are blocked by closing isolation valves. The depressurization valve is opened, and the gas is disposed of via a restriction orifice or fixed choke into the flare (or vent) system. Instead of using a restriction orifice to fix the flowrate, some installations use depressurization valves with a known flow coefficient.

However, the blowdown process is itself a potentially hazardous operation due to the very low temperatures encountered during rapid depressurization. Heat transfer by the fluid within the vessel reduces the temperature of the vessel wall. If the temperature of the vessel wall falls below the ductile-brittle transition temperature of the construction material, brittle fracture of the vessel wall can occur.[1] The shock experienced by a thick-walled vessel due to the combined stresses from rapid temperature and pressure changes arises from non-uniform temperature distribution in the vessel wall, which results in differential expansion and contraction. Such pressurized thermal shocks can lead to embrittlement of the metal wall and, in turn, result in fatigue failure of the vessel.[2]

A depressurization utility, built around a detailed model of a pressure vessel, can be used to simulate emergency plant depressurization. The simulation can predict the depressurization behavior of process equipment with enough accuracy to make better design decisions such as:

- At what rate must gas be released from each equipment item to meet the required depressurization times?
- What is the required total flare capacity?
- What is the lowest metal temperature experienced in each equipment item and in the flare system?
- Which low-temperature materials are required?
- What size restriction orifice or other flowrate-controlling device and flare connections are required for depressurization in each section of the plant?

Models and results. There are versatile and user-friendly depressuring utilities available. However, their predictions can be conservative due to simplifications made in the mathematic models. The business impact from conservative predictions is that new plants are over designed with stainless steel (SS), and existing plants must be modified against high costs and deferred production. If SS is selected where carbon steel (CS) would have been adequate, equipment costs could be twice as high or more.[3]

Accurate dynamic depressurization calculations are required to ensure the selection of the most cost-effective materials for safe operation during depressuring. For existing facilities, reassessment of the temperature during depressuring can lead to changes in operating conditions or changes in process equipment to ensure safe depressurization.

There are many process safety requirements that must be considered when designing new process equipment and units or assessing the operation of existing assets. One of these requirements is the prevention of brittle fracture of the metallic materials used in process equipment. Having reliable and consistent predictions of fluid and minimum wall temperatures during depressurization is fundamental to demonstrating compliance with this requirement. This article discusses the use of a rigorous non-equilibrium vessel model incorporating detailed heat conduction calculations for the vessel wall and insulation to give accurate time-dependent trajectories of vessel fluid and wall conditions during a dynamic depressurization operation.

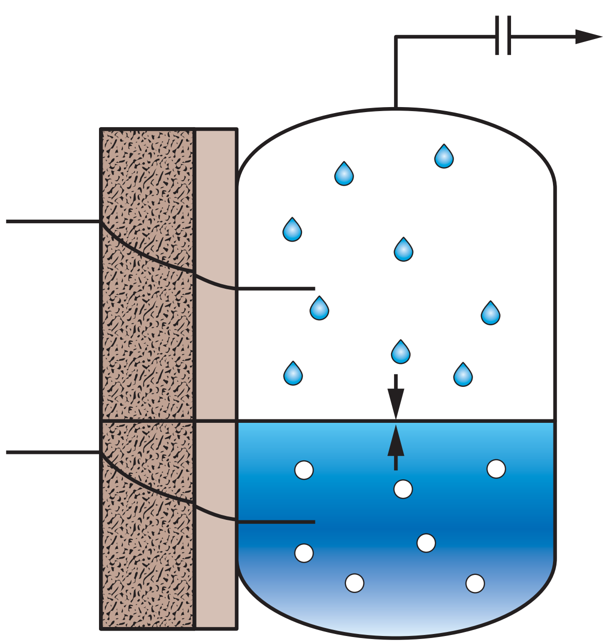

FIG. 1. Unit operation model of a vessel with two zones.

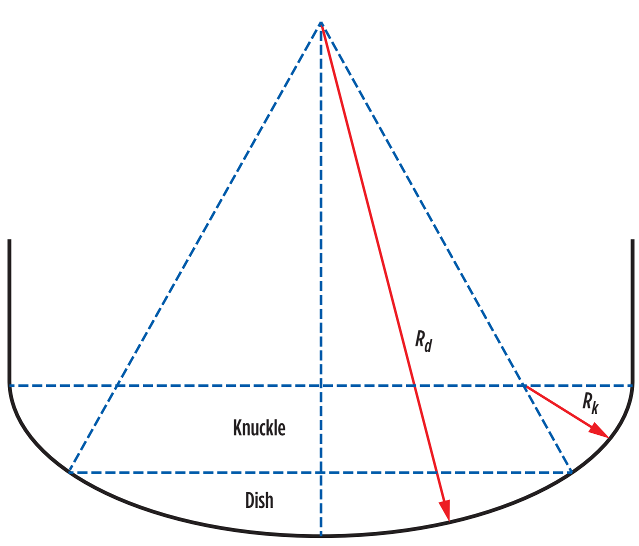

FIG. 2. Cross-section of a torispherical head.

NON-EQUILIBRIUM VESSEL MODEL

A discussion of a non-equilibrium vessel model is available in the literature but it lacks specific mathematical detail.[1] The model described herein improves upon this foundation by rigorously handling three-phase (gas, liquid and water) systems and providing for a wide variety of thermodynamic models. It also incorporates better correlations for heat-transfer coefficients and rigorous formulas for volumes, surfaces and interfacial areas.

Example: A vessel.

The unit operation model for the vessel incorporates three equilibrium zones roughly corresponding to the vapor, liquid and aqueous holdups. This approach enables the model to represent non-equilibrium behavior that is common during depressuring. **FIG. 1** illustrates a vessel with two zones. Droplets forming in the vapor zone move dynamically to the liquid and aqueous zones. Likewise, bubbles forming in the liquid and aqueous zones move dynamically to the vapor zone.

Each zone incorporates heat transfer with adjacent zones, the vessel wall and the environment through heat conduction in the vessel wall and encasing insulation. The heat-transfer coefficient correlations take into account the phases and conditions of the fluids.[4, 5] To ensure that the volumes, surface areas and interfacial areas used in the simulation are accurate, the model incorporates rigorous formulas for these quantities for vertically and horizontally oriented cylindrical vessels having any torispherical (dished) head style.

Vessel geometry calculations.

These calculations address all styles of torispherical heads. Heads are characterized by two dimensionless parameters: the dish radius and knuckle radius factors, which are defined as:

$$f_d = R_d / D \geq 0.5$$
$$f_k = R_k / D \leq 0.5$$

Where D is the inside diameter of the cylinder of the vessel; R_d is the inside radius of the dish; and R_k is the inside radius of the knuckle.[6] **FIG. 2** shows a cross-section of a torispherical head. The head is formed by rotating the cross-section about its central axis.

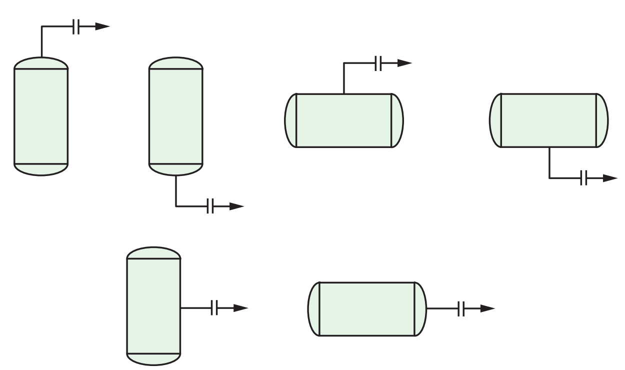

FIG. 3. Vessel orientations and nozzle locations.

Values of the dish radius and knuckle radius factors are well known for many standard torispherical head styles. However, some standard head styles, such as the Standard F&D and Shallow F&D head styles, have a fixed knuckle radius. In this instance, the knuckle radius factor cannot be determined until the diameter of the vessel is specified. Custom-head types can be modeled as long as f_d and f_k can be calculated.

Vessel orientation and outlet calculations. The vessel model allows the configuration of either a vertically or horizontally oriented vessel, as well as different locations of the depressurization outlet. The depressurization outlet is defined by a nozzle, which is configured through specification of the nozzle diameter and center height from the bottom of the vessel. **FIG. 3** shows the different vessel orientations and depressurization nozzle locations that are supported.

The depressurization nozzle can be at the top or bottom or on the side of the vessel. The depressurization nozzle allows accurate modeling of fluid removal from the vessel. The overall composition in the nozzle is determined by mixing outflows from the zones in the vessel. The outflow for a zone is the fraction of the nozzle cross-sectional area covered by the fluid in the zone times the total outflow, which is established by the restriction orifice connected to the depressuring nozzle.

Restriction orifice model. The restriction orifice model provides a pressure-flow relationship that is valid for choked and non-choked flow and fluids at the inlet that are single or multiphase. The flow-pressure relationship is derived starting from a steady-state momentum balance, resulting in a general expression for the mass flux, G, given as:

$$G(P)=C_d\, g(v, P_i, P_o, P_c)$$

where:

P_i = Inlet pressure
P_o = Outlet pressure
P_c = Critical pressure
v = Molar volume

The critical pressure is the pressure associated with the maximum mass flux. The computed discharge coefficient, C_d is a function of the constant discharge coefficient and the inlet phase fractions, φ_I:

$$C_d = C_{d_0}\, h(\varphi_I)$$

This form allows for an accurate representation of liquid, vapor and multiphase flows.

Fire calculations. A vessel exposed to a fire can experience overpressure due to vapor generation from boiling of the liquid contents or decomposition reactions. It can also cause overheating of the vessel wall, thus reducing the wall material strength. The heat transfer model incorporates a number of options to simulate depressurization when a vessel is exposed to an open-pool fire. Two of these options are based on ANSI/API Standard 521 (2007). The API 521 option is the method from API 521 wherein the wetted area is a constant. The API 521 enhanced option dynamically calculates the wetted surface area as the phase condition of the fluid within the vessel changes. A more rigorous option is also provided for modeling heat transfer from a fire through radiation impinging on the outer surface of the vessel and heat conduction through the vessel wall.

TABLE 1. Spadeadam experiment S12

Item	Value
CH_4	66.5 mol%
C_2H_6	3.5 mol%
C_3H_8	30 mol%
Temperature	20°C
Pressure	120 bar
Diameter	1.13 m
Tan-tan height	2.25 m
Orientation	Vertical
Head type	2:1 semi-elliptical
Wall thickness	50 mm
Orifice diameter	10 mm
Back pressure	1.013 bar
External temperature	20°C

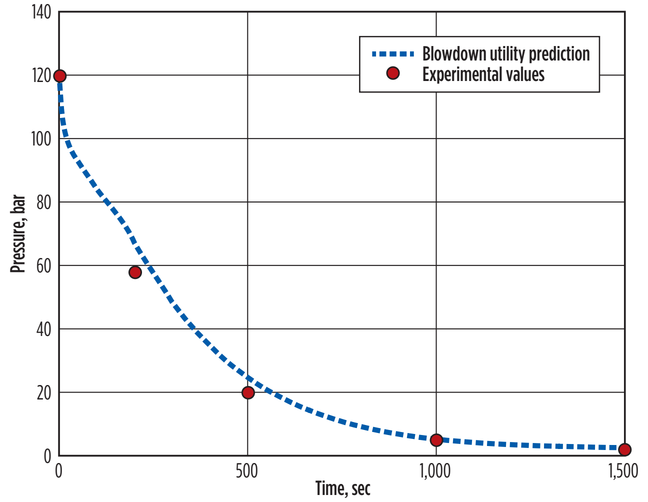

FIG. 4. Pressure profile for Spadeadam experiment S12.

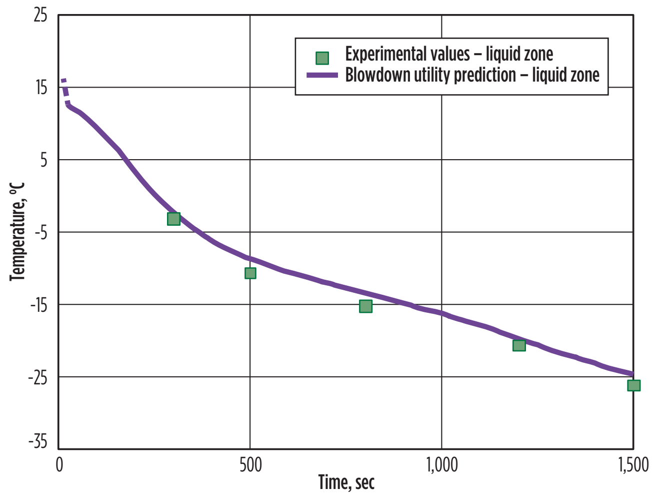

FIG. 5. Liquid-zone temperature profile for Spadeadam experiment S12.

Vessel initialization conditions. Initialization of the fluid in the vessel is based on specifications provided for the initial temperature and pressure of the vessel and total composition, which can be handled in two ways. First, the overall composition can be flashed at a specified temperature and pressure. The resulting phase compositions are used to initialize the compositions of the corresponding zones of the vessel. When the flash predicts that liquid is present, then the initial holdup of liquid must be independently specified. Second, the specified overall composition can be the initial overall composition of the vessel. In this instance, the liquid holdup in the vessel is completely determined by the thermodynamic relationships and cannot be independently specified.

The initial temperature profile through the vessel wall and insulation can have a significant impact on the predictions made by the dynamic model. Consider, for example, initializing the wall and insulation temperature profile to the initial temperature of the fluid holdup in the vessel. When this temperature is greater than the environment temperature, the energy content in the vessel wall and insulation is overestimated. Similarly, when this temperature is less than the environment temperature, the ener-

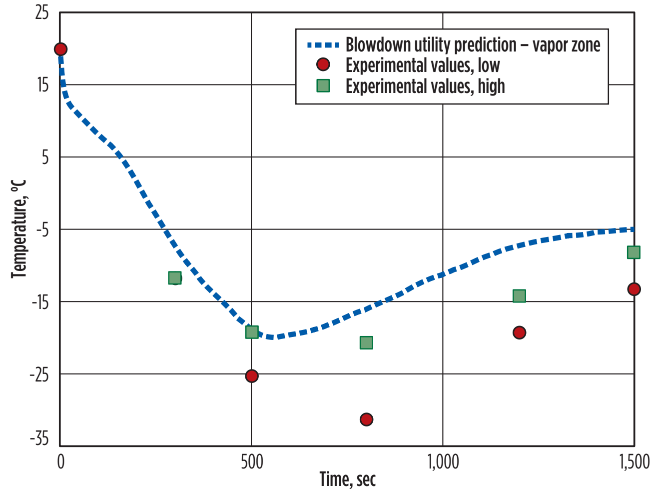

FIG. 6. Vapor-zone temperature profile for Spadeadam experiment S12.

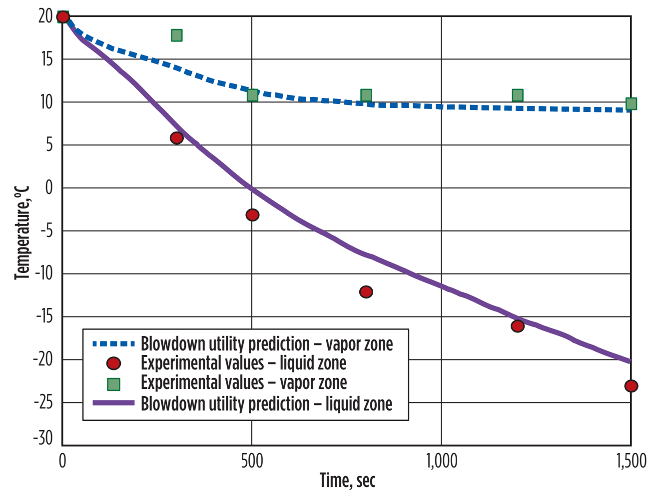

FIG. 7. Wall-temperature profiles for Spadeadam experiment S12.

gy content in the vessel wall and insulation is underestimated. In either case, the predictions of the temperature profile in the vessel wall and insulation and conditions of the fluid holdup will be attenuated during depressuring. Although not strictly correct, a steady-state wall initialization method provides the most realistic initialization of the temperature profile. With this method, the initial temperature profile in the vessel wall and insulation is calculated by solving the steady-state heat conduction equation with the convective boundary condition applied at the inner surface of the wall and the outer surfaces of the insulation.

MODEL IMPLEMENTATION

The dynamic vessel model calculations described here are incorporated into a new dynamic depressurization simulation utility; it was developed to overcome serious deficiencies identified in earlier existing tools, such as:[a]

- Numerical stability. Some tools can stall during calculations, especially for depressurization cases in which the fluid is narrow boiling, the conditions within the vessel are close to the critical conditions of the fluid, or abrupt phase changes occur during depressurization.
- Systems with a water phase. Although theoretically some tools can model a water phase, in practice, the solution of three-phase systems presents many numerical challenges.
- Limited number and type of components
- Limited selection of thermodynamic methods
- Limited capability to set the style of the heads of the vessel
- Calculation of the initial conditions is not rigorous.

The model was implemented using an equation oriented (EO) simultaneous formulation solution to handle the complexity of interactions of the different model mechanisms. Using an EO simultaneous solution formulation allows extension to future optimal design problem formulations in an efficient way.

Model validation. The presented model was tested against a large number of vessel depressurization experiments from the Spadeadam tests.[7] These experiments covered a wide range of compositions, top and bottom blowdown, vessel orientations and orifice sizes. TABLE 1 summarizes the input data for Spadeadam experiment S12.[7]

This experiment was configured and executed with the rigorous dynamic model.[a] Spadeadam experiment S12 demonstrates retrograde condensation, in which condensate forms even though the pressure is dropping due to depressurization. The results are shown in FIGS. 4–7. As illustrated in FIG. 4, there is good agreement between the experimental pressure profile and the predicted pressure.

FIGS. 5 and 6 show the experimental data for the liquid and vapor temperature regions of the vessel compared with the model predictions. The predicted temperature profiles match the experimental data well; they also clearly show that the vessel conditions are not at equilibrium. FIG. 7 shows the experimental inner surface wall temperatures in the vapor and liquid regions of the vessel compared with the model predictions for the same locations. Again, the model predictions agree quite well with the experimental data.

Better design tools for pressurized vessels. A detailed non-equilibrium vessel model was developed and incorporated into a dynamic depressuring utility of the simulator. Dynamic simulation of depressuring adds value in the selection of construction materials for vessels as well as orifice sizing. It overcomes serious deficiencies identified in earlier commercially available tools. The model can provide a high degree of solution accuracy and is robust for three-phase systems. The model consistently predicts liquid formation when it occurs experimentally and demonstrates stable solution behavior in systems with many components. The utility offers a large number of accurate thermodynamic models and can be used to model vessels with any torispherical head style. It also performs rigorous calculation of initial phase equilibrium and vessel conditions. HP

NOTES

[a] The dynamic vessel model calculations described previously have been incorporated in a new dynamic depressurization utility of the UniSim Design process simulator, named the Blowdown Utility.

LITERATURE CITED

Complete literature cited is available at HydrocarbonProcessing.com.

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