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Numerical modeling of rapid depressurization of a pressure vessel containing two-phase hydrocarbon mixture

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ABSTRACT

Blowdown or rapid depressurization of pressure vessels is a well-known safety process that removes overpressure at an emergency situation. Since the thermodynamic and transport properties in a vessel change remarkably during depressurization, rigorous estimation of the properties with respect to time is essential. Particularly, the temperature drop due to the expansion would cause the wall of the vessel to become brittle, and hence, it should be evaluated in an early stage of the design process. This study developed a numerical model to simulate the phenomenon of the rapid depressurization and estimate the non-equilibrium temperature changes of the vapor, liquid and vessel wall during the depressurization process, considering combined convection, nucleate boiling and transient multilayer conduction through the vessel wall. The results of this study were compared with experiment, numerical models from literature and several commercial software and showed good agreement with experimental results.

1. Introduction

The term blowdown can be defined as a rapid depressurizing process of equipment or facilities such as pressure vessels. In an emergency, overpressure causes mechanical failure of equipment or rupture of a vessel, and the flammable fluid from the rupture causes the fire or explosion. Blowdown valves are emergency safety valves that depressurize equipment by discharging fluid for safe operation, often installed in a parallel configuration with pressure relief valves. The discharged gas is sent to the flare network or other suitable disposal process to prevent accidents from overpressure. The API Standard 521 (API, 2007) recommends that efficient depressurization condition is to reduce the operating pressure below 50% of design pressure or 690 kPa in 15 min.

During the depressurization, two aspects are important. The first one is to remove the pressure as soon as it is required, and the second one is to confirm whether the changes in fluid properties harm the pressure vessel itself. During depressurization, the fluid inside the vessel expands quickly due to the decrease in pressure, and the expansion of the fluid in the vessel causes a sudden drop of the temperature. If the wall temperature reaches the ductile-brittle transition temperature (DBTT) of the vessel wall material, the vessels can be ruptured and the leakage of toxic and flammable fluids causes severe problems such as explosion (Cui et al., 2010; Khattak et al., 2016). Therefore, the estimation of a reliable minimum temperature is critical, and it should be evaluated in the early stage of design (Moss and Basic, 2012).

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However, the thermodynamic phenomena in a pressure vessel during rapid depressurization are complex, and the change in properties is not easy to estimate (Haque et al., 1992a). To estimate the temperature and other thermodynamic and transport properties of the fluid during depressurization, the expansion path must be specified. Ideally, the expansion through a valve can be assumed as an isenthalpic process. In a rapid expansion, however, a part of the enthalpy is consumed as P–V work, and the actual expansion path is neither isenthalpic nor isentropic. In addition, as the required time for the depressurization is short, the temperature of the fluid drops faster, and the wall temperature of the vessel cannot be in a thermal equilibrium with the fluid. Accordingly, the wall temperature decreases slower than the fluid temperature, and it is required to solve the convection heat transfer problem between the inner fluid and the vessel wall. After the temperature of the inner fluid and vessel wall decreases, there is additional heat transfer from the outer ambient temperature into the vessel and the fluid. Therefore, a combined heat transfer calculation of both convection and conduction with the changing properties of the fluid is required to describe the phenomena. The metallic property of the vessel is directly related to heat conduction and must be considered. When the fluid temperature reaches the dew point of the fluid, liquid condensation happens in the vessel. The condensed liquid droplets drop to the bottom of the vessel, and vaporize because the wall temperature is still higher than the fluid dew point. The vaporization causes the additional cooling of the local area in the bottom of the vessel contacting the liquid. Therefore, the vessel wall also becomes non-equilibrium system, and the top region of the vessel wall contacting with vapor has higher temperature than that in the bottom part of the vessel wall contacting liquid. Due to the higher heat capacity of the liquid than that of the vapor, the temperature change of the liquid is slower than that of the vapor, it results in non-equilibrium condition between vapor and liquid. Therefore, vapor, liquid, the wall contacting vapor, and the wall contacting liquid would have different temperature during blowdown (Mahgerefteh and Wong, 1999). To simulate these complex phenomena, rigorous numerical model with detailed algorithms is required. In particular, it is important to estimate the properties of the initially condensed liquid and the wall temperature contacting liquid in the vessel. When initially condensed liquid falls and contacts the vessel inside wall, the inner wall temperature drops considerably. Then the initial liquid-side inner wall temperature affects the heat transfer calculation as well as the following estimation of liquid-side inner wall temperature.

Some researchers have been studying the depressurization process to simulate the complex phenomena during blowdown and several numerical models and commercial software have been developed, but only the limited information was opened. Byrnes et al. (1964) conducted experiments on a vertical pressure vessel filled with nitrogen and hydrogen and developed a simple derivative equation model for blowdown with assumptions that the pressure decreases exponentially with a time coefficient, and that the heat exchange occurs only via natural convection. The results showed good average fitting, but the estimated results in low temperature initial condition did not fit with the experiments. Richardson and other researchers (Haque et al., 1990, 1992a,b) developed a numerical model named as "BLOWDOWN." The model used principle of corresponding states with consideration of non-equilibrium conditions among phases including gas and liquid and compared the simulation results with lab-scale experimental results, which depressurized hydrocarbon mixture of C1, C2 and C3 in a pressure vessel. However, the model did not explain about the estimation of initial wall temperature contacting liquid, and used the extended principle of corresponding states that was reported that it had consistency problem and heavy computational work (Mahgerefteh and Wong, 1999). Mahgerefteh and Wong (1999) and Wong (1998) developed a model named as "BLOWSIM" after pointing out limitations in using the corresponding state theory and introducing equation of states to predict the fluid properties. They compared its simulated results with another experimental case from Szczepanski (1994) which depressurized hydrocarbon mixtures of C1, C2, C3 and n-C4. However BLOWSIM assumed only natural convection for heat exchange and a homogeneous vessel wall temperature along the thickness instead of transient conduction with multi-layer, resulting in inaccurate estimation of wall temperature. Speranza and Terenzi (2005) suggested a model named as "BLOW" which used time derivatives of energy and mass balance, and based on the concept of BLOW, D'Alessandro et al. (2015) developed more detailed model named as "VBsim" to estimate EOS-based properties. However, both models considered only conduction without convection, which caused some gap of wall temperature with experimental results by Haque et al. In commercial software packages, VESSFIRE (2009) compared their simulation results with experimental case from Szczepanski (1994) but did not mention any details for modelling. HYSYS took over BLOWDOWN model and included a depressurization model in HYSYS version 9. Its results were compared with experimental cases (Benjamin and Souvik, 2016) but showed different simulated results compared with results of BLOWDOWN (Haque et al., 1990, 1992a,b). The other software, gFlare (Marriott et al., 2011), did not disclose the methodology used for modeling.

This study developed a numerical model to simulate changes of the non-equilibrium properties of the fluid and wall temperature in a pressure vessel during blowdown for two-phase multi-component hydrocarbon fluid based on PR-EOS. For better estimation, an elaborate heat transfer model was reflected including multi-layer transient conduction, combined convection of natural and forced convection, and nucleate boiling at the vessel surface. The separated vapor and liquid zone could estimate the different wall temperature contacting vapor and liquid separately. The simulated results were compared with experimental results and simulation results from BLOWDOWN, BLOWSIM, BLOW, VBSIM, VessFire, and HYSYS V9.

2. Properties calculation

2.1. *Vapor and liquid volume*

Accurate prediction of the fluids properties is the very first step before building a model. In this study, each of the calculated property was validated with references for light hydrocarbons by Younglove and Ely (1987) from the NIST. The pressure range was from atmospheric pressure up to 50 MPa, and the temperature range was from 100 K to 600 K. Properties of liquid and vapor phase were compared with the reference at the saturation line from the triple point to the critical point. In this study, the Peng-Robinson equation of state (PR EOS) was used to calculate the vapor volume of the hydrocarbon mixture (Peng and Robinson, 1976). PR EOS is a well-known EOS for hydrocarbon systems and has the strength of simplicity since only the critical points and the acentric factor are required. As the accuracy of the liquid volume prediction by the PR EOS is not sufficiently high, COSTALD method (Hankinson and Thomson, 1979) was used to calculate the liquid volume. To correct the pressure effect, the Thomson and Hankinson correlation (Thomson et al., 1982) was employed.

2.2. *Critical properties*

Critical properties are the basic inputs for the calculation of EOSs. When a hydrocarbon mixture consists of a large portion of light hydrocarbons, such as methane and ethane, critical pressure of the mixture tends to get higher than that of the pure component. Therefore, a thermodynamic approach to calculate the critical points is required. This study used the API Technical data book to calculate the critical temperature (Daubert and Danner, 1997). In case of critical pressure, the Helmholtz free energy theory suggested by Dimitrakopoulos et al. (2014) was used.