## VENT SIZING APPLICATIONS FOR REACTIVE SYSTEMS

James P. Burelbach Fauske & Associates, Inc. © 16W070 West 83rd Street Burr Ridge, Illinois 60521

# Prepared for Presentation at the AIChE 2001 Spring National Meeting 5<sup>th</sup> Bi-Annual Process Plant Safety Symposium, Pressure Relief Session, April 25 Unpublished

AIChE Shall Not Be Responsible for Statements or Opinions Contained in Papers or Printed in its Publications

Safe process design requires knowledge of chemical reaction rates, character, and energy release. The AIChE Design Institute for Emergency Relief Systems (DIERS) provided the necessary tools to gather such data (Fauske & Leung, 1985). A primary purpose of that effort was evaluation of emergency relief vent requirements for systems under upset conditions, including the effects of two-phase flow. The traditional DIERS vent sizing methodology considers two-phase flow whether the vented material behaves as a vapor (tempered), gassy, or hybrid system. Given the difficulty of predicting two-phase flow regimes, the practice has usually been to design for homogeneous vessel situations, thus erring on the safe side. This can be overly conservative in many cases. Recent articles (Fauske, 1998, 2000) cite large-scale experimental data for several reactive systems supporting a gas/vapor venting approach. The Fauske method makes direct use of relevant experimental data obtainable with a DIERS-based low  $\phi$ -factor calorimeter such as the Advanced Reactive System Screening Tool (ARSST) described by Burelbach (1999). Kinetic modeling and detailed thermophysical properties are not required. Also, it is not necessary to resolve uncertainties in the two-phase flow regime; rather it is sufficient to distinguish between "foamy" and "non-foamy" vapor systems. For systems that are foamy an adequate vent size may be obtained using twice the vapor venting relief area and allowing for modest overpressure. This does not mean that there is no two-phase flow, but just that in many cases an adequate, yet not overly conservative, vent size can be determined without taking a two-phase flow penalty. (Of course for effluent control design, the possibility of two-phase venting should be accounted for even if it is not the basis for the vent design.) This paper applies Fauske's latest approach to specific examples of vapor, gassy, and hybrid systems.

## EXPERIMENTAL APPROACH TO SYSTEM CHARACTERIZATION

A reactive system can be experimentally characterized using the ARSST. This simple adiabatic calorimeter uses a 10-ml sample in a small open glass test cell (low thermal inertia  $\phi$ ) mounted inside a 350-ml pressure containment vessel. More sophisticated low  $\phi$ -factor equipment such as the Vent Sizing Package 2 (VSP2), based on the original DIERS bench-scale apparatus (Fauske & Leung, 1985), may also be used (see Askonas, et al., 2000). The flow charts in Fig. 1 summarize a suggested experimental approach using open-test data. For ARSST users, the first test (Test #1) should be performed with the containment pressure set equal to the maximum allowable accumulated pressure (MAAP) of the process vessel (or 100 psi above the intended relief pressure, whichever is higher). Typically the MAAP is 10% above the (gauge) design pressure or MAWP (maximum allowable working pressure). The subsequent course of action is determined once the reaction has gone to completion (see Fig. 1) based on whether or not noncondensable gas has been generated. The system cannot be gassy or hybrid unless noncondensable gas is formed.

If the system behaves like a vapor system, then any observed pressure rise during Test #1 simply reflects vapor generation plus heating of the initial gas. Subsequent cooldown and condensation returns the system to its initial pressure. If there is negligible mass loss from the open cell test, or if no pressure spike is observed, then the possibility of total pressure containment should be investigated by estimating the vapor pressure curve of the sample mixture. (This can be accomplished in the ARSST by running a second test, initially at a relatively low pressure, and then increasing the pressure in a stepwise manner to identify various tempering points.) Otherwise, Test #2 for a vapor system is set up with the containment backpressure maintained at the intended relief set pressure. Ideally the set pressure is as low as practical so as to minimize the energy release rate during venting and to maximize the available margin for overpressure. *Allowance for overpressure is the key aspect of vent sizing for vapor systems*. Test #2 establishes the boiling (tempering) temperature at the relief set pressure. A good measure of the corresponding self-heat rate is then obtained from Test #1 where boiling was suppressed. With this data (no other information related to kinetics or thermophysical properties is required) a practical vent size can be found using simple formulas from Fauske (2000).



Figure 1: Methodology for System Characterization from Open Test Data.

If the reactive system generates noncondensable gas, then the final pressure in Test #1 exceeds the initial pressure. The Test #1 rate data should then be examined for any evidence of tempering. Typically, such hybrid behavior is suggested by differences in the time and temperature at which the pressure rate and self-heat rate go to zero (one would expect gas generation to outlast self-heating in this case). If these rates go to zero almost simultaneously then the system can be considered gassy, even though tempering may occur at lower pressures. The vent requirement is evaluated using the measured maximum pressure rise rate  $\dot{P}_{max}$  at the MAAP (Fauske, 2000). It is good practice to estimate  $\dot{P}_{max}$  directly from the pressure-time data rather than from a numerically smoothed rate plot. If the calculated vent area is too large then Test #2 may be performed to seek the benefit of tempering. If a hybrid system is indicated, then Test #2 yields the tempering temperature, and the corresponding self-heat and pressure rise rates at that temperature are obtained from the Test #1 data.

For VSP2 users a closed-cell test with automatic pressure tracking is normally run (yielding continuous closed-system pressure-temperature data). Then a vapor system vent size can be determined using the more rigorous  $\omega$ -method (Leung, 1986) as embodied in the VSSP software (Fauske & Associates, Inc., 1997). The closed test provides the self-heat rates at all of the corresponding sample vapor pressures, so the vent sizing requirements can be evaluated at any desired relief set pressure within the scope of the test data. However, if the reaction is anticipated to generate significant noncondensable gas (say from decomposition), then one should either run an open-cell VSP2 test (taking advantage of the 4-liter containment volume) or reduce the sample charge (from typically 80 ml to 50 ml or less). For a hybrid system the closed-cell VSP2 data can again be used for vent sizing using the  $\omega$ -method (Leung, 1992) as embodied in the VSSPH software (Fauske & Associates, Inc., 1994).

Note that for fire exposure one should always consider performing open Test #2 (possibly at ambient backpressure) to properly account for composition changes, including potential gassy decomposition of a reactive heel. Often this later case is most limiting, although tempering during solvent boiloff may weaken the subsequent decomposition relative to what would be observed neat (no solvent). *Open test data are essential to proper characterization of gassy systems.* 

### VENT SIZING EQUATIONS

The following equations can be used to calculate an appropriate vent size based on vapor/gas venting (Fauske, 2000) for critical or highly subcritical flow, respectively:

$$A/V = \frac{1}{0.61 C_{\rm D}} \left[ \frac{\rho c \dot{T}}{\lambda P_{\rm s}} \left( \frac{R T_{\rm s}}{M_{\rm w,v}} \right)^{1/2} + \frac{\rho v \dot{P}}{m_{\rm t} P_{\rm s}} \left( \frac{M_{\rm w,g}}{R T_{\rm s}} \right)^{1/2} \right]$$
(1)

$$A/V = \frac{1}{C_{D}} \left[ \frac{\rho c \dot{T}}{\lambda P_{s}} \left( \frac{RT_{s}}{M_{w,v}} \right)^{1/2} + \frac{\rho v \dot{P}}{m_{t} P_{s}} \left( \frac{M_{w,g}}{RT_{s}} \right)^{1/2} \right] \left( \frac{1}{2(1 - P_{b}/P_{s})} \right)^{1/2}$$
(2)

where

1

$A(m^2)$	=	vent area,
$V(m^3)$	=	reactant volume,
$\rho$ (kg m <sup>-3</sup> )	=	reactant density,
$c (J kg^{-1} K^{-1})$	=	liquid specific heat,
$\dot{T}$ (K s <sup>-1</sup> )	=	self-heat rate,
$\lambda (J \text{ kg}^{-1})$	=	latent heat,
$P_{s}(Pa)$	=	relief set pressure for vapor or hybrid systems (MAAP if gassy),
$v(m^3)$	=	test freeboard volume (standard ARSST vessel is $3.5 \times 10^{-4} \text{ m}^3$ ),
$\dot{P}$ (Pa s <sup>-1</sup> )	=	rate of pressure rise,
$m_t (kg)$	=	test sample mass,
$\mathbf{R} (\mathbf{Pa} \mathbf{m}^3 \mathbf{K}^{-1} \mathbf{kmol}^{-1})$	=	gas constant (8314),
$T_{s}(K)$	=	relieving temperature corresponding to P <sub>s</sub> .
$P_{b}(Pa)$	=	backpressure,
$M_{w,v}$ (kg kmol <sup>-1</sup> )	=	vapor molecular weight,
$M_{w,g}$ (kg kmol <sup>-1</sup> )	=	gas molecular weight,
C <sub>D</sub>	=	discharge coefficient ( $C_D = 1$ for an "ideal" nozzle).

It is convenient for the critical-flow venting examples that follow to rearrange Eq. (1) according to

$$A/V = \frac{C_{1}}{C_{D}} \frac{\dot{T}}{P_{s}} + \frac{C_{2}}{C_{D}} \frac{\dot{P}}{P_{s}}$$
(3)

where

$$C_{1} = 4.0 \times 10^{-6} \frac{\rho c}{\lambda} \left(\frac{RT_{s}}{M_{w,v}}\right)^{1/2} \quad \text{and} \quad C_{2} = 2.73 \times 10^{-2} \frac{\rho v}{m_{t}} \left(\frac{M_{w,g}}{RT_{s}}\right)^{1/2}$$
(4)

The units of  $\dot{T}$  and  $\dot{P}$  are now °C min<sup>-1</sup> and psi min<sup>-1</sup>, respectively, while P<sub>s</sub> is in psia. Equation (2) can be rearranged in a similar way. Fauske (2000) shows that the numerical values of the dimensional property groups in Eq. (4) do not change dramatically from one material to another, and in most cases are bounded by simply using the physical properties of *water*. For screening purposes Eqs. (1) and (2) have thus been further simplified by Fauske (2000) to

A/V = 
$$\frac{C}{C_D P_s} (\dot{T} + \dot{P})$$
, C = 3.5 x 10<sup>-3</sup> (= 7 x 10<sup>-3</sup> for a foamy *vapor* system) (5)

and

A/V = 
$$\frac{C}{C_D \Delta P^{1/2}} (\dot{T} + \dot{P})$$
, C = 4 x 10<sup>-3</sup> (= 8 x 10<sup>-3</sup> for a foamy *vapor* system) (6)

respectively, where again T and P are in °C min<sup>-1</sup> and psi min<sup>-1</sup>, while P<sub>s</sub> and  $\Delta P$  are in psia. The factor C arises from using water properties and ARSST parameters in the above vapor/gas venting equations. For example, suppose both C<sub>1</sub> and C<sub>2</sub> in Eq. (4) are evaluated based on water at 1 atm and 100°C (T<sub>s</sub> = 373 K, M<sub>w,v</sub> = 18 kg kmol<sup>-1</sup>,  $\rho$  = 1000 kg m<sup>-3</sup>, c = 4200 J kg<sup>-1</sup> K<sup>-1</sup>,  $\lambda$  = 2.2 x 10<sup>6</sup> J kg<sup>-1</sup>), conservatively assuming M<sub>w,g</sub> = 44 kg kmol<sup>-1</sup> (i.e. CO<sub>2</sub>), and using the ARSST standard containment volume (v = 3.5 x 10<sup>-4</sup> m<sup>3</sup>) and nominal sample mass (m<sub>t</sub> = 10 g). Then C<sub>1</sub> = 3.2 x 10<sup>-3</sup> and C<sub>2</sub> = 3.6 x 10<sup>-3</sup>, which can each be rounded off to obtain the common factor C = 3.5 x 10<sup>-3</sup> that appears in Eq. (5). For the purposes of the screening equation it does not matter that C<sub>1</sub> and C<sub>2</sub> effectively have different units.

Equations (1) through (6) are shown in their most general (hybrid) form including both vapor ( $\dot{T}$ ) and gas ( $\dot{P}$ ) terms. For a vapor system the gas term is omitted, while for a gassy system the vapor term is omitted. For a vapor system that has not been demonstrated to be non-foamy Eqs. (1) through (6) should include an additional factor-of-two to account for possible foamy two-phase flow while allowing about 40% overpressure relative to the absolute set pressure (Fauske, 2000). The implication for gassy and hybrid systems is that significant gas generation encourages early mass loss and effectively removes the venting limitations presented by foamy systems. When using the screening equations, it is important to keep in mind that v and  $m_t$  are equipment-specific. For example, a VSP2 open test would typically have v = 4000 ml and  $m_t = 80$  g, implying that the measured value of  $\dot{P}$  used in Eq. (5) or (6) should be scaled by a factor of about (4000/350)(10/80)=1.4. Lastly, note that Eqs. (2) and (6) only apply to incompressible (Bernoulli) flow, as say for atmospheric storage tanks.

#### Vapor System Example – Methanol/Acetic Anhydride

Loss of cooling has been identified as a credible upset scenario for a 1500-kg batch of methanol/acetic anhydride in a 2.3 m<sup>3</sup> (600-gal) vessel. The vessel design pressure (MAWP) is 275 psig (MAAP = 302 psig), the relief set pressure is 15 psig, the fill fraction is 81%, and there is no tailpipe. ARSST data are used to characterize the system and size the relief vent.

Test #1 is performed using a chilled 10-g sample (3.86-g methanol, 6.14-g acetic anhydride). The containment is pressurized to 300 psig and sealed, and a slow thermal scan is imposed at 0.5°C min<sup>-1</sup>. Temperature and pressure data for this test are shown in Fig. 2. After cooldown the containment pressure returns to 300 psig. Noncondensible gas is not formed ( $P_{end} = P_{start}$ ), so the mixture is classified as a vapor system. Test #2 is similar to Test #1 except that the backpressure is set at 15 psig. Again the thermal scan rate is about 0.5°C min<sup>-1</sup>. A relief valve is used to minimize backpressure "build up" during the test, which otherwise tends to increase the apparent tempering temperature. The reacting mixture completely tempers at about 98°C, and the relief valve limits the pressure to 17 psig. Figure 3 compares self-heat rate data for the high and low backpressure tests. The self-heat rate at  $T_s = 98°C$  is 20°C min<sup>-1</sup> (from Test #1).

For choked flow Eq. (3) is applied, with an added factor-of-two included to accommodate potentially foamy behavior. This is the prudent approach unless the vapor system can be demonstrated to be non-foamy. If the properties in Eq. (3) are well known they should be evaluated at the relief set temperature  $T_s$ . For convenience one might simply consider the physical properties for methanol at 98°C, which could be rationalized based on the excess of methanol (twice the stoichiometric requirement) and its relative volatility. Then the appropriate parameters for calculating the vent area from Eq. (3) are  $V = 1.86 \text{ m}^3$ ,  $M_{w,v} = 32 \text{ kg kmol}^{-1}$ ,  $\rho = 800 \text{ kg m}^{-3}$ ,  $c = 3200 \text{ J kg}^{-1}$ ,  $K^{-1}$ ,  $\lambda = 1.0 \times 10^6 \text{ J kg}^{-1}$ ,  $\dot{T} = 20^{\circ}\text{C}$  min<sup>-1</sup>,  $P_s = 29.7$  psia, and  $T_s = 371 \text{ K}$ . These values yield  $C = 6.3 \times 10^{-3}$ , leading to A/V = 4.2  $\times 10^{-3} \text{ m}^{-1}$ ,  $A = 7.9 \times 10^{-3} \text{ m}^2$ , and  $d_{ideal} = 3.9$  inches.

A similar (but more involved) calculation may be performed using an ideal solution approach to determine the mixture properties for 50% conversion. Then  $M_{w,v} = 53.4 \text{ kg kmol}^{-1}$ ,  $c = 2500 \text{ J kg}^{-1} \text{ K}^{-1}$ , and  $\lambda = 583,000 \text{ J kg}^{-1}$ , leading to C = 6.6 x  $10^{-3}$  and  $d_{ideal} = 4.1$  inches. However, simply using ambient water properties (with  $\rho = 1000 \text{ kg m}^{-3}$ ) gives  $C = 6.4 \text{ x} 10^{-3}$  and  $d_{ideal} = 4.0$  inches. Finally, the "screening" equation (5) of Fauske (2000) yields  $A/V = 4.7 \text{ x} 10^{-3} \text{ m}^{-1}$ ,  $A = 8.8 \text{ x} 10^{-3} \text{ m}^2$ , and  $d_{ideal} = 4.2$  inches.

It is illustrative to compare the "new" approach of Fauske (2000) to the previously established simplified DIERS method (Fauske, 1988; Creed & Fauske, 1990). For a vapor system the appropriate equation, derived from an emptying time philosophy and assuming two-phase flashing flow and 20% overpressure (absolute) during venting, is

$$A/V = 1.5 \times 10^{-5} \frac{\rho \dot{T}}{F P_s}$$
(7)

where the flow reduction factor F = 1.0 for an ideal nozzle. Again taking  $\rho = 800$  kg m<sup>-3</sup>, and V = 1.86 m<sup>3</sup> results in d<sub>ideal</sub> = 5.5 inches. The latest Fauske (2000) approach is clearly an improvement over Eq. (7), due in large part to the added benefit of allowing 40% overpressure relative to the absolute set pressure. With some loss of conservatism Eq. (7) can also be extended to 40% overpressure by multiplying by the ratio 20%/40% = 1/2, leading to d<sub>ideal</sub> = 3.9 inches, consistent with Fauske (2000).

For comparison, vent-sizing data for this system have also been obtained from a closed-cell VSP2 test. The relief set pressure  $P_s = 15$  psig corresponds to a set temperature  $T_s = 95^{\circ}$ C, and the corresponding self-heat rate is about 18°C min<sup>-1</sup>. The relief requirements have been calculated using the VSSP program. Assuming homogeneous two-phase flow and allowing 40% overpressure (absolute) the required ideal vent area is  $1.15 \times 10^{-2} m^2$ , corresponding to  $d_{ideal} = 4.8$  inches. The vapor vent area in this case (no overpressure) is calculated to be  $2.72 \times 10^{-3} m^2$ . Using twice this vapor vent area (presuming foamy behavior) gives  $d_{ideal} = 3.3$  inches. This vent size is somewhat smaller than that calculated above using Eq. (3) mainly because the simplified approach effectively uses a slightly higher relief set temperature and therefore a higher self-heat rate. Also, the latent heat estimated by the VSSP program using the Clapeyron equation ( $\lambda = 647,000 \text{ J kg}^{-1}$ ) is larger than the ideal solution estimate used in the simplified analysis. To better compare the hand calculation with the computer result the VSSP analysis has been repeated using the ideal solution latent heat and an effective set pressure of  $P_s = 18.6$  psig (i.e. the closed system VSP2 vapor pressure corresponding to  $T_s = 98^{\circ}$ C measured in the low backpressure ARSST test). This results in an ideal vent area of  $1.63 \times 10^{-2} m^2$ , corresponding to  $d_{ideal} = 5.7$  inches. Now the vapor vent area is  $A = 3.72 \times 10^{-3} m^2$ . Again taking twice this area gives  $d_{ideal} = 3.8$  inches, consistent with Fauske (2000).

Lastly, it can be demonstrated using the ARSST Flow Regime Detector (Burelbach, 1999) that the methanol/acetic anhydride system is actually not foamy. The required vent area can then be reduced to half that calculated above from Eq. (5), and  $d_{ideal} = 2.9$  inches. A detailed and time-consuming property evaluation would provide only a marginal reduction in vent size, notwithstanding uncertainty in the extent of chemical conversion. Rather, it is expedient and reasonable to simply use the screening equations of Fauske (2000) for calculating the relief requirements. Fauske's comparison to large-scale data provides the technical basis for this approach. Clearly, for tempered systems a lower set-pressure is better. Furthermore, the significant uncertainties in the details of two-phase discharge are "enveloped" by designing for 40% overpressure relative to the (absolute) relief set pressure.

### Gassy System Example - 37.5% 3,4,4-Trimethyl Hexanoyl Peroxide in n-Dodecane

ARSST data are again used to determine the relief requirements, in this case for a 1000-kg storage tank of 37.5% 3,4,4-trimethyl hexanoyl peroxide in n-dodecane subject to a 2°C min<sup>-1</sup> fire. The vessel MAWP is 275 psig (MAAP = 302 psig), the relief set pressure is 55 psig, and there is no tailpipe.



Figure 2: Temperature and Pressure Histories for Vapor System Test #1.



Figure 3: Self-Heat Rates for Vapor System Example.



Figure 4: Temperature and Pressure Histories for Gassy System Test #1.

Test #1 is performed using an 8.3-g sample. The containment vessel is pressurized to 300 psig and sealed, and a thermal scan is imposed at 2°C min<sup>-1</sup>. Temperature and pressure data for this test are shown in Fig. 4. After cooldown the containment pressure shows a gain of 15 psi. Non-condensable gas was formed. The self-heat and pressure rates both go to zero at about the same time, so the system is gassy at high backpressure. (Note that at such high rates a slight difference between the times that  $\dot{T}$  and  $\dot{P}$  approach zero can result in an artificial offset in temperatures between the endpoints of the two rate curves.) Test #2 is similar to Test #1 except that the backpressure is set lower, at the relief set pressure of 55 psig. The aim of this test is to see if any tempering benefit can be achieved. Again the thermal scan rate is about 2.0°C min<sup>-1</sup>. Fig. 5 compares pressure rate data from Tests #1 and #2. The mixture does not exhibit significant tempering (T<sub>max</sub> from Test #1 is 204°C, while T<sub>max</sub> from Test #2 is 202°C). After cooldown the containment pressure again shows a gain of 15 psi, and the system is classified as gassy.

The ideal vent area is estimated from Eq. (3) using the following parameters:  $V = 1.33 \text{ m}^3$ ,  $\rho = 750 \text{ kg m}^{-3}$ ,  $v = 3.5 \times 10^{-4} \text{ m}^3$ ,  $m_t = 0.0083 \text{ kg}$ ,  $M_{w,g} = 44 \text{ kg kmol}^{-1}$  (i.e. CO<sub>2</sub>),  $\dot{P} = \dot{P}_{max} = 5700 \text{ psi min}^{-1}$ ,  $P_s = MAAP = 302 \text{ psig} = 317 \text{ psia}$ , and  $T_s = 165^{\circ}\text{C} = 438 \text{ K}$ .  $\dot{P}_{max}$  is estimated from an expanded Test #2 pressure/time plot. The relieving temperature  $T_s$  coincides with the peak pressure rate. These values result in C = 3.0 x 10^{-3}, leading to A/V = 0.054 m<sup>-1</sup>, A = 0.072 m<sup>2</sup>, and  $d_{ideal} = 11.9$  inches. Simply using Fauske's "screening" equation (5) gives comparable results.

It is illustrative to again compare the "new" approach of Fauske (2000) to the previous simplified DIERS method (Fauske, 1988; Creed & Fauske, 1990). For a gassy system the appropriate equation is

$$A/V = 3 \times 10^{-6} \left(\frac{1}{F}\right) \left(\frac{\rho}{m_t}\right) \frac{\dot{P}}{P^{3/2}}$$
(8)

which assumes no early mass loss of reactants, and homogeneous two-phase flow at the peak gas generation rate. Eq. (8) results in  $d_{ideal} = 27$  inches. The Fauske (2000) approach is a big improvement, whereas considering two-phase flow at peak reactive conditions can greatly overestimate the required vent area. Calorimetric data demonstrate that significant material losses occur well before reaching peak reactive conditions, supporting the assumption of gas venting only. This "early mass loss effect" can be demonstrated in the ARSST by using the Flow Regime Detector (Burelbach, 1999).

#### Hybrid System Example – 25% Di-Tert-Butyl Peroxide (DTBP) in Toluene

A 400-gal vessel containing 1000 kg of 25% DTBP in toluene has a MAWP of 275 psig (MAAP = 302 psig) and the relief set pressure is 40 psig. There exists a 3" rupture disc and a long tailpipe with several elbows extending 20 ft upward. The ideal vent area is calculated first, using ARSST data, and then the impact of the tailpipe is analyzed.

Test #1 is performed using an 8.7-g sample. The containment vessel is pressurized to 300 psig and sealed, and a thermal scan at 2°C min<sup>-1</sup> is imposed. Temperature and pressure data for this test are shown in Fig. 6. After cooldown the containment pressure shows a gain of 17 psi. Non-condensable gas was formed. The self-heat and pressure rates both go to zero at about the same time (at  $T_{max} = 248$ °C), so the system is gassy at high backpressure. Test #2 again uses a lower backpressure, normally set at P<sub>s</sub>. However, in this example the backpressure is set at 46 psig. The additional 6 psi of backpressure represents the potential tailpipe backpressure arising from an elevation change of h = 20 ft = 6.1 m. Assuming a liquid density  $\rho = 730$  kg m<sup>-3</sup>, along with the gravitational constant g = 9.8 m s<sup>-2</sup>, the limiting hydrostatic head is  $\Delta P = \rho gh = 44$  kPa = 6 psi. Thus, setting the backpressure in Test #2 at 46 psig accommodates elevation changes in the subsequent tailpipe analysis. The scan rate in Test #2 is again 2°C min<sup>-1</sup>. Figure 7 compares self-heat rates from the two tests. The mixture clearly exhibits significant tempering starting at about 157°C, and after cooldown the containment pressure shows a gain of 9 psi. The system is classified as hybrid, since it exhibits both tempering and gas evolution.

The ideal vent area can be estimated from Eq. (3) using the following parameters:  $V = 730 \text{ kg m}^{-3}$ ,  $M_{w,v} = 92 \text{ kg kmol}^{-1}$ ,  $M_{w,g} = 44 \text{ kg kmol}^{-1}$ ,  $c = 2100 \text{ J kg}^{-1} \text{ K}^{-1}$ ,  $\lambda = 3.3 \text{ x} 10^5 \text{ J kg}^{-1}$ ,  $v = 3.5 \text{ x} 10^{-4} \text{ m}^3$ ,  $m_t = 0.0087 \text{ g}$ ,  $\dot{T} = 7^{\circ}\text{C} \text{ min}^{-1}$ ,  $\dot{P} = 1 \text{ psi min}^{-1}$ ,  $P_s = 40 \text{ psig} = 54.7 \text{ psia}$ , and  $T_s = 157^{\circ}\text{C} = 430 \text{ K}$ . Note that  $\dot{T}$  and  $\dot{P}$  are taken from the Test #1 rate data at  $T_s = 157^{\circ}\text{C}$ , the Test #2 tempering temperature. These values result in  $C_1 = 3.66 \text{ x} 10^{-3}$  and  $C_2 = 2.81 \text{ x} 10^{-3}$ , leading to  $A/V = 5.2 \text{ x} 10^{-4} \text{ m}^{-1}$ ,  $A = 7.1 \text{ x} 10^{-4} \text{ m}^2$ , and  $d_{ideal} = 1.2$  inches. Simply using Fauske's "screening" equation (5) yields  $A/V = 5.1 \text{ x} 10^{-4} \text{ m}^{-1}$ ,







Figure 6: Temperature and Pressure Histories for Hybrid System Test #1.



Figure 7: Self-Heat Rates for Hybrid System Example.

A = 7.0 x  $10^{-4}$  m<sup>2</sup>, and d<sub>ideal</sub> = 1.2 inches. It is not surprising that the results of Eq. (5) are nearly identical to the results of Eq. (3), considering that C<sub>1</sub> and C<sub>2</sub> above are nearly identical to Fauske's constant C = 3.5 x  $10^{-3}$ .

Once again the approach of Fauske (2000) is compared to the previous simplified DIERS method (Fauske, 1988; Creed & Fauske, 1990). For a tempered-hybrid system that earlier technique uses the larger of the areas calculated from either the vapor system formula Eq. (7) using  $\dot{T}$  (from Test #1 at the Test #2 tempering temperature), or the hybrid system equation

A/V = 5.6 x 10<sup>-6</sup> 
$$\left(\frac{1}{F}\right) \left(\frac{\rho}{m_t}\right) \frac{\dot{P}}{P_s^{3/2}}$$
 (9)

using  $\dot{P}$  (again from Test #1 at the tempering point). Equation (7) with  $\dot{T} = 7^{\circ}C \min^{-1}$  yields  $A/V = 1.4 \times 10^{-3} \text{ m}^{-1}$ ,  $A = 1.9 \times 10^{-3} \text{ m}^2$ , and  $d_{ideal} = 2.0$  inches. ). Equation (9) with  $\dot{P} = 1$  psi min<sup>-1</sup> yields  $A/V = 1.2 \times 10^{-3} \text{ m}^{-1}$ ,  $A = 1.6 \times 10^{-3} \text{ m}^2$ , and  $d_{ideal} = 1.8$  inches. In this case the vapor equation gives the limiting (larger) vent area. Note that this area  $(1.9 \times 10^{-3} \text{ m}^2 = 3.0 \text{ in}^2)$  is more than twice the area calculated from the Fauske (2000) method  $(2 \times 7.1 \times 10^{-4} = 1.4 \times 10^{-3} \text{ m}^2 = 2.2 \text{ in}^2)$ .

#### **Discharge Piping Example**

This example considers the tailpipe for the above Hybrid System Example. It would appear that the existing 3" rupture disc is adequate, given that  $d_{ideal} = 1.2$  inches. However, it is prudent to demonstrate that the velocity head losses in the relief piping do not reduce the relief flow (i.e. mass flux) to the point that the required actual (effective) diameter exceeds the available 3" piping. The actual minimum pipe diameter is calculated by first estimating the total equivalent velocity head loss for the existing Schedule 40 tailpipe. The ERS (emergency relief system) includes a 6" nozzle, 6' of 6" pipe, a 6"x3" reducer, the 3" rupture disc, three 45° 3" elbows, three 90° 3" elbows, and 40' of 3" pipe. The flow resistance coefficient K for each fitting is taken from API-521, 4th edition, p. 61, along with a certified K<sub>R</sub> for the rupture disc. The Fanning friction factor f = 0.005 is appropriate for two-phase flow, and the reducer is treated as an ANSI contraction. The velocity head losses for the 3" and 6" sections are summed separately as follows:

$$\sum K_{3^*} = 4f \frac{L}{D} + K_R + 2K_{45} + 4K_{90} + K_{6x3} + K_{exit}$$
  
= 4(0.005)(40/0.25) + 2.0 + 2(0.21)  $\left(1 + \frac{1}{3}\right) + 4(0.32) \left(1 + \frac{1}{3}\right) + 0.173 + 1.0 = 8.64$   
$$\sum K_{6^*} = K_{entrance} + 4f \frac{L}{D} = 0.5 + 4(0.005)(3.0/0.5) = 0.62$$

Then

$$K_{TOT,3^{*}} = \sum K_{3^{*}} + \sum K_{6^{*}} \left(\frac{3}{6}\right)^{*} = 8.68$$

which represents an equivalent 4fL/D, or L/D = 430. Although this formulation is strictly correct only for incompressible or highly subcritical flow, it is conservative for the present application. Elevation changes have already been accounted for by imposing an added backpressure during the ARSST experiment. An effective discharge coefficient (i.e. flow reduction factor)  $C_D$  may be estimated by taking  $\omega = 1$  (gas flow) in the design charts from Leung'  $\omega$ -method (Leung, 1996), which is conservative for flashing two-phase flow (lower  $C_D$ ). Alternatively, one can use the approximation  $C_D = (1 + 4fL/D)^{-0.4}$ , which gives  $C_D = 0.40$ , consistent with the values tabulated by Fauske (2000). The actual required vent diameter is then  $d_{actual} = d_{ideal} / \sqrt{C_D} = 1.2 / \sqrt{0.40} = 1.9$  inches. The existing ERS is adequate. Lastly, note that for highly subcritical (incompressible) flow  $C_D = (1 + 4fL/D)^{-0.5}$ , which is analogous to  $\omega = 0$  (liquid flow) in Leung's  $\omega$  method.

#### **Summary**

The ARSST and a new simplified methodology based on vapor/gas venting (Fauske, 2000) are used to experimentally characterize examples of vapor, gassy, and hybrid reactive systems and quickly arrive at adequate but not overly conservative vent sizes. Allowance for modest overpressure is the key aspect of vent sizing for vapor systems, effectively enveloping significant uncertainties in the details of two-phase discharge. For gassy and hybrid systems the recognition that early mass loss can occur well before peak reactive conditions reduces the vent area requirements by an order-of-magnitude relative to previous methods. Open test data are essential to proper characterization of gassy systems.

### **References**

- Askonas, C. F., Burelbach, J. P., and Leung, J. C., 2000, "The Versatile VSP2: A Tool for Adiabatic Thermal Analysis and Vent Sizing Applications," Presented at the 28<sup>th</sup> Annual North American Thermal Analysis Society (NATAS) Conference, Orlando, Florida, October 4-6.
- Burelbach, J. P., 1999, "Advanced Reactive System Screening Tool (ARSST)," Presented at the Mary Kay O'Connor Process Safety Center Symposium, College Station, Texas, October 26-27.
- Creed, M. J. and Fauske, H. K., 1990, "An Easy, Inexpensive Approach to the DIERS Procedure," Chemical Engineering Progress <u>86(3)</u>.
- Fauske, H. K., 1988, "Emergency Relief System Design for Reactive and Non-Reactive Systems: Extension of the DIERS Methodology," Plant/Operations Progress <u>7</u>(3).
- Fauske, H. K, 1998, "The Reactive System Screening Tool (RSST): An Inexpensive and Practical Approach to Sizing Emergency Relief Vents," Presented at the 1998 Process Plant Safety Symposium, Sheraton Astrodome Hotel, Houston, Texas, October 26-27.
- Fauske, H. K., 2000, "Properly Size Vents for Nonreactive and Reactive Chemicals," Chemical Engineering Progress, pp. 17-29, February.
- Fauske, H. K, and Leung, J. C., 1985, "New Experimental Technique for Characterizing Runaway Chemical Reactions," Chemical Engineering Progress, pp. 39-46, August.
- Fauske & Associates, Inc., 1997, "Vent Sizing Software Program (VSSP)", FAI, Burr Ridge, Illinois.
- Fauske & Associates, Inc., 1994, "Vent Sizing Software Program for Hybrid System (VSSPH)", FAI, Burr Ridge, Illinois.
- Leung, J. C., 1986, "Simplified Vent Sizing Equations for Emergency Relief Requirements in Reactors and Storage Vessels," AIChE Journal, 32 (10), pp. 1622-1634.
- Leung, J. C., 1992, "Venting of Runaway Reactions with Gas Generation," AIChE Journal, 38 (5), pp. 723-733.