Generalized Vent Sizing Monogram for Runaway Chemical Reactions

A method which is realistic yet also simple enough to be easily used by non-specialist engineers.

Hans K. Fauske., Fauske & Associates, Inc., Burr Ridge, IL 60521

This paper outlines for the first time a generalized vent sizing monogram for runaway chemical reactions. The method is shown to be realistic yet also simple enough to be used by non-specialist engineers. Typically, only a knowledge of the adiabatic self-heat rate corresponding to tempered reaction conditions at the specified set pressure of the relief device is necessary in order to carry out the assessment; no other thermo-kinetic and physical property information are required.

VENT SIZING MONOGRAM

On the basis of available information in the open literature [*1*] the following guidelines are suggested for sizing emergency relief systems for runaway chemical reactions.*

- Two-phase discharges must be considered.
- Partial vapor disengagement is difficult to be credited in design.
- For tempered reactions a homogeneous discharge assures a safe design.
- Vent line flows should be based upon homogeneous equilibrium flow assumptions. Non-equilibrium flow models such as Henry-Fauske, Moody, and Lockhart-Martinelli are not recommended for design.
- For tempered reactions (including hybrid systems) a modest overpressure (~20% of actual set pressure) is permissible.

The above guidelines have been used to construct the generalized vent sizing monogram illustrated in Figure 1.

For a given self-heat rate and set pressure the chart provides a vent-sizing envelope for both runaway chemical reactions including gassy reactions and for uncontrolled heating with or without chemical reactions, as long as these are tempered at the specified relief set pressure and the turbulent flow regime prevails in the vent line.

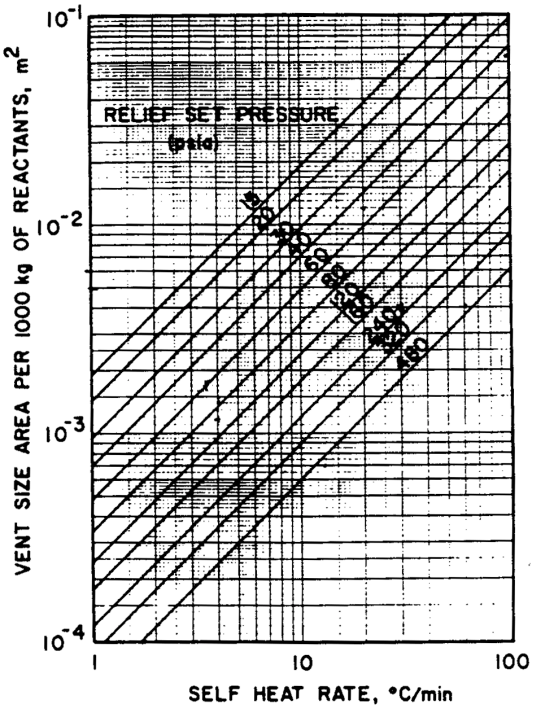

Figure 1. A generalized vent-sizing monogram for both runaway chemical reactions and for uncontrolled heating with or without chemical reaction.

APPLICATION OF VENT SIZING MONOGRAM

In this section the generalized vent sizing monogram is compared to several specific vent sizing calculational tools and loss data.

* These guidelines are also consistent with the recently completed Design Institute for Emergency Relief Systems (DIERS) R&D program [*2*] carried out under the auspices of the American Institute of Chemical Engineers (AIChE).

Monsanto Correlation for Phenol-Formaldehyde Reactions

Reference [*3*] recommends the following correlation for safe prediction of vent sizes (based upon experience) for runaway phenol-formaldehyde reactions

$$D = 0.3\sqrt{V} \qquad (3.1)$$

where D is the vent diameter given in inches and V is volume of reactants given in gallons. Equation (3.1) is noted to be valid for a set pressure of 15-16 psia, (i.e., a horizontal vent line is mandatory to avoid pressure buildup from a static head of liquid) and a self-heat rate of the order of 6.5°C/min.

Per 1000 kg of reactants the Monsanto correlation suggests a vent area of 1.25 x 10^{-2}m^2. Using the specified set pressure and the corresponding self-heat rate, the generalized vent sizing monogram suggests an area of 1.2 x 10^{-2} m^2 per 1000 kg of reactants.

The 1978 Chloroprene Accident

Reference [*4*] reported a serious chloroprene runaway accident which caused a 2000-gallon tank to explode. The vessel, which contained ~5400 kg of monomer, was equipped with a 4-inch diameter, 75-psig safety disc. The adiabatic self-heat rate at the set pressure of 75 psig has been determined to be ~15ºC/min.

For the above conditions, the generalized vent sizing chart suggests an area of 4.8 x 10^{-3} m^2 per 1000 kg of reactants. This translates to an 8-inch diameter, 75-psig safety disc required for the safe relief of the chloroprene runaway reaction.

The British Plastics Federation Computer Code

Reference [*5*] describes a detailed computational tool for evaluating emergency relief systems for runaway phenol-formaldehyde reactions. For an initial charge of 3628 kg (38.3% formaldehyde + phenol) with a relief set pressure of 2.07 bar the computer simulation resulted in a vent diameter of 30 cm with a maximum overpressure of 2.3 bar, (i.e., 11.1% overpressure). The length-to-diameter ratio of the vent line was ~100. The adiabatic self-heat rate at the relief set pressure was given as 15.4ºC/min.

Using the above self-heat rate and the corresponding set pressure, the generalized vent sizing monogram predicts an area of 1.45 x 10^{-2} m^2 per 1000 kg of reactants for 20% overpressure. Correcting for overpressure, i.e., multiplying the above value with (20/11.1) one obtains 2.6 x 10^{-2} m^2 per 1000 kg of reactants. This value translates to a vent diameter of 34. cm.

Huff's Computer Simulation

Reference [*6*] describes the most generalized computer simulation of runaway reaction venting published to date. Several computer simulations are provided, including the phenol-formaldehyde condensation reaction and comparison to the British Plastics Federation Computer code. Assuming homogeneous-froth vessel behavior and homogeneous equilibrium vent line flow, Huff's computer simulation yields a vent diameter of 33.7 cm for the runaway reaction conditions (self heat rate of 15.4ºC/min and an overpressure of 11.1%) described in the preceding section [*7*]. We recall that the generalized vent sizing monogram produced a vent-size diameter of ~34 cm.

The DIERS' Computer Code, SAFIRE

Reference [*8*] describes the latest and most advanced computer program developed for sizing emergency relief systems for runaway chemical reactions. For an initial charge of 5000 kg (80% styrene-20% ethylbenzene) with a relief set pressure of 75 psig (corresponding self-heat rate is ~15.8ºC/min), the computer simulation predicts the following vent diameters of d = 15.8 cm (L/D ~ 100), d = 16.8 cm (L/D ~ 200) and d = 18 cm (L/D ~ 400) for an overpressure of 20% based on actual set pressure.

Using the above self-heat rate and corresponding set pressure, the generalized vent sizing monogram suggest a vent area of 5.2 x 10^{-3} m^2 per 1000 kg of reactants which translates to a recommended vent diameter of d ~ 18.5 cm.

The FIA Vent Sizing Chart

The methodology behind the generalized vent sizing monogram can readily be used to quantify the often used empirical FIA chart [*9*]. The four FIA reaction categories can be quantified in terms of first order design variables including the adiabatic energy release rate, q, corresponding to the set pressure of the relief system and allowable overpressure. Figure 2 illustrates the quantification for an overpressure of 20 psi. This corresponds to ~20% overpressure for the vessels used in the FIA chart [*10*]. *As such it is important to note that the FIA chart as presented is generally valid only for one set pressure.*

CONCLUDING REMARKS

The ERS design is only as good as the most difficult part of the design strategy, i.e., the definition of the credible worst case based upon possible upset emergency conditions. As such the generalized vent sizing monogram presented in this paper is believed to provide an adequate balance in terms of the available vent sizing methodology as well as predictive conservatism.

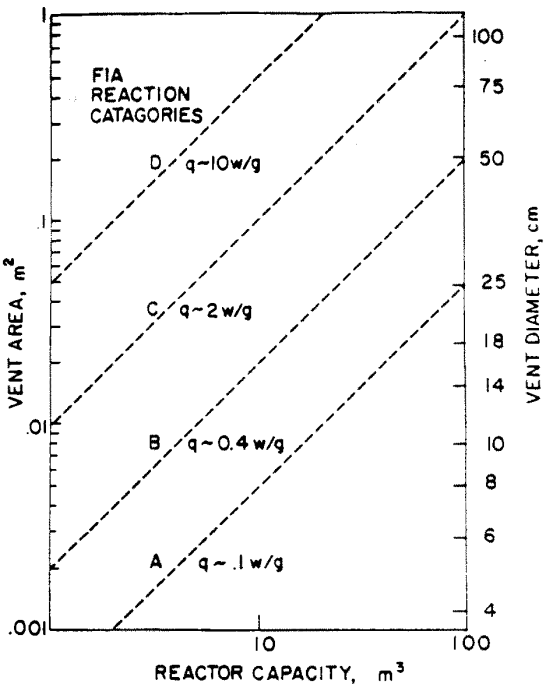

Figure 2. Quantification of the FIA chart based upon 20 psi overpressure. Vent area is simply obtained by specifying the energy release, q, corresponding to the set pressure of the relief system. Taken from [1].

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Hans K. Fauske earned the D.Sc. degree from the Norwegian Institute of Technology in 1963. He has published more than one hundred scientific articles in the areas of reactor safety and multiphase flow application and has served as a consultant to the U.S. Advisory Committee on Reactor Safeguards and the President's Commission on the accident at Three Mile Island. He now consults for domestic and foreign corporations in the chemical and nuclear industries. He is a member of the Editorial Board of the International Journal of Multi-phase Flow, a member of the American Institute of Chemical Engineers and a Fellow of the American Nuclear Society. He received one of the first University of Chicago awards for Distinguished Performance at the Argonne National Laboratory and in 1982 he became the third recipient of the Tommy Thompson Award, the highest honor the American Nuclear Society gives in the field of reactor safety.