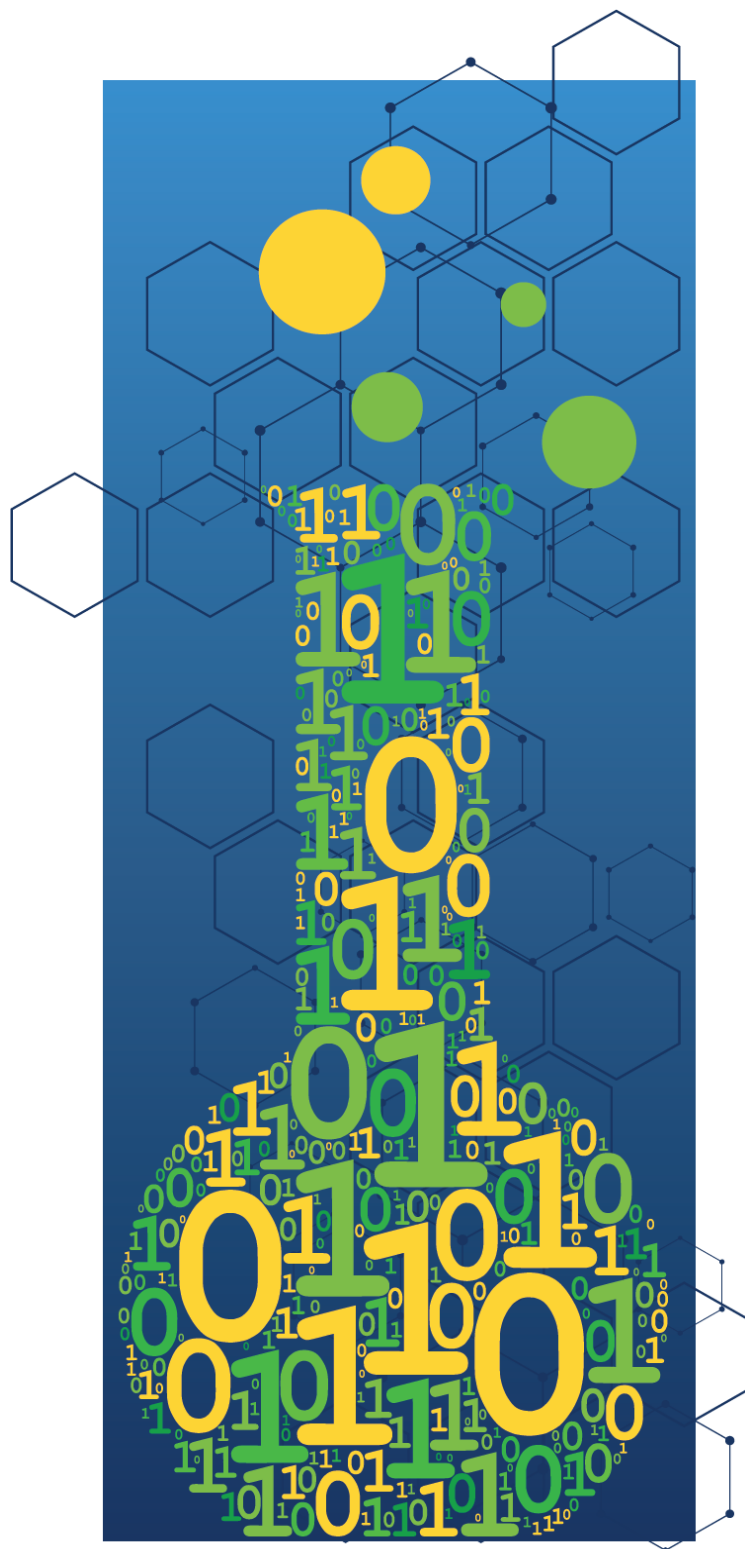


# Two-phase Flow Onset and Disengagement Methods



An ioMosaic Corporation White  
Paper

**G. A. Melhem, Ph.D., FAIChE**  
[melhem@iomosaic.com](mailto:melhem@iomosaic.com)

IO MOSAIC CORPORATION

# **Two-phase Flow Onset and Disengagement Methods**

*Pressure Relief Systems Practices*

authored by

Georges A. MELHEM, Ph.D., FAIChE

November 9, 2020

# **Contents**

<b>1 Introduction</b>	<b>2</b>
<b>2 Two-phase Flow Implications</b>	<b>2</b>
<b>3 Two-phase Flow Patterns</b>	<b>3</b>
<b>4 Two-phase Flow Dynamics</b>	<b>4</b>
<b>5 Simple Methods for Onset/Disengagement</b>	<b>5</b>
<b>6 The DIERS Coupling Equation</b>	<b>5</b>
6.1 Two-phase Flow Onset and Disengagement . . . . .	5
6.2 Vapor Quality Entering Vent . . . . .	7
<b>7 Solving the Coupling Equation</b>	<b>7</b>
<b>8 Application of the Coupling Equation to Quench Tanks</b>	<b>8</b>
<b>9 Non-boiling Height Considerations</b>	<b>8</b>
<b>10 Wall Heating Considerations</b>	<b>9</b>
<b>11 Liquid Entrainment During Vessel Blowdown</b>	<b>11</b>
<b>12 Thermodynamic Consistency of Slip Flow</b>	<b>11</b>
<b>13 Liquid Surface Tension Considerations</b>	<b>12</b>
<b>14 Testing the Performance of the Coupling Equation</b>	<b>13</b>
<b>15 Conclusions</b>	<b>14</b>

## 1 Introduction

Two-phase flow is often considered in system hydraulics as well as the evaluation and design of pressure relief and effluent handling systems. A variety of scenarios can lead to two-phase flow under relief conditions.

In general, two-phase flow during relief can occur because of flow hydrodynamics and poor vapor/liquid disengagement where (a) the liquid swells due to generation of vapor bubbles in the liquid<sup>1</sup>, (b) fluid expansion occurs due to heating, and/or (c) the superficial vapor velocity is high enough through the pressure relief device. Oversized relief devices can induce two-phase flow because a large relief flow area yields a higher superficial vapor velocity. Runaway chemical reactions and/or chemical systems that are viscous and/or foamy almost always lead to homogeneous two-phase flow.

Two-phase flow can also occur by entrainment, for example, where gas is sparged at a high enough rate in the liquid. In some systems, condensation leading to two-phase flow in the discharge piping can also occur due to expansion cooling caused by pressure reduction through a control valve or a pressure relief device.

Numerous two-phase flow models have appeared in the literature. These models represent broad ranges of theory. Some are based on single-phase critical flow, others on homogeneous equilibrium flow, frozen flow, separated flow, slip flow, and/or non-equilibrium flow.

Homogeneous equilibrium flow models assume equal vapor and liquid velocities and calculate the change of quality with pressure using an isenthalpic or isentropic thermodynamic path. Homogeneous frozen models assume equal vapor and liquid flow velocities and that the quality is frozen along the flow path, i.e., no change with respect to pressure or temperature. The separated flow models assume different vapor and liquid flow velocities and account for mass, momentum and heat transfer between the separate phases.

## 2 Two-phase Flow Implications

It is preferred to eliminate or significantly reduce the potential for two-phase flow. This can be accomplished by either (a) reducing the risk/likelihood of the scenarios that can lead to two-phase flow to a tolerable level and/or (b) specific relief and effluent handling systems design considerations and implementations<sup>2</sup>.

More mass is vented from a vessel during two-phase flow than during all vapor flow. During all vapor flow, the liquid has to make up the lost vapor and beneficial energy tempering occurs. This helps to reduce the relief requirements for fire exposure scenarios for example.

As a result of more mass being discharged due to two-phase flow, potential dispersion, fire, and explosion hazard footprints can become significantly larger. Vent containment and/or flow separa-

---

<sup>1</sup>Generation of bubbles can occur due to mechanical means and/or chemical reactions including decomposition reactions.

<sup>2</sup>This includes the use of quenching systems that suppress chemical reactions that can cause two-phase flow, such as the introduction of a quench fluid, and/or the quick injection of an inhibitor or a neutralizing agent.

tion are often required to reduce the risks of two-phase flow. When homogeneous two-phase flow occurs, the specific ratio of vapor to liquid does not change in the vessel during venting and as result beneficial energy tempering does not occur. When more vapor is vented relative to liquid, beneficial energy tempering occurs because the liquid has to make up the lost vapor. This is one of the primary reasons why homogeneous two-phase flow results in large relief requirements for vessels exposed to external fire, external or internal heating, and/or where chemical runaway reactions are the cause of the homogeneous two-phase flow.

It is therefore important to be able to determine:

- (a) what configurations and/or process conditions can lead to two-phase flow,
- (b) the vapor quality entering the vent, and
- (c) the rate at which two-phase flow occurs.

Undoubtedly, one of the most important contributions of the American Institute of Chemical Engineers (AIChE) design institute of emergency relief systems (DIERS) to chemical process safety is the development of the coupling equation which can be used to determine if and when two-phase will occur and what the vapor quality entering the vent will be. DIERS also published methods for the estimation of two-phase flow rates.

### 3 Two-phase Flow Patterns

The treatment of two-phase flow is complex by nature because a sequence of flow patterns can develop within a given process pipe or unit. Figure 1 shows typical two-phase flow patterns occurring in horizontal and vertical piping configurations.

**Stratified** Gas<sup>3</sup> and liquid are separated in two cocurrently flowing phases, with liquid flowing as a layer along the channel bottom.

**Wavy** Stratified flow where flow instabilities cause a wavy gas-liquid interface excluding low flow rates conditions.

**Slug** Liquid waves tend to bridge the gap between the liquid surface and the channel top, causing the gas phase to move as a slug.

**Plug** Gas bubbles tend to agglomerate and nearly fill the cross section of the channel, moving as asymmetrical bullet shaped entities.

**Bubbly** The gas tend to distribute as discrete bubbles in the continuous liquid phase, with bubbles rising towards the top of the channel. A good example is soapy water or bubbly beer.

**Churn** Similar to bubble flow where the liquid phase is continuous. Typifies clean water or un-contaminated refrigerants where extensive bubble coalescence occurs.

---

<sup>3</sup>Gas and/or vapor may be used interchangeably in this paper

**Droplet** The vapor forms a continuous phase where the vapor superficial velocity exceeds the liquid entrainment velocity.

**Annular** At high flow rates the liquid climbs the walls of the channel, forming a ring of nonuniform thickness around a central core of gas. The gas-liquid interface is highly irregular and waves tend to break off, giving rise to dispersed annular flow. At sufficiently high gas flow rates the flow becomes dispersed, during which liquid droplets are distributed in the continuous gas phase.

## 4 Two-phase Flow Dynamics

Consider a vessel containing a two-phase mixture with an adequately sized relief device. The vapor space is maintained at a pressure that is above the bubble point of the liquid through the use of a nitrogen pad, i.e. the system is subcooled. Let us assume that a puncture / line break develops in the vapor space or the relief device is actuated due to external fire or internal chemical reaction.

We expect that mostly nitrogen will be vented first and the pressure in the vapor space to start decreasing. As the pressure reaches the bubble point, the liquid starts to flash and vapor bubbles are formed. As a result the liquid level swells (expands), and depending on the initial fill level and the liquid characteristics, the swell level can reach the relief device or puncture/break point and a two-phase mixture is discharged. If the liquid is cooled or tempered as it flashes to vapor, i.e. internal energy is converted to vaporization energy, the system is referred to as tempered.

As previously discussed, another mechanism by which two-phase flow can occur for top vessel venting or discharge is when the superficial vapor velocity at the relief device or break entrance is higher than the liquid entrainment velocity, and thus the liquid droplets are carried into the relief device or break entrance. This is mostly important for high liquid fill levels or vessels with oversized relief devices.

Under some vessel conditions the vapor could disengage completely from the liquid inside the vessel so that the swelled liquid level remains below the discharge point and all vapor flow occurs. This is referred to as partial vapor disengagement and can happen as soon as the relief device or break occurs or after a certain period of two-phase flow. Foamy liquids exhibit little vapor disengagement and as a result a large portion of the vessel contents is vented as a two-phase mixture. It is difficult to determine a priori whether or not a fluid is foamy. This is best done by testing (see [www.iokinetic.com](http://www.iokinetic.com)) using calorimetry or other suitable means.

The level of liquid swell in the vessel depends on fluid characteristics, flow regime and dynamics of bubble rise and liquid disengagement. The bubble rise velocity depends on buoyancy and surface tension and is retarded by the viscosity and foaminess of the liquid. Typical flow regimes include:

1. bubbly flow,
2. churn-turbulent, and
3. droplet flow.

When non-condensable gases are generated due to chemical reaction, the system is referred to as gassy. For foamy liquids, i.e. where the liquid phase remains continuous to essentially 100 % void fraction, the discharge should be assumed to be homogeneous two-phase at all times.

## 5 Simple Methods for Onset/Disengagement

A simple method for onset/disengagement is presented by Fauske [1] for non-foamy materials. Vapor flow occurs around a void fraction of 50 %:

$$z_l < \frac{z_h}{2} \quad (1)$$

Two phase flow occurs when:

$$0.6 \left( \frac{D_h}{D} \right)^2 \sqrt{R_g T_0 / M_w} > u_\infty \left[ \frac{z_h - z_l}{z_h} \right] \left[ \frac{z_l}{z_h} \right] \quad (2)$$

where

$$u_\infty = 1.20 \frac{[\sigma g (\rho_l - \rho_v)]^{0.25}}{\sqrt{\rho_l}} \quad (3)$$

The left hand side of Equation 2 is the vessel superficial vapor velocity based on choked flow through the hole and the right hand side is the characteristics two-phase drift velocity for bubbly flow.

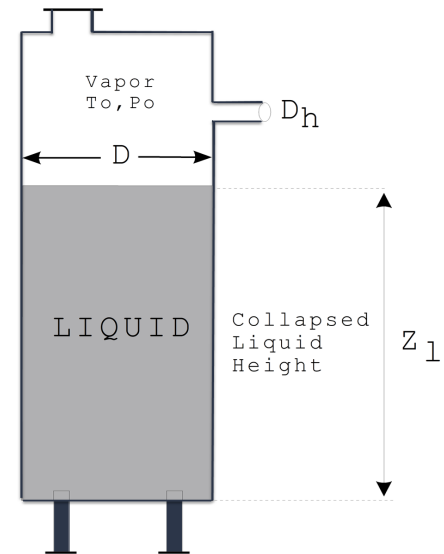
Bubbly flow regimes are more likely in typical process vessels because they are favored by the presence of small quantities of impurities, while for example churn-turbulent flow is typical for clean water-like flow conditions.

## 6 The DIERS Coupling Equation

A more detailed method for predicting the onset and disengagement of two-phase flow for non-foamy liquids from a vertical vessel during depressurization or emergency relief was developed and validated by DIERS [2]. Vapor holdup is predicted using a first order lumped parameter drift-flux formulation.

### 6.1 Two-phase Flow Onset and Disengagement

The vapor-liquid flow regimes that are addressed with this method include bubbly and churn-turbulent. The DIERS method proceeds as follows:



1. Determine the vapor capacity of the relief device or the orifice,  $\dot{M}$ .
2. Calculate the superficial vapor velocity:

$$u_{sv} = j_{g\infty} = \frac{\dot{M}}{\rho_v A} \quad (4)$$

where  $A$  is the vessel cross sectional area in  $\text{m}^2$ . Grolmes and Fisher [3] showed that all onset/disengagement models based on constant cross-sectional area for vertical cylindrical geometries can be used with little error for horizontal cylinders and spheres. For a sphere, assume an equivalent vertical cylinder with a cross sectional area equal to 2/3 the area of the sphere (or diameter = 0.8165 times the diameter of the sphere). For a horizontal cylindrical configuration, assume an equivalent vertical cylinder with a diameter equal to the square root of the horizontal cylinder diameter by length. One can also simply divide the total volume by the vertical dimension of the vessel to obtain an equivalent vertical cylindrical vessel cross sectional area.

3. Calculate the bubble rise velocity:

$$u_{\infty} = c \frac{[g\sigma(\rho_l - \rho_v)]^{1/4}}{\sqrt{\rho_l}} \quad (5)$$

where  $c$  is a constant which is flow regime dependent. Its value is 1.53 for churn flow and 1.18 for bubbly flow.

4. Calculate the dimensionless superficial vapor velocity due to flow:

$$\psi_F = \frac{j_{g\infty}}{u_{\infty}} = \frac{u_{sv}}{u_{\infty}} \quad (6)$$

5. Calculate the dimensionless superficial velocity at which two-phase flow commences. For bubbly flow it is:

$$\psi = \frac{\alpha(1 - \alpha)^2}{(1 - \alpha^3)(1 - C_0\alpha)} \quad (7)$$

where  $\alpha$  is the vessel average void fraction and  $C_0$  is a correlating parameter determined from experimental data. Its value ranges from 1.01 (conservative) to 1.2 (best estimate).

For churn flow,  $\psi$  is given by:

$$\psi = \frac{2\alpha}{1 - C_0\alpha} \quad (8)$$

The value of  $C_0$  ranges from 1 (conservative) to 1.5 (best estimate).



6. If  $\psi_F \geq \psi$ , two-phase flow is predicted.  
     If  $\psi_F < \psi$  vapor flow is predicted.  
     If  $\psi_F < \psi$  and two-phase flow is in progress, disengagement is predicted.

The  $\alpha$  vs.  $\psi$  curve is shown in Figure 10. To determine if a particular vapor venting rate will result in two-phase flow, one can simply locate the associated  $\psi$  and void fraction point on the chart. If the point is above the selected flow regime curve, then all vapor flow is predicted. If the point is below the curve, then two-phase flow will occur. Note that the purple curve (Co=1.20, Actual - Bubbly) represents the results of a dynamic vessel simulation consisting of many  $\alpha$  vs.  $\psi$  points throughout the simulation.

## 6.2 Vapor Quality Entering Vent

If two-phase flow conditions are predicted, the weight fraction of vapor entering the relief device or break is the one which satisfies the following relation:

$$\frac{\mathcal{Y}G_m A_h}{\epsilon \zeta u_\infty \rho_v A} = \frac{1}{1 - C_0 \epsilon \frac{\rho_v}{\rho_l} \frac{1 - \mathcal{Y}}{\mathcal{Y}}} \quad (9)$$

where  $\epsilon$  and  $\zeta$  are flow dependent parameters given as function of the vessel average void fraction. This equation is often referred to as the DIERS coupling equation. For bubbly flow:

$$\epsilon = \frac{\alpha}{1 - C_0 \alpha} \quad \text{and} \quad \zeta = \frac{(1 - \alpha)^2}{1 - \alpha^3} \quad (10)$$

For churn flow:

$$\epsilon = \frac{2\alpha}{1 - C_0 \alpha} \quad \text{and} \quad \zeta = 1 \quad (11)$$

Calculations involving partial vapor-liquid disengagement can be computationally intensive as they require calculation of  $G$  at each estimate of  $\mathcal{Y}$ . Note that at very large superficial vapor velocities (large vents), the disengagement will occur at a vessel liquid level equal to  $\left(\frac{C_0 - 1}{C_0}\right)$ .

## 7 Solving the Coupling Equation

The solution of the DIERS coupling equation requires trial and error. The form represented by Equation 9 has to be rearranged in order to produce a solution without numerical discontinuities as shown by Melhem [4, 5]. The preferred form for a numerical solution is:

$$f(\mathcal{Y}) = G_m \left(\frac{A_h}{A}\right) \left(\mathcal{Y} - C_0 \epsilon \frac{\rho_v}{\rho_l} (1 - \mathcal{Y})\right) - \epsilon \zeta u_\infty \rho_v = 0 \quad (12)$$

The solution begins by guessing the vapor quality entering the vent,  $\mathcal{Y}$ , and then by estimating the mass flow through the vent,  $G_m$ , using an appropriate two-phase flow model (often homogeneous equilibrium). The calculated value of  $G_m$  is inserted in Equation 12 and  $f(\mathcal{Y})$  is then evaluated. With this form of the DIERS coupling equation the actual solution of  $\mathcal{Y}$  will always be bounded between 0 and 1.

## 8 Application of the Coupling Equation to Quench Tanks

The level swell in a quench tank which involves gas/vapor bottom sparging instead of volumetric gas generation can be determined from the following equation for  $\psi$ :

$$\psi = \frac{\alpha}{1 - C_0\alpha} \quad (13)$$

This equation [6] uses the non-integral form of the churn turbulent drift flux relationship (see Zuber [7] and Wallis [8]). It will predict more level swell than Equation 8 since the maximum gas rate occurs throughout the entire two-phase column.

The DIERS coupling equation only predicts two-phase flow due to level swell. In order to account for two-phase flow due to liquid entrainment caused by gas bubbling through the liquid column, the following relation is typically used (also see [9]):

$$\frac{\dot{m}_{liq}}{\dot{M}_{gas}} = 0.18 \frac{u_{sv}^3 \rho_v^{1.5}}{[g(\rho_l - \rho_v)\sigma]^{\frac{3}{4}}} \quad (14)$$

where  $\dot{m}_{liq}$  is the liquid entrainment rate in kg/s. Note that two-phase flow caused by level swell will not occur simultaneously with two-phase flow caused by liquid entrainment. If the swell does not reach the vessel top, only liquid entrainment will occur. If the swell reaches the vessel top, liquid entrainment will not occur.

## 9 Non-boiling Height Considerations

The DIERS coupling equation key parameters include the average void fraction in the swelled liquid, the superficial vapor velocity at the liquid surface, and the bubble rise velocity [10]. There are practical scenarios where boiling and/or vapor generation does not occur throughout the entire liquid volume but only occurs at the top portion of the liquid. As a result, liquid swell does not occur below the top liquid portion because the bottom liquid portion does not contain bubbles. The churn-turbulent model can be extended to handle top-biased vapor generation by using the average void fraction of the top portion of the liquid,  $\hat{\alpha}$ . This is referred to as the nonboiling height vessel model. The same value of  $\psi$  is used in the DIERS coupling equation, but with  $\hat{\alpha}$ :

$$\psi = \frac{2\hat{\alpha}}{1 - C_0\hat{\alpha}} \quad (15)$$

$$\hat{\alpha} = \frac{\alpha}{1 + \delta(\alpha - 1)} \quad (16)$$

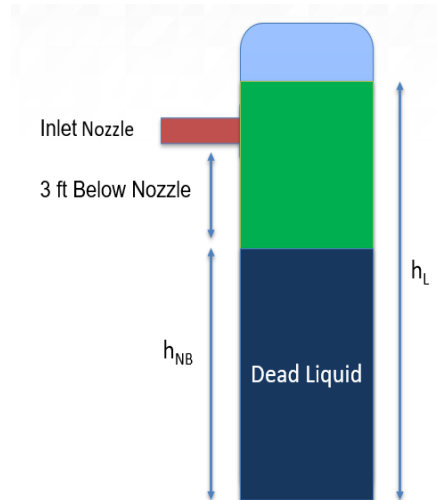
where  $\alpha$  is the vessel overall average void fraction, and  $\delta$  is the ratio of nonboiling liquid region height to the unaerated rest height of the total liquid. Although the physical basis for nonboiling height is not directly applicable to gas sparged systems, a reasonable value of  $\delta$  can be specified to reflect the location where the gas is being sparged into the liquid relative to overall liquid height. Where there is a physical basis for determining the nonboiling liquid height due to strong recirculation effects in the boiling region caused by rising vapor bubbles,  $\delta$  can be approximated from:

$$\delta = \frac{1}{1 + 0.76 \left(\frac{1}{D^{0.2}}\right) \left(\frac{1}{\rho_l}\right) \left(\frac{dP_s}{dt}\right)} \quad (17)$$

where  $D$  is the vessel diameter in meters,  $\rho_l$  is the liquid density in  $\text{kg}/\text{m}^3$ , and  $\frac{dP_s}{dt}$  is the rate of saturation pressure change with time in  $\text{Pa}/\text{s}$  during venting. Effectively, the non-boiling height model causes the churn turbulent model to be executed with a higher value of  $\alpha$  which leads to quicker vapor/liquid disengagement.

The non-boiling height model can be extended to applications where vapor is introduced below the liquid level through a nozzle or a pipe. In this application the liquid towards the bottom of the vessel is considered to be "dead" liquid without any bubbles. The values of  $\delta$  can be set at:

$$\delta = \frac{h_{NB}}{h_L} \quad (18)$$



The "dead" liquid layer has to be clear of bubbles from any internal or external sources. Instead of using 3 ft below the nozzle, one can approximate the gas penetration depth as the point at which the horizontal velocity of the incoming gas and entrained liquid equals the bubble rise velocity from Equation 5 for churn turbulent flow.

## 10 Wall Heating Considerations

Another variation to the DIERS coupling equation was proposed by Fisher and Forrest [11] for large vessels under fire exposure where bubble generation only occurs at the walls. This model applies where the bottom of the large vessel is not exposed to fire such as large flat bottom tanks designed per API 620/650 where the fire can only heat the side walls.

This model does not apply to mixtures which are chemically reactive or where gas is being sparged or bubbled into the liquid. A new definition of void fraction required to avoid two-phase flow to

wall heating is provided:

$$\hat{\alpha} = 2\alpha_{BL}\beta\frac{H_l}{D} \quad (19)$$

$$\beta = 0.089 + 0.001136F_{wall} \quad (20)$$

$$\alpha_{BL} = 0.0576F_{wall}^{2/3} \quad (21)$$

$$F_{wall} = 28.34\frac{q_{fire}}{\rho_v u_\infty \lambda} \quad (22)$$

where  $\alpha_{BL}$  is the average void fraction in the boundary layer,  $\beta$  is the boundary layer thickness growth rate,  $H_l$  is the liquid height in the vessel,  $D$  is the vessel diameter,  $q_{fire}$  is the fire flux<sup>4</sup> in  $W/m^2$ ,  $\rho_v$  is the vapor density in  $kg/m^3$ ,  $u_\infty$  is the chrun turbulent flow regime bubble rise velocity defined in Equation 5 in  $m/s$ , and  $\lambda$  is the latent heat of vaporization in  $J/kg$ .

Fisher and Forrest [11] further modified the vapor/liquid disengagement criteria by defining a void fraction required to avoid two-phase flow due to liquid entrainment:

$$\alpha_{ent} = \frac{F_{BHT}}{H_{tank}} \quad (23)$$

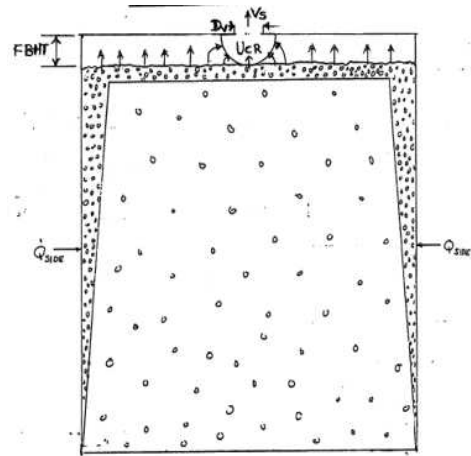
$$F_{BHT} = R_v \sqrt{\frac{u}{2u_e}} \quad (24)$$

where  $R_v$  is the relief device flow radius,  $u_e$  is the critical liquid entrainment velocity defined in Equation 32,  $F_{BHT}$  is the required free board height in the vessel to avoid liquid entrainment,  $H_{tank}$  is the tank height, and  $u$  is the pseudo vent discharge gas velocity  $\frac{\dot{m}_g}{\rho_g A_v}$ . Two-phase flow is predicted if:

$$(1 - \alpha_o) + (1 - \alpha_{ent})\hat{\alpha} + \alpha_{ent} \geq 1 \quad (25)$$

$$\alpha_o = \frac{V_T - V_l}{V_T} \quad (26)$$

$$(27)$$



where  $\alpha_o$  is the overall vessel average void fraction. The free board height relation (see equation 24) is derived by assuming that the flow through the imaginary surface area of half sphere of radius  $F_{BHT}$  at the entrance of the vent is equal to the vent flow at entrainment:

$$2\pi F_{BHT}^2 u_e = \pi R_v^2 u \quad (28)$$

$$F_{BHT} = \frac{\pi R_v^2 u}{2\pi u_e} = R_v \sqrt{\frac{u}{2u_e}} \quad (29)$$

<sup>4</sup>Depending on what simulation method is used,  $q_{fire}$  may require the computation of vessel wetted area at relief temperature, which in turns requires the computation of the void fraction needed to avoid two-phase flow.

## 11 Liquid Entrainment During Vessel Blowdown

Liquid can also be entrained during vessel blowdown if the liquid level is high enough and the gas/vapor velocity in the plane of the vent is high enough. Liquid is entrained from the liquid surface by the gas motion induced by vessel blowdown through vents in the vapor space above the liquid surface (see Figure 2). A semi-empirical relationship for predicting the onset and magnitude of liquid entrainment can be used to determine the ratio of the entrained liquid flow rate to the gas flow rate discharged from the vent:

$$\frac{\dot{m}_{l,e}}{\dot{m}_g} = E_0 \left( \frac{\rho_l}{\rho_g} \right)^{0.5} \left( \frac{R_v}{H} \right) \left[ \frac{1}{2} \frac{u}{u_e} \frac{R_v}{H} - 1 \right] \quad (30)$$

where  $\dot{m}_{l,e}$  is the entrained liquid mass flow rate,  $\dot{m}_g$  is the gas mass flow rate,  $E_0$  is an entrainment coefficient ( $\simeq 0.1$ ),  $\rho_l$  is the liquid density,  $\rho_g$  is the gas density (at vessel conditions),  $R_v$  is the vent radius,  $H$  is the freeboard (vertical distance between vent plane and liquid interface),  $u$  is the pseudo vent discharge gas velocity  $\frac{\dot{m}_g}{\rho_g A_v}$  or the gas velocity in the plane of the vent where the flow is considered to become uniform, and  $u_e$  is the minimum entrainment velocity.

The last term on the right hand side of Equation 30 must be positive. As a result, a minimum freeboard required for entrainment can be established:

$$H_b = u \left( \frac{R_v}{2u_e} \right) = \left( \frac{\dot{m}_g}{\rho_g A_v} \right) \left( \frac{R_v}{2u_e} \right) \quad (31)$$

where  $H_b$  is the freeboard height required for the onset of entrainment. The minimum velocity required for entrainment,  $u_e$  is given by:

$$u_e = 3.1 \left( \frac{\sigma g \rho_l}{\rho_g^2} \right)^{1/4} \quad (32)$$

where  $\sigma$  is the liquid surface tension and  $g$  is the gravitational constant. Equation 30 can be used in conjunction with a transient blowdown simulation to calculate the liquid entrainment rate as a function of time. Some literature references have applied Equation 30 to estimate the amount of liquid that is aerosolized in deflagrations occurring in the vapor space of vessels containing liquids (see [12], [13], and [14]).

## 12 Thermodynamic Consistency of Slip Flow

Nozzle flow where slip exists between the vapor and liquid phases and/or flow from a vessel where the vapor quality entering the vent is different from the vessel average vapor quality are consistent with thermodynamic equilibrium [15]. Simply stated, the vapor and liquid phases can still be in thermodynamic equilibrium at the same temperature and pressure regardless of the relative amount of flowing vapor to flowing liquid. This is true because the individual mole fractions in each phase

are still equilibrium mole fractions. The flowing overall composition will be different than the source overall composition and can be easily calculated by combining the vapor and liquid phases that are in equilibrium:

$$z_i = \frac{x_i(1 - x_e) + y_i x_e}{\sum_i [x_i(1 - x_e) + y_i x_e]} \quad (33)$$

where  $z_i$  is the overall mass fraction of component  $i$  entering the nozzle or vent,  $y_i$  is the equilibrium vapor mass fraction,  $x_i$  is the equilibrium liquid mass fraction, and  $x_e$  is the vapor quality entering the vent.  $z_i$  will equal to  $y_i$  when  $x_e = 1$ ,  $x_i$  when  $x_e = 0$ , and the vessel average composition when  $x_e$  is equal to the vessel average vapor quality.

### 13 Liquid Surface Tension Considerations

The liquid surface tension,  $\sigma$ , is used in the calculation of the bubble rise velocity (see Equation 5). Accurate values can be directly measured and/or obtained from published data for pure components. Mixture data, especially for mixtures with wide boiling point differences or mixtures with non-condensable components such as methane or carbon monoxide or carbon dioxide, should be carefully calculated and must consider the vapor/liquid equilibrium of the mixture at the prevailing system temperature and pressure conditions. An accurate value of mixture surface tension is also important when calculating bubble nucleation rates for non-equilibrium multicomponent two-phase flow, vapor-liquid separator design, rapid phase transitions, and/or rapid vessel blowdown.

One method that can be used and has shown to be reliable is the parachor method. In the simple case of a pure component,  $\sigma$  can be calculated from the following equation:

$$\sigma^{1/n} = \mathcal{P}(\rho_l - \rho_v) \quad (34)$$

$$n \simeq 4 \quad (35)$$

where  $\mathcal{P}$  is the parachor,  $\sigma$  is the liquid surface tension in N/m,  $\rho_v$  is the molar density of vapor in kmol/m<sup>3</sup> in equilibrium with the liquid and  $\rho_l$  is the molar density of liquid in kmol/m<sup>3</sup>.

Equation 34 can be extended to mixtures:

$$\sigma_m = \left[ \sum_i \mathcal{P}_i (\rho_{l,m} x_i - \rho_{v,m} y_i) \right]^n \quad (36)$$

$$\mathcal{P}_i = \frac{\sigma_i^{1/n}}{(\rho_{l_i} - \rho_{v_i})} \quad (37)$$

where  $n$  ranges between 3.5 and 4.5 but typically set to 4,  $\rho_{l,m}$  and  $\rho_{v,m}$  are the mixture liquid and vapor molar densities at equilibrium conditions,  $x_i$  is the liquid equilibrium mole fraction, and  $y_i$  is the vapor equilibrium mole fraction. The mixture vapor/liquid equilibrium conditions are calculated at the bubble pressure or temperature conditions using an equation of state or at

constant volume for dynamic vessel relief simulations. Note the parachor value increases sharply when approaching the critical temperature conditions.

The parachor [16] may be estimated from the critical properties of a chemical using the following equation:

$$\mathcal{P} = 0.324 T_c^{1/4} v_c^{7/8} \quad (38)$$

where  $T_c$  is the critical temperature in Kelvin and  $v_c$  is the specific molar volume in  $\text{m}^3/\text{kmol}$ . In general the pure component surface tension depends on reduced temperature:

$$\sigma = \sigma_0 \left(1 - \frac{T}{T_c}\right)^n \quad (39)$$

where  $n$  is approximately 1.2,  $\sigma_0$  is an empirical constant (in  $\text{N/m}$ ) that can be regressed from measured data or from a reference value of the surface tension, and  $T$  is temperature in Kelvin. Note that for polymers, surface tension increases with polymer molecular weight:

$$\sigma = \sigma_\infty - \frac{k_e}{M^{2/3}} \quad (40)$$

where  $\sigma_\infty$  is the polymer surface tension at infinite molecular weight,  $k_e$  is a polymer specific constant, and  $M$  the polymer molecular weight.

## 14 Testing the Performance of the Coupling Equation

We consider two DIERS large scale tests [10] using water and water with 1000 ppm of detergent to illustrate the solution and performance of the coupling for churn-turbulent flow (Test T2C) and for bubbly flow (Test T12A). All the solutions for this example were produced using SuperChems Expert<sup>TM</sup>.

The vessel used in both tests has a volume of 2190 liters (588 gallons,  $L=3.048$  m,  $ID=0.9144$  m). Details of the tests are shown in Table 1.

Two solutions for Test T2C were produced using SuperChems Expert for Churn Turbulent flow using the recommended DIERS best estimate value of  $C_o = 1.5$  and the DIERS recommended conservative estimate of  $C_o = 1.0$ . The pressure predictions are shown in Figure 3. A similar pressure profile was predicted in reference [10] for  $C_o = 1.5$ . The average vessel void fraction estimates are shown in Figure 4. Similar predictions were also reported in reference [10]. A slightly better pressure prediction was reported in reference [10] by using churn turbulent flow with a non-boiling height correction for average void fraction.

The actual numerical solution implementation technique provided in SuperChems Expertis illustrated in Figures 5 and 6 for a single time step. Figure 5 illustrates the behavior of  $f(\mathcal{Y})$  as a function of the quantity of vapor entering the vent. We note that  $f(\mathcal{Y})$  is well behaved and a solution is easy to obtain.

Table 1: DIERS Large Scale Test Data Summary

	T2C	T12A
Material	Water	Water + 1000 ppm Detergent
Void Fraction	0.05	0.05
Pressure. kPa	927	510
Flow Type	Nozzle	Nozzle
Vent Location	Top	Top
Discharge Coefficient	1	1
Vent Diameter. mm	32.2	50.8

Figure 6 illustrates the behavior of the DIERS coupling Equation 1 if one attempts to obtain a direct solution of  $G_m$  using the coupling equation once  $\mathcal{Y}$  is specified. This method of solution has a numerical discontinuity (not shown in Figure 6) and is not reliable.

The results for Test T12A are shown in Figures 7, 8, and 9. All the solutions are performed without a non-boiling height correction. As with Test T2C, similar results are reported in the DIERS Project Manual [10].

Figure 10 superimposes the  $\alpha$  vs.  $\psi$  calculated by SuperChems Expert for T12A with a  $C_o = 1.2$  over the best case and conservative churn turbulent and bubbly  $\alpha$  vs.  $\psi$  curves. As mentioned earlier, to determine if a particular vapor venting rate will result in two-phase flow, one can simply locate the associated  $\psi$  and void fraction point on the chart. If the point is above the selected flow regime curve, then all vapor flow is predicted. If the point is below the curve, then two-phase flow will occur. The purple curve ( $Co=1.20$ , Actual - Bubbly) represents the results of T12A dynamic vessel simulation consisting of many  $\alpha$  vs.  $\psi$  points throughout the simulation.

## 15 Conclusions

The DIERS coupling equation is an essential modeling tool for the onset/disengagement of two-phase flow. SuperChems Expert includes a detailed implementation of the coupling equation which can be used with venting dynamics for simple and complex arrangements of vessels and/or piping. Although the coupling equation can be used to represent if two-phase will onset or disengage at a single specific set of conditions, it is most valuable when used in dynamic simulations of venting and depressuring systems with/without reactions. When used in that context, substantial improvements in process safety and cost effective risk reduction can be realized.



Figure 1: Approximate two-phase flow patterns

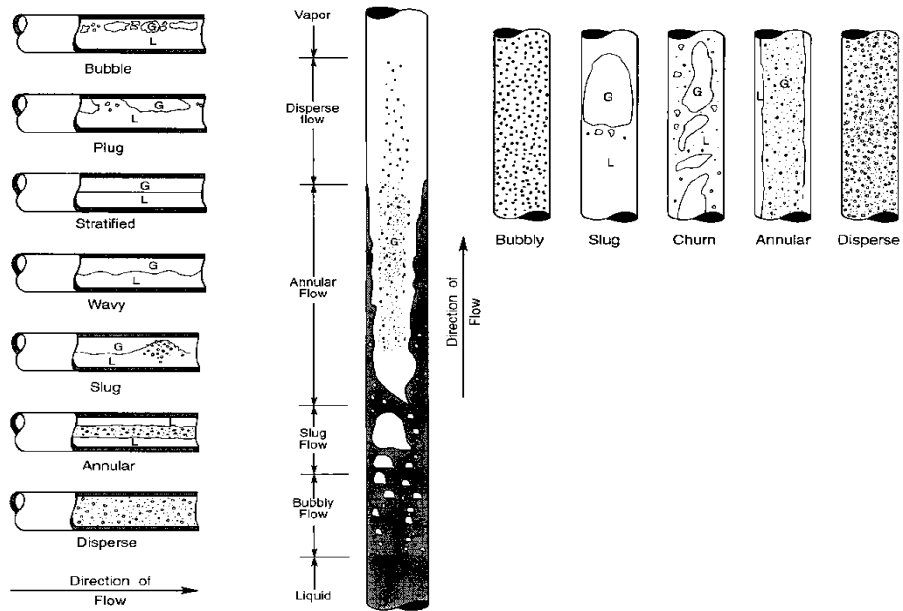


Figure 2: Liquid entrainment caused by vessel blowdown

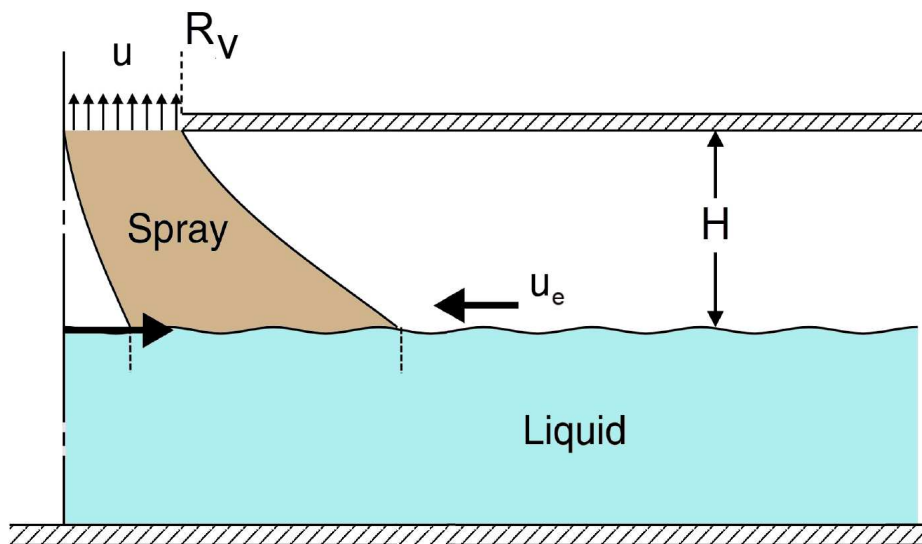


Figure 3: SuperChems ExpertChurn turbulent estimates of pressure for test T2C

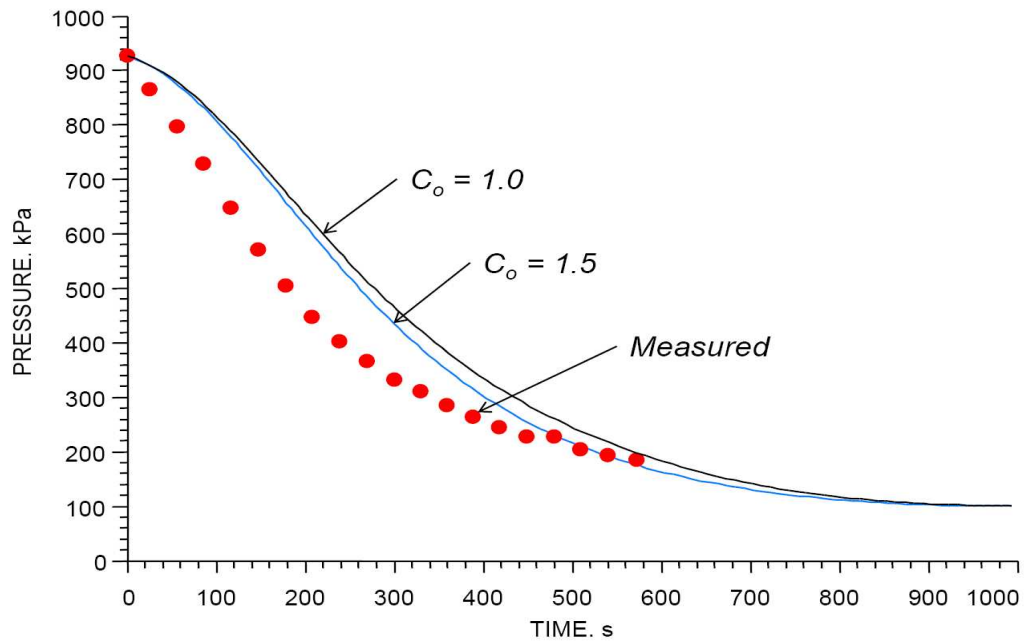


Figure 4: SuperChems ExpertChurn turbulent estimates of vessel void fraction for test T2C

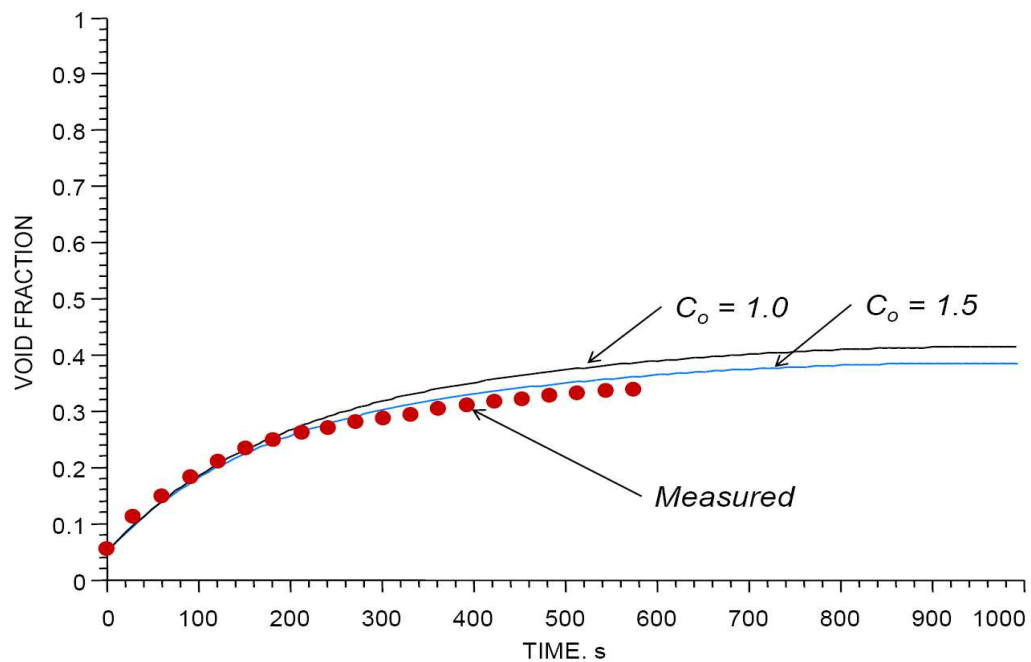


Figure 5: SuperChems ExpertChurn turbulent numerical solution of Equation 1 using  $f(\mathcal{Y})$

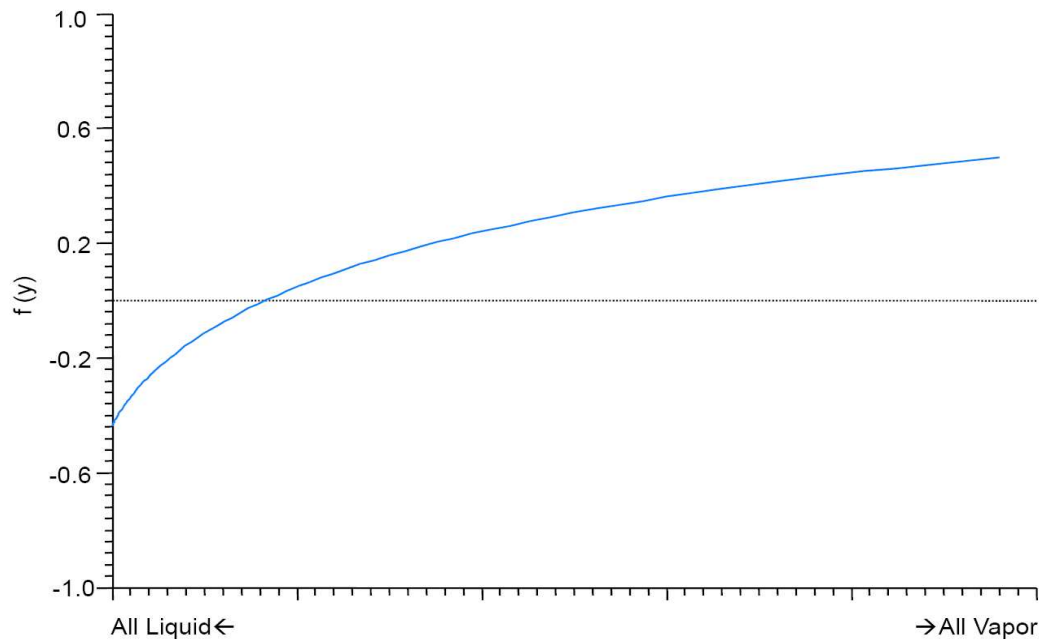


Figure 6: SuperChems ExpertChurn turbulent numerical solution of Equation 1 using  $G_m$

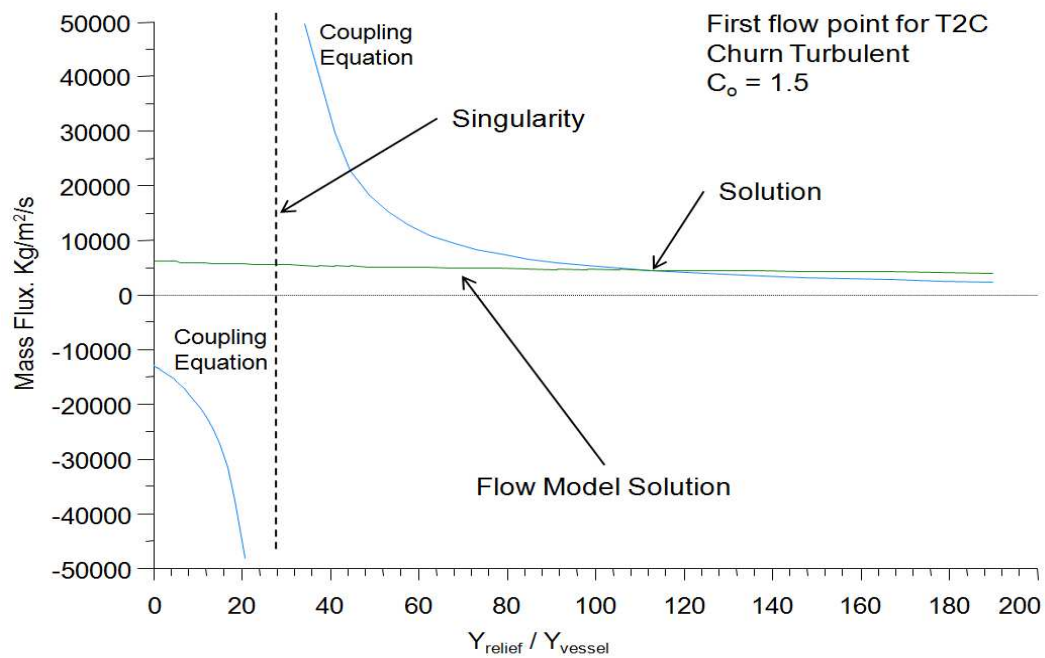


Figure 7: SuperChems ExpertBubbly estimates of pressure for test T12A

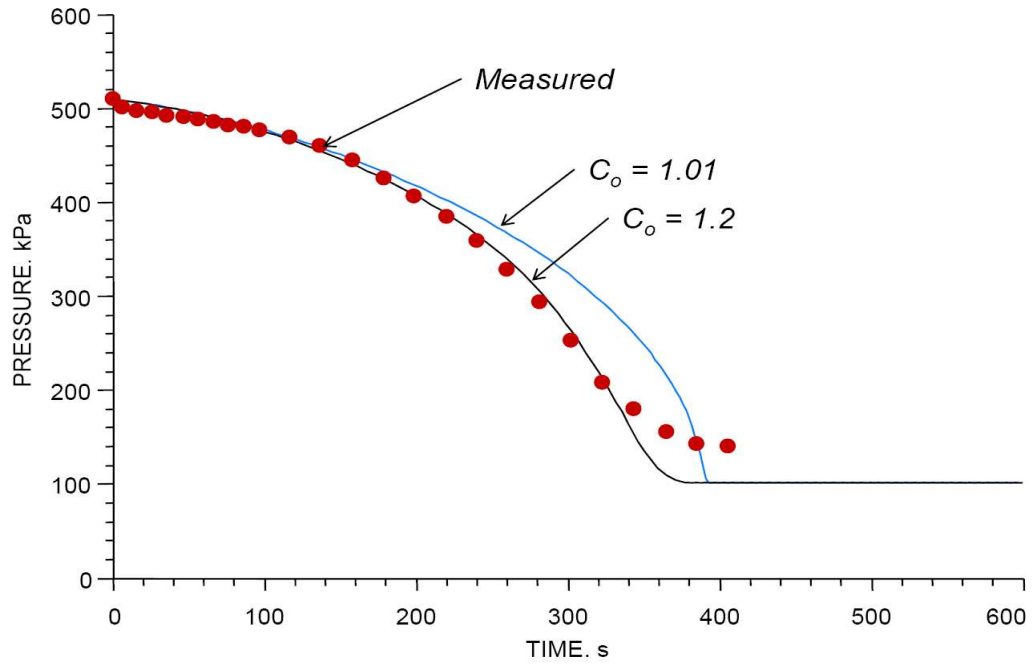


Figure 8: SuperChems ExpertBubbly estimates of vessel void fraction for test T12A

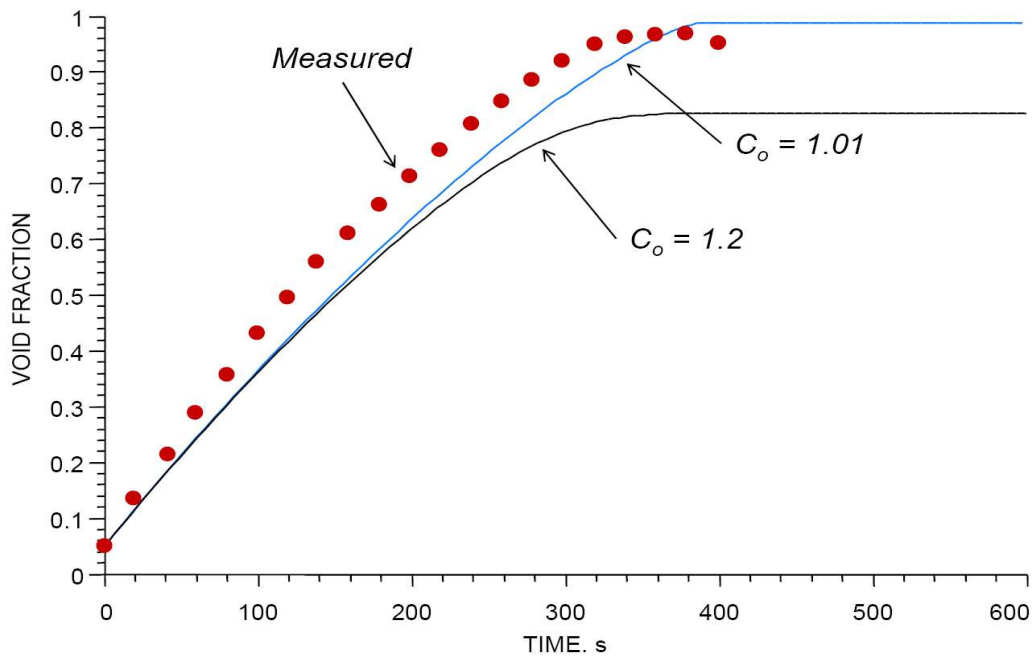


Figure 9: SuperChems ExpertBubbly estimates of vessel mass flow for test T12A

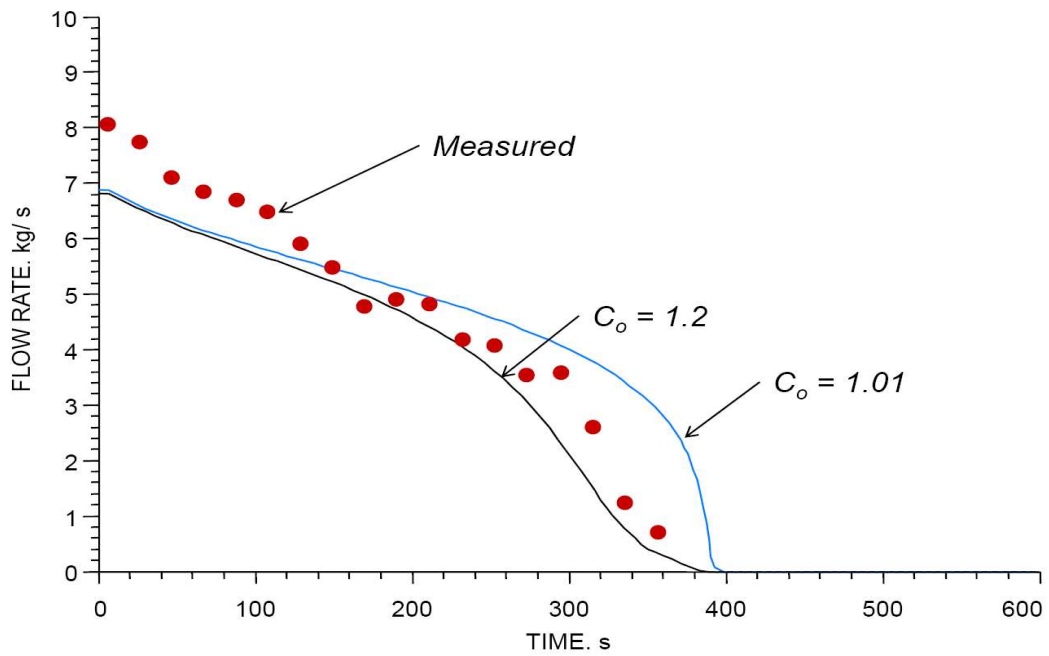
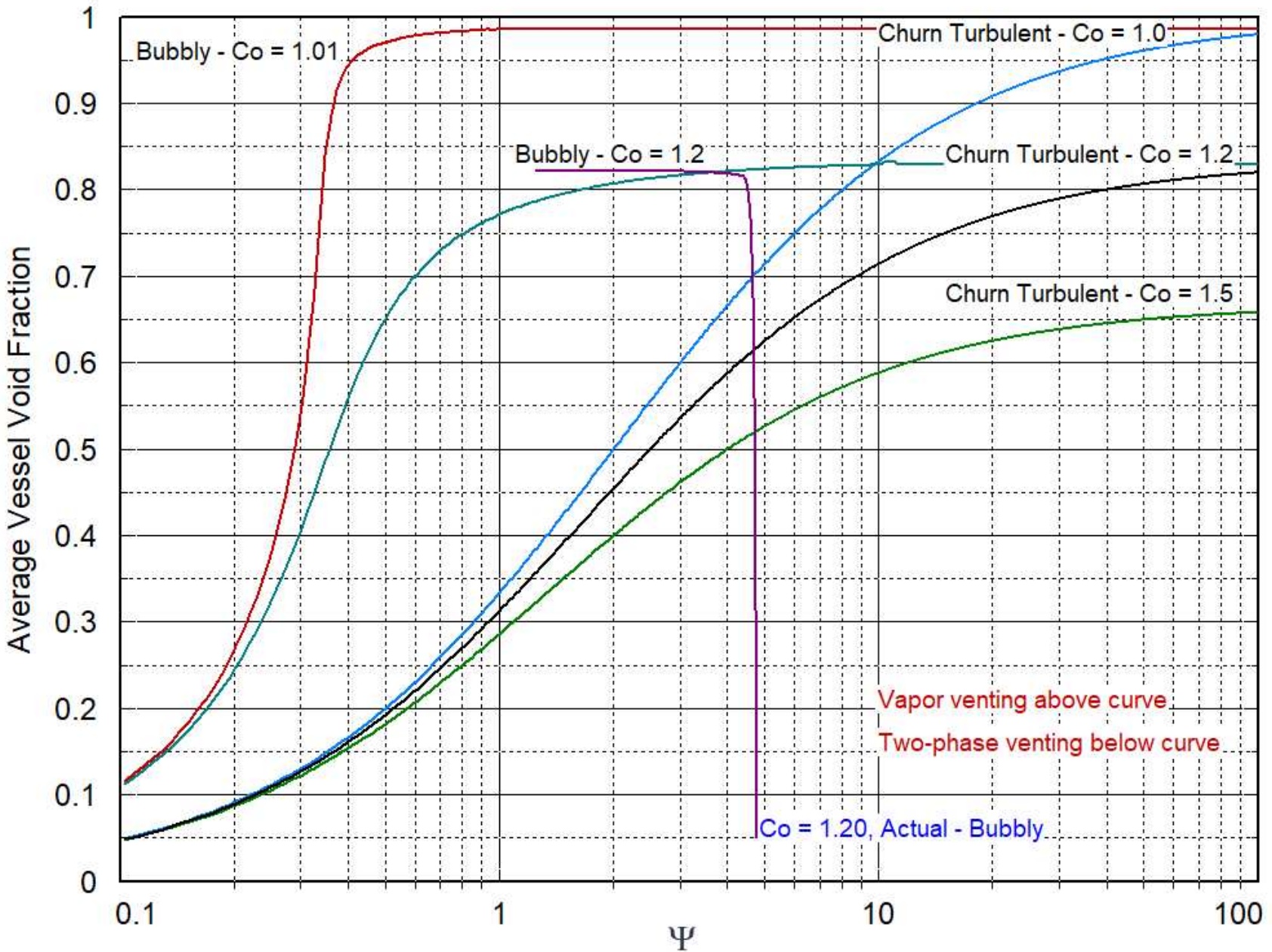


Figure 10: SuperChems ExpertBubbly estimate of  $\alpha$  vs.  $\psi$  for test T12A

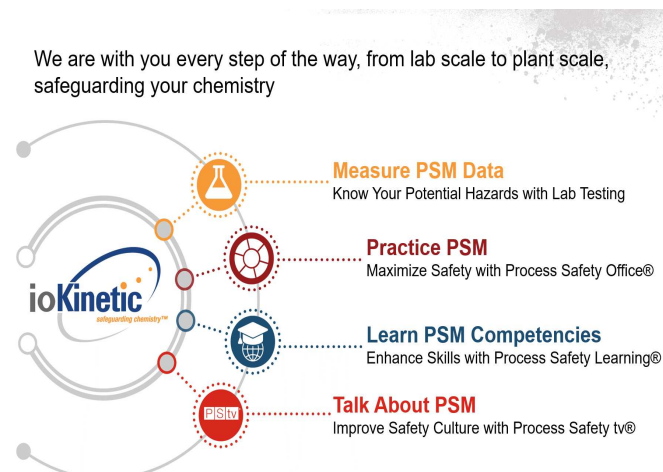


## How can we help?

In addition to our deep experience in process safety management (PSM) and the conduct of large-scale site wide relief systems evaluations by both static and dynamic methods, we understand the many non-technical and subtle aspects of regulatory compliance and legal requirements. When you work with ioMosaic you have a trusted ISO certified partner that you can rely on for assistance and support with the lifecycle costs of relief systems to achieve optimal risk reduction and PSM compliance that you can evergreen. We invite you to connect the dots with ioMosaic.

We also offer laboratory testing services through ioKinetic for the characterization of chemical reactivity and dust/flammability hazards. ioKinetic is an ISO accredited, ultra-modern testing facility that can assist in minimizing operational risks. Our experienced professionals will help you define what you need, conduct the testing, interpret the data, and conduct detailed analysis. All with the goal of helping you identify your hazards, define and control your risk.

Please visit [www.iomosaic.com](http://www.iomosaic.com) and [www.iokinetic.com](http://www.iokinetic.com) to preview numerous publications on process safety management, chemical reactivity and dust hazards characterization, safety moments, video papers, software solutions, and online training.



## References

- [1] H. K. Fauske and M. Epstein. Source term considerations in connection with chemical accidents and vapor cloud modeling. *Journal of Loss Prevention Process Ind.*, 1:75–83, 1988.
- [2] Fauske and Associates Inc. Emergency relief systems for runaway chemical reactions and storage vessels: a summary of multiphase flow methods. Technology summary, AIChE/DIERS, 1986.
- [3] M. Grolmes and H. Fisher. Vapor liquid onset/disengagement modeling for emergency relief discharge evaluation. In *AIChE Summer National Meeting*, 1994.
- [4] G. A. Melhem. Eliminate the DIERS coupling equation singularity. In *DIERS Users Group Meeting*. AIChE, Fall 2008.
- [5] M. Levin. Developments in disengagement. In *DIERS Users Group Meeting*. AIChE, Fall 2015.
- [6] AIChE/DIERS. Emergency relief systems for runaway chemical reactions and storage vessels: A summary of multiphase flow methods. Technical Report FAI/83-27, Fauske and Associates Inc., 1983.
- [7] H. K. Forester and N. Zuber. Growth of a vapor bubble in a superheated liquid. *Journal of Applied Physics*, 25(4):474–478, 1954.
- [8] G. B. Wallis. *One-Dimensional Two-Phase Flow*. McGraw-Hill Book Company, New York, 1st edition, 1969.
- [9] K. Nakajima, J. W. Palen, and J. Taborek. Analysis and prediction of entrainment and its application to kettle reboiler shell sizing. Technical Report B-K-1/2, Heat Transfer Research, Inc. HTRI, 1970.
- [10] H. G. Fisher et al. *Emergency relief system design using DIERS technology. The DIERS project manual*. AIChE/DIERS, 1992.
- [11] H. G. Fisher and H. S. Forrest. Protection of storage tanks from two-phase flow due to fire exposure. *Process Safety Progress*, 14(3):183–199, July 1995.
- [12] J. Mishima and D. Pinkston. Doe handbook airborne release fractions/rates and respirable fractions for nonreactor nuclear facilities. Technical Report DOE-HDBK-3010-94, Vol. 1, U.S. Dept. of Energy, Washington, D.C., 1994.
- [13] D. F. Paddleford and J. K. Thomas. Waste tank deflagration source generation mechanisms. Technical Report WSRCMS-95-0001, Westinghouse Savannah River Co., Aiken, SC, 1995.
- [14] B. E. Hey and D. S. Leach. A model for predicting respirable releases from pressurized leaks. Technical Report WHC-SD-GN-SWD-20007, Westinghouse Hanford Co., Richland, WA, 1994.



- [15] D. A. Shaw. Thermodynamic consistency of the DIERS coupling equation. In *DIERS Users Group Meeting*. DIERS, AIChE, October 2000.
- [16] S. N. Balasubrahmanyam. Einstein, parachor and molecular volume: Some history and a suggestion. *Current Science*, 94(2):1650–1658, JUNE 2008.

## About the Author



Dr. Melhem is an internationally known pressure relief and flare systems, chemical reaction systems, process safety, and risk analysis expert. In this regard he has provided consulting, design services, expert testimony, incident investigation, and incident reconstruction for a large number of clients. Since 1988, he has conducted and participated in numerous studies focused on the risks associated with process industries fixed facilities, facility siting, business interruption, and transportation.

Prior to founding ioMosaic Corporation, Dr. Melhem was president of Pyxsys Corporation; a technology subsidiary of Arthur D. Little Inc. Prior to Pyxsys and during his twelve years tenure at Arthur D. Little, Dr. Melhem was a vice president of Arthur D. Little and managing director of its Global Safety and Risk Management Practice and Process Safety and Reaction Engineering Laboratories.

Dr. Melhem holds a Ph.D. and an M.S. in Chemical Engineering, as well as a B.S. in Chemical Engineering with a minor in Industrial Engineering, all from Northeastern University. In addition, he has completed executive training in the areas of Finance and Strategic Sales Management at the Harvard Business School. Dr. Melhem is a Fellow of the American Institute of Chemical Engineers (AIChE) and Vice Chair of the AIChE Design Institute for Emergency Relief Systems (DiERS).

### Contact Information

Georges. A. Melhem, Ph.D., FAIChE  
E-mail. [melhem@iomosaic.com](mailto:melhem@iomosaic.com)

ioMosaic Corporation  
93 Stiles Road  
Salem, New Hampshire 03079  
Tel. 603.893.7009, x 1001  
Fax. 603.251.8384  
web. [www.iomosaic.com](http://www.iomosaic.com)

## **Index**

Dust, 21

Flammability, 21

ioKinetic, 21

ioMosaic, 21

ISO, 21



## US Offices

New Hampshire (Salem) –  
Headquarters

Texas (Houston)

Minnesota (Minneapolis)

California (Berkeley)

## International Offices

Kingdom of Bahrain (Al Seef)

United Kingdom (Bath)

## Software Solutions



### [Process Safety Enterprise<sup>®</sup>](#)

Centralize the process safety management lifecycle to accelerate business goals



### [Process Safety Office<sup>®</sup>](#)

Identify, evaluate, and control process hazards with tools used by process safety consultants



### [Process Safety Learning<sup>®</sup>](#)

Build your process safety competencies incrementally with online training



### [Process Safety tv<sup>®</sup>](#)

View, share, and discuss PSM worldwide on a secure platform

## Contact Us

[www.ioMosaic.com](http://www.ioMosaic.com)

[sales@ioMosaic.com](mailto:sales@ioMosaic.com)

1.844.ioMosaic

## About ioMosaic Corporation

Through innovation and dedication to continual improvement, ioMosaic has become a leading provider of integrated process safety and risk management solutions. ioMosaic has expertise in a wide variety of areas, including pressure relief systems design, process safety management, expert litigation support, laboratory services, training and software development.

As a certified ISO 9001:2015 Quality Management System (QMS) company, ioMosaic offers integrated process safety and risk management services to help you manage and reduce episodic risk. Because when safety, efficiency, and compliance are improved, you can sleep better at night. Our extensive expertise allows us the flexibility, resources, and capabilities to determine what you need to reduce and manage episodic risk, maintain compliance, and prevent injuries and catastrophic incidents.

Our mission is to help you protect your people, plant, stakeholder value, and our planet.

## [Consulting Services](#)

- Asset Integrity
- Auditing and Due Diligence
- Combustible Dust Hazard Analysis and Testing
- Facility Siting
- Fault Tree/SIL/SIS Analysis
- Fire and Explosion Dynamics
- Incident Investigation, Litigation Support and Expert Testimony
- Liquefied Natural Gas Safety
- Pipeline Safety
- Process Engineering Design and Support
- Process Hazards Analysis (PHA)
- Process Safety Management (PSM)
- Reactive Chemicals Evaluation and Testing
- Relief and Flare Systems Design and Evaluations
- Risk Management Program Development
- Quantitative Risk Assessments (QRA)
- Software Solutions
- Structural Dynamics
- Training

## [Laboratory Testing Services \(ISO accredited\)](#)

- Chemical Reactivity
- Battery Safety
- Combustible Dust
- Specialized Testing