Introduction to Fire Modeling

An ioMosaic® Publication

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ioMosaic® Corporation

Introduction to Fire Modeling

Process Safety and Risk Management Practices

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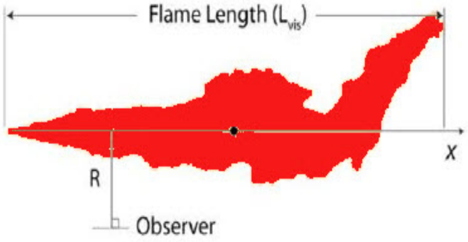
1 Introduction

Fire hazards following loss of containment include pool fires, jet fires or flame jets, flash fires or vapor cloud fires, and fireballs. A pool fire occurs when a liquid pool is ignited following a liquid spill on land or water. A flame jet occurs following a pressurized release and ignition of a flammable gas or two-phase mixture. A flash fire results from the delayed ignition of a flammable vapor cloud. Flash fires can burn back to the source of release and can produce severe blast waves if flame acceleration occurs. Fireballs typically occur following catastrophic vessel failures and immediate ignition of released flammable materials. Fireballs are often observed following a boiling liquid expanding vapor explosion (BLEVE) caused by catastrophic vessel failure due to external fire heating or runaway chemical reaction heating.

In what follows, we discuss methods that can be used to assess thermal radiation hazards resulting from pool fires, flame jets, fireballs, and flash fires.

Several models are commonly used to assess the thermal radiation hazards of pool fires, vapor cloud fires, fireballs, flame jets, and flares. These models are generally divided into three classes: (a) point source or line source models, (b) solid flame models, and (c) computational fluid dynamics (CFD) models. A line source model is made up of multiple point sources. A solid flame model represents the flame and flame surfaces using idealized cylindrical and/or rectangular geometries.

Figure 1: Point source model



2 Point Source Models

The simplest model for the estimation of thermal radiation hazards from fires is the point source model. The incident flux, I, at any location is described using the following relation:

$$I(x_t, y_t, z_t) \quad = \quad \cos\theta \frac{\tau \chi_r \dot{Q}_T}{4\pi s^2} = \cos\theta \frac{\tau \chi_r \dot{M} \Delta H_c}{4\pi s^2} \tag{1}$$

where s is the distance in m from the point source to target surface receiving the incident flux, θ is the angle between normal to the surface and line of sight from the point source, τ is the atmospheric transmissivity, and χ_r is the fraction of total combustion energy radiated by the fire in all directions to the surroundings (except to the liquid pool surface), ΔH_c is the total heat of combustion in $\mathrm{J/kg}$, $\dot{M}$ is the mass burning rate in $\mathrm{kg/s}$, x_t, y_t, and z_t are the Cartesian coordinates of the target surface receiving thermal radiation, and x, y, and z are the Cartesian coordinates of the point source usually selected at the center of the fire.

The heat release rate, $\dot{Q}_T$, represents the total combustion energy of the pool liquid or liquid mixture in $\mathrm{J/s}$, and $I(x_t, y_t, z_t)$ is the incident thermal radiation heat flux received by the target surface in $\mathrm{J/s/m^2}$ or $\mathrm{W/m^2}$.

If the point source is located at coordinates $(x, 0, z)$, then $\cos\theta$ can be evaluated for a horizontal target,

$$\cos\theta = \frac{z - z_t}{s} \text{ for } z_t < z \tag{2}$$

a vertical target which is perpendicular to the x-axis,

$$\cos\theta = \frac{x_t - x}{s} \text{ for } x_t > x \tag{3}$$

and a vertical target which is parallel to the x-axis:

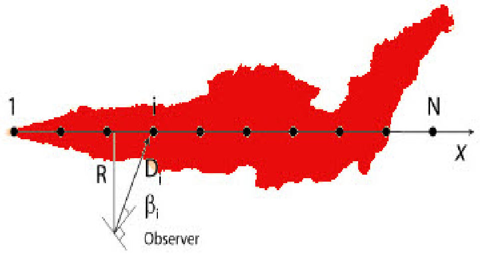
$$\cos\theta = \frac{y_t}{s} \tag{4}$$

where s is defined as:

$$s^2 = (z_t - z)^2 + y_t^2 + (x_t - x)^2 \tag{5}$$

The point source model underestimates thermal radiation levels close to the source. At large distances, the fire will appear as a point source to the target, and as a result thermal radiation levels at large distances are more reasonably predicted by a point source model. We note from Equation 1 that the incident flux in inversely proportional to the square of the target distance ($\propto \frac{1}{s^2}$) from the point source which is why thermal radiation hazards of fires are almost always localized to the immediate surroundings of the release location.

Figure 2: Multiple point source or line source model

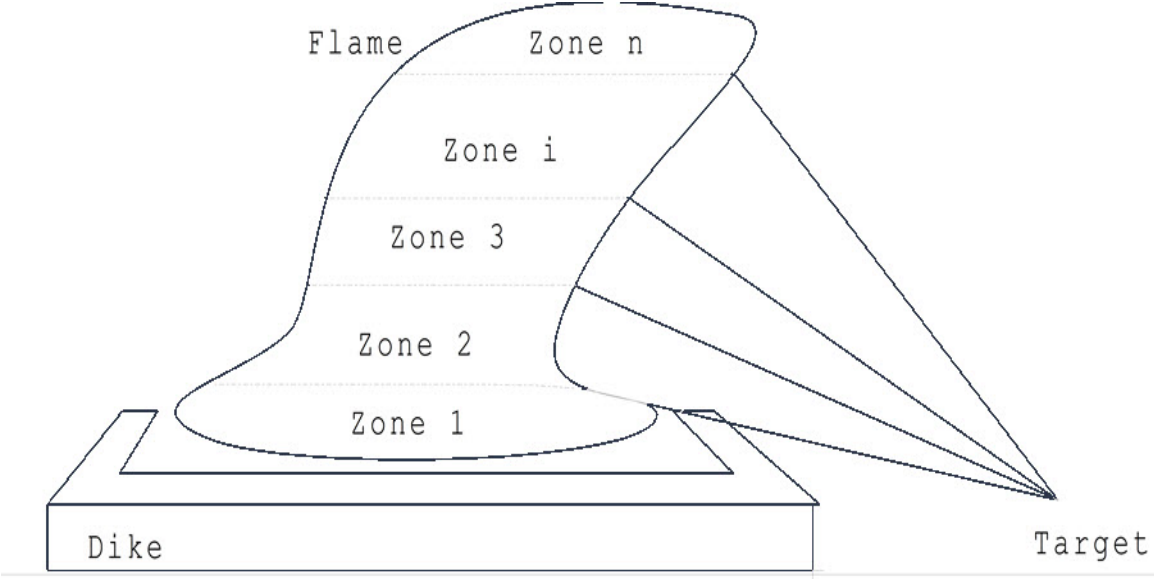


3 Line or Multiple Point Source Models

Line source models are more accurate than point source models for thermal radiation estimates in the near field, i.e., close to the fire location. The flame path is represented using a curvilinear or straight line, and the fraction of energy radiated from the flame is divided over the entire flame path or length. This is equivalent to creating multiple point sources along the flame path and adding their individual contributions when calculating an incident fire flux at a specific distance from the flame. At long distances from the flame, the flame path will resemble a single point source. At short distances, incident fire flux values are more accurate when calculated using multiple point sources (line source). A single point source will often underestimate incident fire flux values close to the flame.

4 Solid Flame Models

Figure 4: Solid flame geometry



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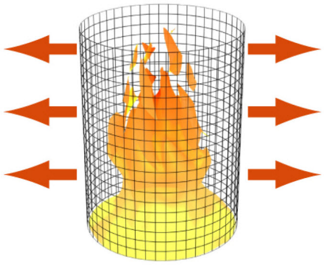
A more realistic method for fire modeling is the solid flame geometry model. Here the flame is represented as one or more simple solid geometrical shapes with radiation being emitted in all directions from different sections or zones of the flame surface (see Figures 3 and 4):

$$I = \left(\sum_i F_i E_i \tau_i \right) - \epsilon_s \sigma T_s^4 \tag{6}$$

where I is the overall incident flux, τ_i is the atmospheric transmissivity of flame surface section i, F_i is the geometric view factor of flame surface section i, E_i is the emissive power of flame surface section i, T_s is the receiving surface temperature, and ϵ_s is the emissivity of the receiving surface. At long distances from the flame surface, the entire flame surface can be approximated by a point source.

Figure 3: Solid flame model



The flame surface emissive power of section i can be calculated from Stefan's law:

$$E_i = \epsilon_{f,i} \sigma T_{f,i}^4 \tag{7}$$

where $\epsilon_{f,i}$ is the flame emissivity of section i, $T_{f,i}$ is the flame temperature of section i, and σ is the Stefan-Boltzmann constant. The emissivity is 1 for a blackbody and less than 1 for a gray body. Flame radiation temperatures are difficult to measure for turbulent diffusion flames.

5 Computational Fluid Dynamics (CFD) Models

These models solve the Navier-Stokes equations for fluid flow. To simulate flares, flame jets, or pool fires, sub-models are needed to describe the fire chemical reactions and turbulence. Although CFD models are becoming more popular and available because of high speed computing, they still need to be validated against test data. Once validated, CFD models can be used to model fires in complex geometries. CFD models are still not practical or necessary for hazard or consequence modeling or for quantitative risk assessment (QRA) studies. QRA studies for large plants can include thousands of potential hazard scenarios which makes CFD fire modeling impractical. In addition, uncertainties in scenario frequencies far outweigh uncertainties associated with semi-empirical models such as the solid flame models and point source or line models described earlier.

6 API-521 Fire Flux and Flame Emissive Power

In recent editions of API-521 [1, 2], a fundamental equation (Annex A, A.1) for incident fire flux is provided. Equation A.1 enables a better assessment of both relief requirement and vessel integrity depending on fire type and duration.

$$I_{fire,w} = \underbrace{\alpha_w \epsilon_f \sigma T_f^4}_{\text{Radiative Flux}} + \underbrace{h\left(T_{f,g} - T_{w,t}\right)}_{\text{Convective Flux}} - \underbrace{\epsilon_w \sigma T_{w,t}^4}_{\text{Re-radiated Flux}} \tag{8}$$

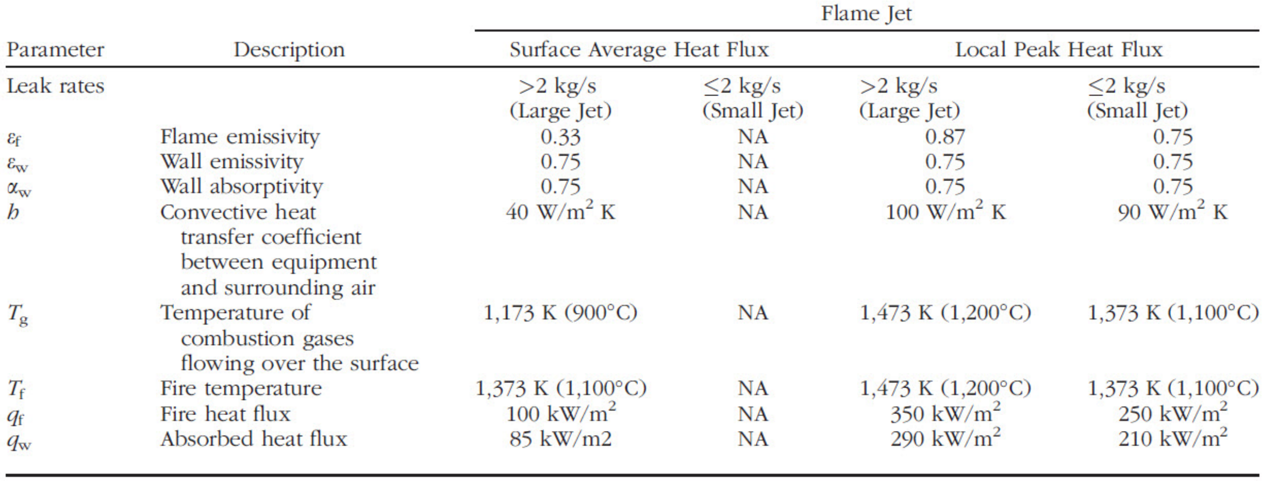
The first term in Equation 8 is the flame radiative heat flux into the external wall or insulation surface. The second term is the hot combustion gases convective heat flux into the external wall or insulation surface. The third term is the heat flux that is re-radiated by the external wall or insulation surface. Note that temperature in this equation must be absolute. The radiative heat flux is the dominant component of fire flux.

A vessel or piping segment does not have to be engulfed by fire in order to receive large heating rates by thermal radiation [3]. Thermal radiation is independent of elevation, which is why fire heating of vessels and equipment should not be limited to vessel sections or vessels that are only within the 25 feet elevation [4] limit used by API-521 or the 30 ft limit used by NFPA-30. This is especially important for vessels containing reactive chemicals.

When SI units are used, $I_{fire,w}$ is the net heat flux reaching the outer wall or insulation surface in $\mathrm{W/m^2}$, α_w is the external wall surface or insulation absorptivity, ϵ_f is the flame surface emissivity, σ is the Stefan-Boltzmann constant = $5.67 \times 10^{-8}\ \mathrm{W/m^2/K^4}$, T_f is the flame surface temperature in K, h is the combustion gases convective heat transfer coefficient in $\mathrm{W/m^2/K}$, $T_{f,g}$ is the combustion gases temperature in K, $T_{w,t}$ is the time dependent wall surface temperature, and ϵ_w is the outer wall or insulation surface emissivity (note that hydrocarbons fire exposure scenarios can cause the vessels walls to be coated with soot).

Recommended values are provided by API-521 [1] for a typical unconfined heptane pool fire engulfing an uninsulated carbon steel vessel for a surface average heat flux ($\alpha_w = 0.75$, $\epsilon_f = 0.75$, $T_f = 750\ ^\circ\mathrm{C}\ \ (1023\ \mathrm{K})$, $h = 20\ \mathrm{W/m^2/K}$, $T_{f,g} = 600\ ^\circ\mathrm{C}\ \ (873\ \mathrm{K})$, and $\epsilon_w = 0.75$) and local peak heat flux parameters ($\alpha_w = 0.75$, $\epsilon_f = 0.75$, $T_f = 1050\ ^\circ\mathrm{C}\ \ (1323\ \mathrm{K})$, $h = 20\ \mathrm{W/m^2/K}$, $T_{f,g} = 1050\ ^\circ\mathrm{C}\ \ (1323\ \mathrm{K})$, and $\epsilon_w = 0.75$). These recommended values are consistent with a fire

Table 1: Recommended parameter values for Equation 8 for flame jets by API-521 [1] where other data or information are not available



Parameter	Description	Flame Jet			
		Surface Average Heat Flux		Local Peak Heat Flux	
Leak rates		>2 kg/s (Large Jet)	≤2 kg/s (Small Jet)	>2 kg/s (Large Jet)	≤2 kg/s (Small Jet)
ε_f	Flame emissivity	0.33	NA	0.87	0.75
ε_w	Wall emissivity	0.75	NA	0.75	0.75
α_w	Wall absorptivity	0.75	NA	0.75	0.75
h	Convective heat transfer coefficient between equipment and surrounding air	40 W/m^2 K	NA	100 W/m^2 K	90 W/m^2 K
T_g	Temperature of combustion gases flowing over the surface	1,173 K (900°C)	NA	1,473 K (1,200°C)	1,373 K (1,100°C)
T_f	Fire temperature	1,373 K (1,100°C)	NA	1,473 K (1,200°C)	1,373 K (1,100°C)
q_f	Fire heat flux	100 kW/m^2	NA	350 kW/m^2	250 kW/m^2
q_w	Absorbed heat flux	85 kW/m2	NA	290 kW/m^2	210 kW/m^2

flux of 60 $\mathrm{kW/m^2}$ and 150 $\mathrm{kW/m^2}$ for surface-averaged and local peak values and wall absorbed values of 45 $\mathrm{kW/m^2}$ and 120 $\mathrm{kW/m^2}$, respectively. Recommended values for jet fires are also provided by API-521 [1](as shown in Table 1) where actual test data are not readily available for establishing the flame characteristics.

API-521 [1] also provides an empirical equation to directly calculate the heating rate absorbed by the vessel contents since Equation A.1 (8) only provides the fire flux that the vessel outer wall or insulation is exposed to. The heating rate absorbed by vessel contents is calculated empirically [1]:

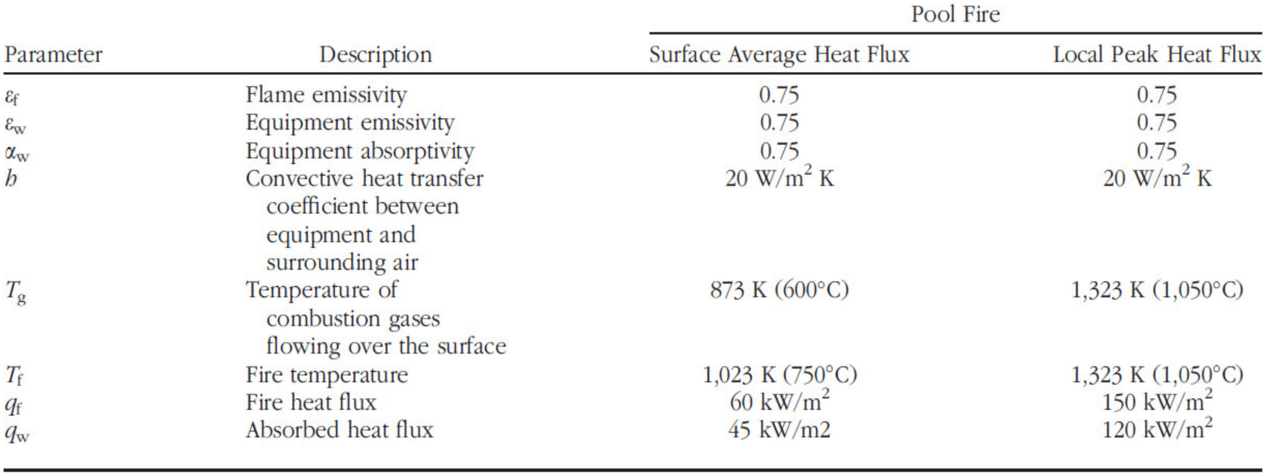
$$Q_{fire} \quad = \quad qFA_w^a \tag{9}$$

Where Q_{fire} is the total heating rate absorbed by the liquid in $\mathrm{J/s}$ or W, F is a mitigation factor that is used to allow reduction of the heating rate because of water sprays, firefighting, and/or insulation, and A_w is the wetted surface area in m^2, i.e. the inner wall surface area contacted by liquid. The constant q represents the heat flux absorbed by the liquid corrected for the presence of adequate drainage. Note that q includes a unit conversion factor associated with the fact that the wetted surface area is raised to a power less than 1. A similar form is used by NFPA-30 [5]. Also note that NFPA and API correlations differ for wetted surface areas that are less than 2,800 ft^2 where NFPA yields a higher heating rate.

Equation 9 correlates the heat absorbed by the vessel liquid contents to the wetted surface area raised to the power $a = 0.82$ typically. Confined pool fires lead to higher heating rates. A value of $a = 1$ is substituted for $a = 0.82$ in API-521.

Melhem [6] showed that the simple API-521 equation (Equation 9) can be recovered from Equation 8 when the fire heating and relief dynamics are properly modeled. Equation 8 can be used to develop both the relief requirements and to assess the failure potential as well as the effectiveness of a variety of potential mitigation options. Melhem [6] also independently demonstrated that Equation 8, when used with Process Safety Office® SuperChems® Expert vessel and wall dynamics, can accurately reproduce measured large scale [7, 8, 9] fire exposure test data including

Table 2: Recommended parameter values for Equation 8 for pool fires by API-521 [1] where other data or information are not available



		Pool Fire	
Parameter	Description	Surface Average Heat Flux	Local Peak Heat Flux
ε_f	Flame emissivity	0.75	0.75
ε_w	Equipment emissivity	0.75	0.75
α_w	Equipment absorptivity	0.75	0.75
h	Convective heat transfer coefficient between equipment and surrounding air	20 W/m^2 K	20 W/m^2 K
T_g	Temperature of combustion gases flowing over the surface	873 K (600°C)	1,323 K (1,050°C)
T_f	Fire temperature	1,023 K (750°C)	1,323 K (1,050°C)
q_f	Fire heat flux	60 kW/m^2	150 kW/m^2
q_w	Absorbed heat flux	45 kW/m2	120 kW/m^2

wall temperatures and vessel failure pressure.

The fire flux provided by Equation 8 is used by detailed dynamic simulation software such as SuperChems® Expert to provide time dependent estimates of wall segment temperatures, estimated time to failure, fluid temperatures, and single/multiphase venting rates with and without chemical reactions.

7 Fire Modeling with SuperChems® Expert

Fire models that are available in SuperChems® Expert include (a) gas flame jet and flare, (b) twophase flame jet, (c) pool fire, (d) fireball, and (d) vapor cloud fire.

7.1 Flame Jets and Flares

The flame jet and flare models are multiple point source models. They rely on jet dispersion to first establish the flame jet length and curvilinear path and then integrate the multiple point source energy release rates along the entire flame jet path. The fraction of combustion energy available for radiation is based on Shore's [10] method or can be user defined. Tools are available for the assessment of thermal radiation on nearby structures as well as the calculation and visualization noise and thermal radiation contours with user defined options for sound power level weighting and combustion spectrum efficiency selection. The thermal radiation or noise contours from one or more sources/flares can be added and displayed on site maps.

7.2 Pool Fires

The pool fire model in SuperChems® Expert is a dynamic model that considers both spreading and burning on different surfaces or water. The dynamics of spreading on surfaces or water solve the shallow water equations and consider surface roughness as well as dissolution into water or percolation into the soil. Several default spill surfaces are provided and the user can specify diking and the geometry of the dike to be either circular or rectangular. The energy balance dynamics include consideration for fire heating, ground heat transfer exchange with the bulk liquid of the pool, and the non-ideal vapor/liquid equilibrium of the liquid leading to preferential depletion and fractionation of the liquid volatile components or light ends. The user can specify the flame temperature, the flame emissivity, as well as the fraction of combustion energy transferred by the flame to the liquid pool surface.

The pool fire model uses a solid flame model and allows for the impact of wind speed on flame tilt, length, and drag. Upwind, crosswind, and downwind thermal radiation incident flux can be calculated as well as isopleth for specific thermal radiation limiting flux values, dosage, or probability of injury. The model considers the impact of escape for healthy individuals and is particularly useful in developing the design basis for fire exposure scenarios on equipment involving hydrocarbon fuels, biofuels, or any other type of fuel mixtures. The fire flux is used for both consequence and risk modeling as well pressure relief design and estimated time to failure of process equipment and vessels. The pool fire model includes a variety of user tools such as tools for the calculation of burning rates or the fraction of combustion energy radiated to the liquid surface. The thermal raditions contours can be shown on site maps.

7.3 Fireballs and Vapor Cloud Fires

In addition to pool fire and flame jet models where the fire duration can be long enough to enable a healthy individual to run away from the fire, there can be release and dispersion scenarios where an intense dose of thermal radiation is delivered over a very short period of time.

Fireballs and vapor cloud fires are examples of such scenarios. Fireballs can deliver upwards of 400 $\mathrm{kW/m^2}$ of intense thermal radiation over a short duration of seconds or tens of seconds depending on the size of the fireball.

Fireball thermal radiation is so intense, it is typically assumed that people receiving such high doses of thermal radiation can get injured even if the thermal radiation is visible through building windows. In the 1992 NFPA BLEVE large scale tests [9], sand bags turned to glass. The sand bags were used to protect instrumentation in close proximity to the 500 gal propane tanks that failed and caused the fireball.

SuperChems® Expert calculates the maximum fireball dimensions based on semi-empirical relationships, but dynamically integrates the heat transfer rate as a function of time at any radial location in the vicinity of the fireball.

Vapor cloud fires can burn at the rate of 10 to 15 $\mathrm{m/s}$ and can deliver intense thermal radiation in excess of 200 $\mathrm{kW/m^2}$. Anyone within the the vapor cloud fire reach would be assumed to be fatally injured from exposure to such high levels of thermal radiation and/or from inhalation of the hot combustion products.

Vapor cloud fires can occur when a liquid spill forms a liquid pool and the vapor formation from the pool disperses without immediate ignition. When the dispersing vapor cloud encounters an ignition source, the delayed ignition causes the flammable vapor cloud to burn back all the way to the liquid pool source causing a pool fire. The vapor cloud fire typically burns at a velocity of 10 to 15 m/s and can accelerate in the presence of turbulence and obstructions to a deflagration and under some very unique conditions to a detonation.

SuperChems® Expert establishes the vapor cloud fire boundaries by dispersing the vapor cloud using either either heavy gas or Gaussian models to the lower flammability limit downwind and to 1/2 the lower flammable limit cross-wind to allow for pocketing.

8 Recommended Additional Reading

Please refer to additional ioMosaic® publications in the fire modeling series for more details on understanding thermal radiation modeling and atmospheric transmissivity, the calculation of geometric view factors for solid flame geometries, the calculation of flame emissive power and fraction radiated for pool fires and flame jets/flares, and the calculation of short duration exposure to thermal radiation from fireballs and vapor cloud fires. These technical publications can be made available upon request.

9 References

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About the Authors

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).

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