

# A Model Structuring Dust, Mist, Gas/Vapour and Hybrid Explosion Behavior: the Chemical-Engineering Model

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The Chemical-Engineering model describes how the synergetic combination of chemical and engineering factors determines gas, particulate, and hybrid explosion behavior. Explosion behavior is expressed as explosion sensitivity (e.g. probability of explosion), explosion severity (e.g. adverse effects of explosion), and explosion types (deflagration or detonation). Chemical factors are ranked using NFPA methodology. Engineering includes whether explosion occurs in open or enclosed spaces, equipment shape/size, and initial T, p, and flow conditions. The model is semi-quantitative; its virtues are its unique integration of chemical and engineering factors in determining explosion risk, its didactic qualities, provision of insight, and practical utility to engineers who are not experts in combustion science.

## 1. Introduction

Explosion behaviour is here characterized in terms of Explosion Severity and Explosion Sensitivity, the latter concerning ignition probability. Table 1 lists important explosion sensitivity terms, definitions, and units. In general the lower the absolute values of explosion sensitivity terms (e.g. lower MIE-values), the greater the probability of ignition and occurrence of explosion. Explosion Severity relates to possible adverse effects of explosion; greater explosion severity (e.g. detonation rather than deflagration) causes more damaging effects. Table 2 lists important Explosion Severity terms, meanings and units. Together, Explosion Sensitivity (probability) and Explosion Severity (adverse effects) relate to explosion risk, risk being a term composed of probabilities of given adverse effects. Estimating explosion risk requires knowledge of both Explosion Sensitivity and Explosion Severity (Tables 1 and 2, next page) and how these are affected by changes in Chemistry and Engineering parameters.

## 2. Explanation of terms ‘Chemistry’ and ‘Engineering’ as used in the ‘Chemical-Engineering’ model

“Chemistry” relates to the “Chemistry” half of the “Chemical-Engineering” model (Figure 1). For given substances, the relative quantitative value of “Chemistry” in terms of explosion risk follow from fundamental chemical properties and from instrumentally determined parameters of the substances in question. Fundamental are the chemical thermodynamics and kinetics of relevant combustion and/or decomposition reactions, as these determine the mass-based volumetric rate of heat production ( $W/kg/m^3$ ), which is a key parameter for both Explosion Sensitivity and Severity. In spite of QSAR development, at this moment reliable quantitative values of most of the Explosion Severity and Sensitivity parameters are still most accurately determined via standardized test procedures.

‘Chemistry’ hazard is quantified relatively using the well-known and applied NFPA-system (Head and Wagner, 1995) that ranks substances in terms of two separate explosion-related categories, Flammability and Instability/Reactivity, each of which has a five tier system of no hazard (zero) to highest hazard (4). For liquids (and for certain solids of high volatility, e.g. naphthalene). Flammability is based largely on the combination of Lower Flash Point, LFP (Table 1) and tendency to disperse in air. The lower the LFP the higher the volatility (i.e. higher vapour pressure), and therefore the greater the Flammability. Ease of dispersion in air is a second

criterion. Obviously vapours, formed by liquids with low LFPs, and gases, disperse most easily in air. Also considered are finely divided solids in air (dusts); idem liquids (mists). Pyrophoric substances, which spontaneously ignite in air (i.e. MIE = zero), in any phase form (e.g. solid micro-/nano-particles of most metals), have, along with flammable gases, the highest Flammability classification (4).

Instability/Reactivity is based on reactivity with water (e.g. forming hydrogen) and, in particular, tendency to explosively decompose, especially tendency to detonate. Largest values (4) are given to high explosives (e.g. TNT, nitroglycerine) and highly unstable substances; i.e. having highly exothermic decomposition enthalpies of decomposition (e.g. chlorine dioxide; pure liquid ozone) making detonation highly likely.

Alternatively,  $K_G$ - and  $K_{St}$ -values can be used to estimate relative Chemistry-based explosion hazard of gases, resp., air-particulate mixtures.

'Engineering' is characterized by the "environment" in which explosion occurs and ignition factors, meaning open air or in vessels; if the latter, shape, size, and inter-connectedness; initial temperature, pressure, and turbulence; location/energy of ignition.

*Table 1: Important explosion sensitivity terms and relevant units*

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Lower Explosion Limit (LEL), for gases and for particulates suspended in air. For gases/vapours: mol-% or volume-%; for particulates: typically g/m <sup>3</sup>
Upper Explosion Limit (UEL), for gases and for particulates suspended in air. For gases/vapours: mol-% or volume-%; for particulates: typically g/m <sup>3</sup>
Explosive range (UEL) – (LEL), for gases and for particulates suspended in air: units as above
Minimum Ignition Energy (MIE), for gases and for particulates suspended in air: mJ
Minimum Ignition Temperature (MIT), for gases and for particulates suspended in air: °C or K
Minimum Ignition Temperature (MIT), for a layer of particulates deposited on a (hot) surface: °C (for a given layer thickness, cm)
Lower Flash Point (LFP): °C
Upper Flash Point (UFP): °C
Maximum Experimental Safe Gap (MESG), in practice only for gases; theoretically also applicable for particulates suspended in air: mm
Limiting Oxygen Concentration (LOC), for gases and for particulates suspended in air or in another gas (e.g. nitrogen): mol-% O <sub>2</sub>

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*Table 2: Important explosion sensitivity terms and relevant units*

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Adiabatic flame temperature: the maximum theoretical temperature reached when no heat loss occurs. Relates to constant pressure or constant volume, the latter being higher: °C or K
Maximum explosion pressure, $p_{max}$ : bara
Maximum rate of pressure rise, $(dp/dt)_{max}$ : bar/s
For deflagrations, volume-standardized measure of explosion violence, the K-factor: $K = [(dp/dt)]_{max} \cdot V^{1/3}$ : bar.m/s, where V = vessel volume (m <sup>3</sup> )
Flame speed, velocity of flame relative to a fixed observer: for deflagrations: m/s
Deflagration-to-detonation transition (DDT): $p_{max}$ -values: bara; DDT run-up distance: m
Pressure-piling: maximum pressures (bar), maximum rates of pressure rise, $(dp/dt)_{max}$ : bar/s

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### 3. The 'Chemical-Engineering' model

The Chemical-Engineering model (Figure 1) schematically illustrates how Explosion Sensitivity and Explosion Severity, which together determine explosion hazard, are based on the combination of Chemistry-based and Engineering-based phenomena. The top part of the Chemical-Engineering model, based on heat balances, concerns Explosion Sensitivity, which relates to probability of ignition (Table 1). The bottom part, Explosion Severity, which is based on gas dynamics (e.g. gas expansion, turbulence), relates to the destructive potential ("hazard") of explosion in terms of type of explosion occurring (i.e. deflagration or detonation); for both: maximum pressures (static and dynamic), and, for deflagration, rate of pressure rise (Table 2). The left side relates to Chemical aspects of the exploding substances, such as kinetics (rates of chemical reactions) and thermodynamic properties (amounts of heat produced) these latter two determine volumetric rate of heat production (W/m<sup>3</sup>) A noted above, relative "Chemistry" hazards of substances are quantified using the relevant "Flammability" and "Reactivity/Instability" ratings of the NFPA-substance hazard system, larger numbers (up to 4) indicating greater hazard.

The right side relates to ‘Engineering’ aspects of the physical “environment” in which explosion occurs, such as open or closed spaces; if the latter, dimensions, geometry; inter-connectedness of process equipment; (turbulent) flow and initial pressure and temperature. The bottom right side relates to the (huge) influence of turbulence. Together with Chemistry’, these parameters determine volumetric rate of heat loss (upper right part Figure 1a) and gas dynamic behaviour, such as (acceleration of) flame speed (lower right part Figure 1a).

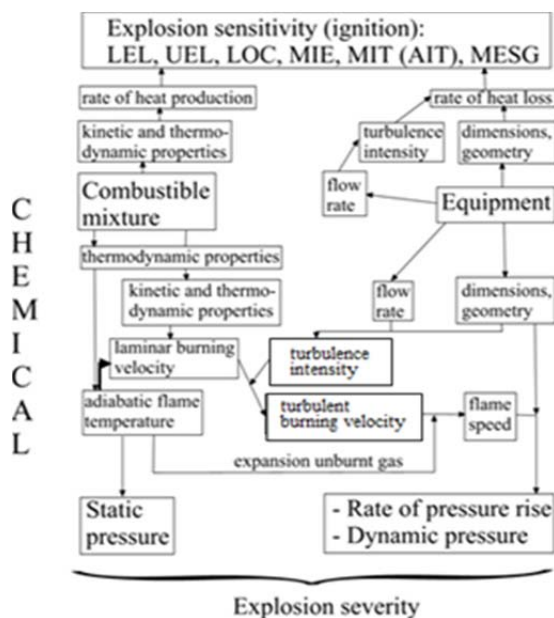


Figure 1a. The ‘Chemical-Engineering’ model.

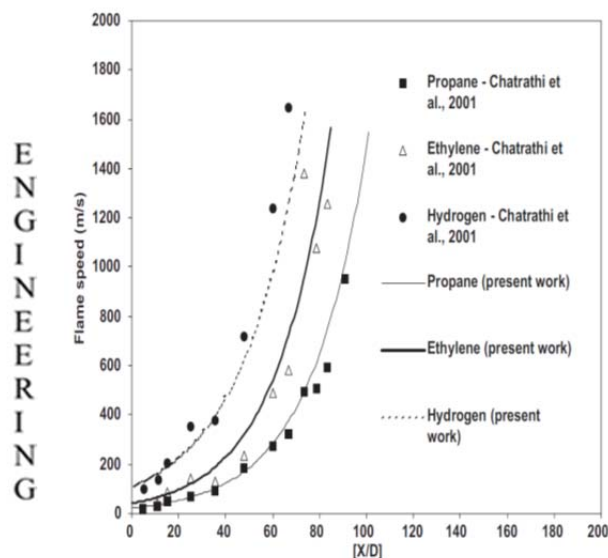


Figure 1b. Flame speed (acceleration) in cylinder;  $D = 0.15$  m.  $X/D =$  ratio of [distance flame travelled in (m)]/[diameter of cylinder (0.15 m)]. Silvestrini et al, 2008

A previous article (Lemkowitz and Schotte, 1999) describes in detail the theoretical basis of the methodology, which is based on simplified chemical thermodynamics, kinetics and physical transport phenomena, as applied to estimating how changes in ‘Chemistry’ and ‘Engineering’ affect explosion behaviour of gas explosions in closed spherical vessels. This theory, not repeated here, is extended in this article to explosion severity in two other general cases, explosions in cylinders and explosions in a type of interconnected equipment. (Applied to Explosion Sensitivity (i.e. ignition parameters) in the two cases considered here, the theory presented in the 1999 article leads to the same results as for explosions in spherical vessels.) While many books (e.g. Bartknecht, 1994; Ogle, 2017) and articles (e.g. Proust, 2015) describe phenomena here discussed, none give explanation in terms of the simple, concise, and, in particular, integrative ‘Chemical-Engineering’ approach presented here.

### 3.1 Severity of explosion of gas or gases + particulates in cylinders (e.g. pipelines)

The ‘Chemistry’ of a substance or mixture is ranked using the NFPA-approach described above (or, alternatively, the K-value system). Note that all substances entrained in air (or other gas supporting combustion) and having an NFPA-rating (or K-value) greater than zero can potentially explode and, and many, if not all, can under certain ‘Engineering’ circumstances (explained below), even detonate.

‘Engineering’ is, in addition to the description above (e.g. form, dimensions), for this case extended to include parameters such as whether the cylinder is open or closed (if closed at both ends; or closed at only one end) and the location of ignition; i.e. at open end or at closed end. What occurs after ignition of a flammable mixture in a cylinder (pipeline) depends on the combination of ‘Chemistry’ and ‘Engineering’.

After initial ignition of a flammable mixture of given ‘Chemistry’ flame propagation can occur, or not occur. For a given ‘Chemistry’ and ‘Engineering’ (here: cylinder) heat balances – i.e. rate of heat production relative to rate of heat loss - determine whether or not flame propagation occurs. By approximation, heat production occurs in the flame’s area, which increases with diameter squared. Also by approximation, heat loss occurs in the flame’s perimeter, which increases only linearly with diameter. Increasing diameter thus increases heat

production more than heat loss, making flame propagation possible. If diameter is too small (below a critical diameter), then rate of heat loss is larger than rate of heat production; flame propagation is then impossible.

Rate of heat production is a chemical parameter (chemical thermodynamics and chemical kinetics). The most reactive substances (e.g. acetylene) generally have, thermodynamically, the highest values of heat production and also, kinetically, the highest rates of chemical reactions, particularly at or near stoichiometric concentrations in air (and especially so in pure oxygen). Additionally, increasing temperature and pressure usually more strongly increase rate of heat production than rate of heat loss. While rate of heat production is a strong function of composition (i.e. maximum at or near stoichiometric) rate of heat loss is usually relatively (much) less strongly affected by changes in composition. The values of explosion sensitivity factors specified in (upper part of) Figure 1), all of which relate to ignition and flame propagation at extreme minima (e.g. Lower Explosion Limits), follow from heat balances.

After initial ignition, effects of Engineering on a given chemical composition are as follows. If cylinder diameter is greater than critical diameter, AND if ignition occurs at the OPEN END, then the resulting flame tends to burn into the closed end of the cylinder at a more or less slow constant velocity. In this case the flame is burning its way into a quiescent (i.e. non-moving: zero turbulence) mixture. The hot combustion gases are flowing in the direction opposite to that of the flame. The flame is thus not influenced by the hot expanding combustion gases. This more or less constant and relatively slow (order of magnitude typically 0.1. – 1.0 m/s) flame speed is known as the laminar flame speed (laminar since the flame is propagating into the unburnt gas, which is stationary and thus totally laminar: Reynolds number = 0). The laminar flame speed (often called the laminar burning velocity) is thus largely a Chemical property, being, for gases, greatest for highly reactive substances at their respective (near) stoichiometric concentrations (e.g. hydrogen) and lowest for the least reactive flammable substances (e.g. methane).

Consider now the same cylinder (open at one end, closed at other) containing the same methane-air mixture (same p and T). Except: ignition at closed end of cylinder instead of open end. Thus: same Chemistry (methane-air mixture) – but different Engineering. And (possibly) totally different results. Figure 2 illustrates this case: rather than moving in opposite directions, flame and hot expanding gases move in the same direction. The flame is pushed forward/accelerated by hot expanding combustion gases. Shear forces generated by gas flow along cylinder walls generate turbulence, creating turbulent eddies, increasing flame surface area, which changes from two-dimensional to three-dimensional. Increased flame area increases rate of combustion, which increases rate of heat production, which increases flow, which increases turbulence, which increase flame area, enz. This positive-feedback mechanism is well-known. In the extreme case the turbulent flame can even engulf pockets of unburned gas, which ignite/explode.

Via the above-sketch mechanism flame speed can accelerate from mild deflagration (cm/s) to more violent deflagration (102 m/s), and even transform from deflagration to detonation, or even to a short-lived “super” (i.e. over-driven) detonation: a Deflagration-Detonation Transition (DDT). Such behavior will again be influenced by the combination of “Chemistry” (i.e. reactivity of mixture) and “Engineering” (i.e. cylinder L and D, even surface roughness and obstacles in the cylinder, both of which generate extra turbulence). Such behavior can occur with both combustible gases as well as with gases containing combustible particulates (dusts, mists), as Table 3 summarizes.

### 3.2 Inter-connected equipment: two spherical/cubical vessels connected to each other via a cylinder

The combination of “Chemistry” and “Engineering” determine explosion severity in inter-connected equipment. Chemical factors are the same as those discussed earlier; i.e. the more reactive the substance/mixture involved (e.g. mixtures containing hydrogen; (near) stoichiometric composition; powders with high  $K_{St}$ -values (> ca. 300 bar.m/s), the greater the potential for increased explosion severity.

Engineering is here more complex than in the case with cylinders. Consider the following scenario, for an installation illustrated in Figure 2: a larger vessel  $V_1$ , connected to a smaller vessel,  $V_2$ , via a pipeline of length L and diameter D. The installation is filled with a combustible gaseous mixture at room temperature and atmospheric pressure. Figure 2 illustrates ignition to deflagration in the larger vessel. The expanding deflagrative (thus subsonic) explosion in the larger vessel,  $V_1$ , compresses the unreacted gases, increasing their pressure and thus causing flow into the second, smaller, vessel,  $V_2$ , increasing its temperature, pressure, and turbulence intensity. If the ratio  $V_2/V_1$  is sufficiently large, and the dimensions of inter-connecting pipelines such that  $V_2$  approaches the same maximum explosion as  $V_1$  (typically 8 bara), then ignition occurs in  $V_2$  in a heated turbulent mixture at an initial pressure of ca. 8 bara. In this particular case maximum final explosion in  $V_2$  could theoretically approach roughly  $8 \times 8 \text{ bara} = \text{ca. } 60 \text{ bara}$ , with correspondingly much higher values of  $(dp/dt)_{\max}$  than in  $V_1$ . Figure 2 does not exhibit such extreme behavior, but obvious from the measured results are the strongly increased explosion pressure and  $(dp/dt)_{\max}$  in the second vessel. This phenomenon is known as pressure piling.

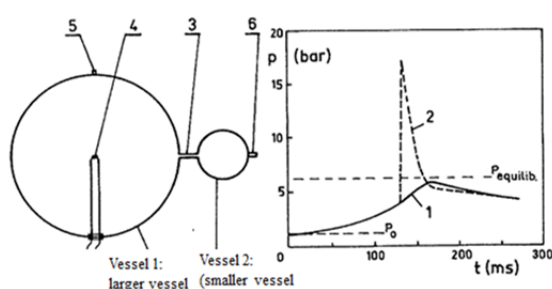


Figure 2: Pressure piling:  $p$ - $t$  behaviour in Vessel 1, where ignition occurs, and smaller vessel, Vessel 2. Increased explosion pressure and, in particular, greatly increased  $dp/dt$  in Vessel 2. Larger ratios  $V_2/V_1$  increase effect pressure piling. More extreme behaviour would also seem possible. Kaufman et al, 1995

A more extreme scenario would also seem theoretically possible; namely maximum deflagrative pressure piling into  $V_2$  (i.e. large ratio  $V_2/V_1$ ) followed by detonation in  $V_2$ . In this hypothetical case, L- and D-dimensions of connecting cylindrical piping allow flow of unreacted gases into  $V_2$  such that in  $V_2$  these gases reach a pressure of ca. 8 bara. Somewhat later in time, DDT occurs in connecting pipelines. Gases in  $V_2$  are thus ignited by a detonative flame, causing them to detonate directly rather than deflagrate. Resulting pressure explosion pressure will therefore be much higher than ca. 60 bara mentioned above, more in order of ca.  $(15-20) \bullet 8 \text{ bara} = \text{ca. } 120-160 \text{ bar}$  and the (near) infinite ( $dp/dt$ ) of a detonation. Chemical factors influencing probability of increased Explosion Severity are basically the same as those listed in Table 3 (e.g. mixtures of substances with higher/highest NFPA Flammability (e.g. hydrogen, acetylene) Reactivity/Instability ratings (e.g. ethylene oxide) and/or high K-values. Idem for flammable mixtures containing reactive particulates (e.g. finely divided reactive metals, such as Al, Mg, Ti, in particular, micro- and nano-particulates of such metals whose surfaces are not oxidized).

Table 3: Chemical and engineering factors increasing Explosion Severity in cylinders containing flammable gases alone and gaseous mixtures containing flammable particulates

Chemistry: gases	"Engineering" factors	Gases containing particulates
1. (Mixtures of) Gases with higher/highest NFPA Flammability and Reactivity/ Instability ratings (e.g. $H_2$ )	1. Ignition at/near closed end of cylindrical equipment	1. Originally soft deflagrations of particulate-air mixtures can transform violent deflagrations.
2. (Near) stoichiometric mixtures	2. Ignition in cylindrical equipment with $L/D \geq 5$ , such as silos.	2. Even DDTs can occur in particulate explosions in cylinders (in industrial practice, only in exceptional cases)
3. Increasing temperature (increases reactivity and reaction rate)	3. Ignition in long pipelines ( $L/D \gg 10$ )	3. Engineering factors applying to gas explosions also apply to particulates explosions (cylinders, $L/D \gg 10$ )
4. Increasing pressure (increases energy concentration ( $J/m^3$ ) and, usually, also reaction rate)	4. High flow rates (creates turbulence)	4. Typical chemical factors increasing violence of explosions in cylinders involving particulates:
High $O_2$ -concentrations at (near) stoichiometric composition	5. Pipelines: Ideal diameter (not too small, not too big)	a. Mixtures containing gases with higher/highest NFPA-Reactivity/Instability ratings (e.g. $H_2$ )
	6. Pipelines: Wall roughness and obstacles (generate turbulence)	b. Drier/finer particulates
	Interconnected equipment, especially larger volume vessel connected to smaller volume vessel via (long) pipelines; risk of flame acceleration and 'pressure piling' (de-scribed further below)	c. Reactive particulates; e.g. finely divided reactive metals, esp. when surfaces not (fully) oxidised);
		d. Hybrid mixtures: mixtures containing flammable gases/ vapours as well as flammable particulates
		e. Higher oxygen concentrations
		f. Thermodynamically unstable substances (i.e. substances with strongly exothermic enthalpies of decomposition); e.g. ethylene oxide and/or powdered high explosives, such as TNT

Table 4 lists how changes in Engineering affect Explosion Severity in two spherical vessels connected via a cylinder (i.e. piping).

*Table 4: Possible effects of 'Engineering' factors on explosion severity in two spherical vessels interconnected via a cylinder: pressure piling, and/or flame acceleration, and/or DDT*

Changes 'Engineering'	Effect on Explosion Severity
Ignition in larger vessel rather than smaller vessel	Larger $V_1/V_2$ ratios allows pressure in $V_2$ to approach maximum explosion pressure in $V_1$ (i.e. ca. 8 time initial pressure) before ignition in $V_2$ occurs. Result: significant pressure piling effects. Small $V_1/V_2$ ratios hardly raise pressure in $V_2$
Diameter connecting piping $> D_{critical}$ allowing flame propagation	If pipe diameter less than critical value, then pipe extinguishes flame: no explosion in $V_2$ . If pipe diameter greater than critical diameter flame acceleration possible, probability and intensity increasing with greater chemical reactivity.
Idem, but additionally: Piping long enough to assure appreciable flame acceleration	No appreciable flame acceleration in short pipe. Longer lengths allow greater flame acceleration, increasing turbulence and T of unreacted gases in $V_2$ . Flame acceleration increases causes flame to more powerful ignite unreacted gases in $V_2$ . In extreme cases, acceleration to DDT potentially possible.

### 3.3 The contrasting effects of turbulence

Increased turbulence generally decreases explosion sensitivity. Reason is that explosion sensitivity terms relate to the extreme possibilities of ignition (i.e. lowest LEL; highest UEL; lowest MIE). Increased turbulence causes increased mixing with unreacted gases, hampering ignition by removing heat. While turbulence generally reduces explosion sensitivity, turbulence can both increase and decrease explosion severity. Near to explosion limits, increased turbulence tends to extinguish combustion by mixing a weakly combustible mixture with cold air. However, as reactivity of a given mixture increases (e.g. more reactive substances; stoichiometric concentrations), increased turbulence increases explosion severity. The main mechanism is increased flame surface area. Since risk is a function of probability of occurrence (i.e. ignition) and severity of effects, it is probable that a certain level of turbulence creates maximum risk.

## 4. Conclusions

Explosion behavior of gases and mixtures of gases and particulates can be understood, explained and semi-quantitatively estimated using a unique 'Chemistry-Engineering' approach. Chemical hazards of substances are ranked using NFPA-methodology (or K-factors). Engineering aspects are considered in terms factors like shape, form, inter-connectedness of equipment, pressure, temperature, and location of ignition. Applied to explosions in cylinders, the model explains and estimates increasing likelihood of flame acceleration, even deflagration to detonation transition (DDT), as mixture reactivity increases, ignition occurs at the closed end of a cylinder open at one end, mixture reactivity increases, cylinder length increases and cylinder diameter increases to a value ensuring maximum turbulence. Applied to explosions occurring in equipment consisting of two spherical vessels connected via a cylinder (i.e. piping), explosion severity (e.g. flame acceleration) increases with increasing mixture reactivity, ignition occurring in the larger of the two vessels, greater cylinder length, and an ideal diameter favoring maximum turbulence. The model's greatest utility is providing insight into explosion risks to engineers who are not explosion specialists.

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