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January 24-25, 2022 | 16th Annual Global Software Users Group Meeting | Virtual

## Master Explosion Dynamics with SuperChems<sup>™</sup>

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QMS\_7.3\_7.4.F06 Rev.9

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# Meet your presenter

- ▶ Over 30 years of Engineering and Process Safety Experience
- ▶ Pressure Relief and Flare Systems
- ▶ PRV Stability and Fluid Dynamics
- ▶ Chemical Reaction Systems
- ▶ Fire, Explosion, and Dispersion Dynamics
- ▶ Quantitative and Transportation Risk Analysis
- ▶ LNG, LPG, and Hydrogen Safety
- ▶ Process Safety Management
- ▶ Litigation Support & Public Testimony



G. A. Melhem, Ph.D., FAIChE  
President and CEO

# In this presentation we will learn about useful fundamental SuperChems explosion building blocks and models

- ▶ Equilibrium calculations for multiphase and hybrid systems to represent the flame front
- ▶ Single volume deflagration dynamics
- ▶ Rankine-Hugoniot modeling to develop reduced analytical models for 1D dynamics
- ▶ Detailed 1D explosion dynamics
- ▶ Example Case studies

Vapor Cloud Explosion: TNT Equivalence	
Vapor Cloud Explosion: TNO Shockwave	
Vapor Cloud Explosion: TNO Multienergy	
Vapor Cloud Explosion: Baker-Strehlow	
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Vessel Burst: Vapor	
Vessel Burst: Two Phase	
Vessel Burst: Fragment Trajectory	
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Vapor and Dust Deflagration in Vessels (Dynamic)	
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•• Hugoniot. Last Executed: 11:18:07 AM, Sat Jan 08 2022	
✓ •• 1D Explosion Dynamics. Last Executed: 03:57:19 PM, Fri Jan 21 2022	
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NFPA-68: Venting Deflagrations of Dusts and Hybrid Mixture	
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NFPA-68: Venting Deflagrations of Gas Mixtures and Mists	
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<b>High Pressure Relief Design for Vapor - BM</b>	
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High Pressure Relief Design for Vapor - Reduced Set Point	

# This presentation is based in part on this recent ioMosaic white paper (available for download)

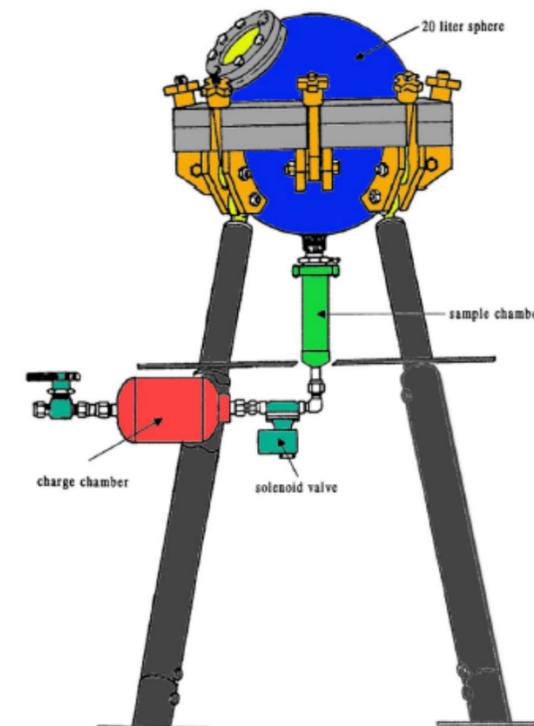
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## Quantify Explosion Venting Dynamics in Vessels, Enclosures, and Energy Storage Systems



An ioMosaic Corporation White Paper

G. A. Melhem, Ph.D., FAICHe

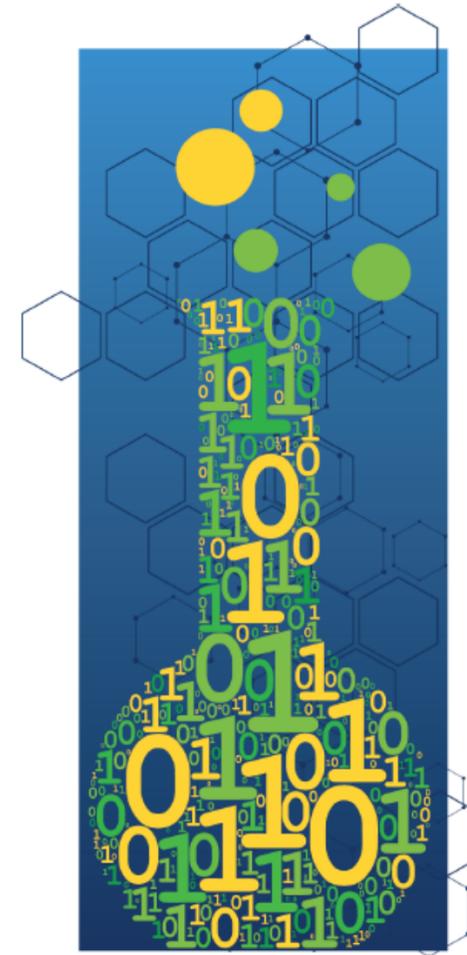
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# This presentation is also based on this additional recent ioMosaic white paper (available for download)

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## Development of Reduced Analytical Models for Explosion Dynamics

An ioMosaic Corporation White Paper

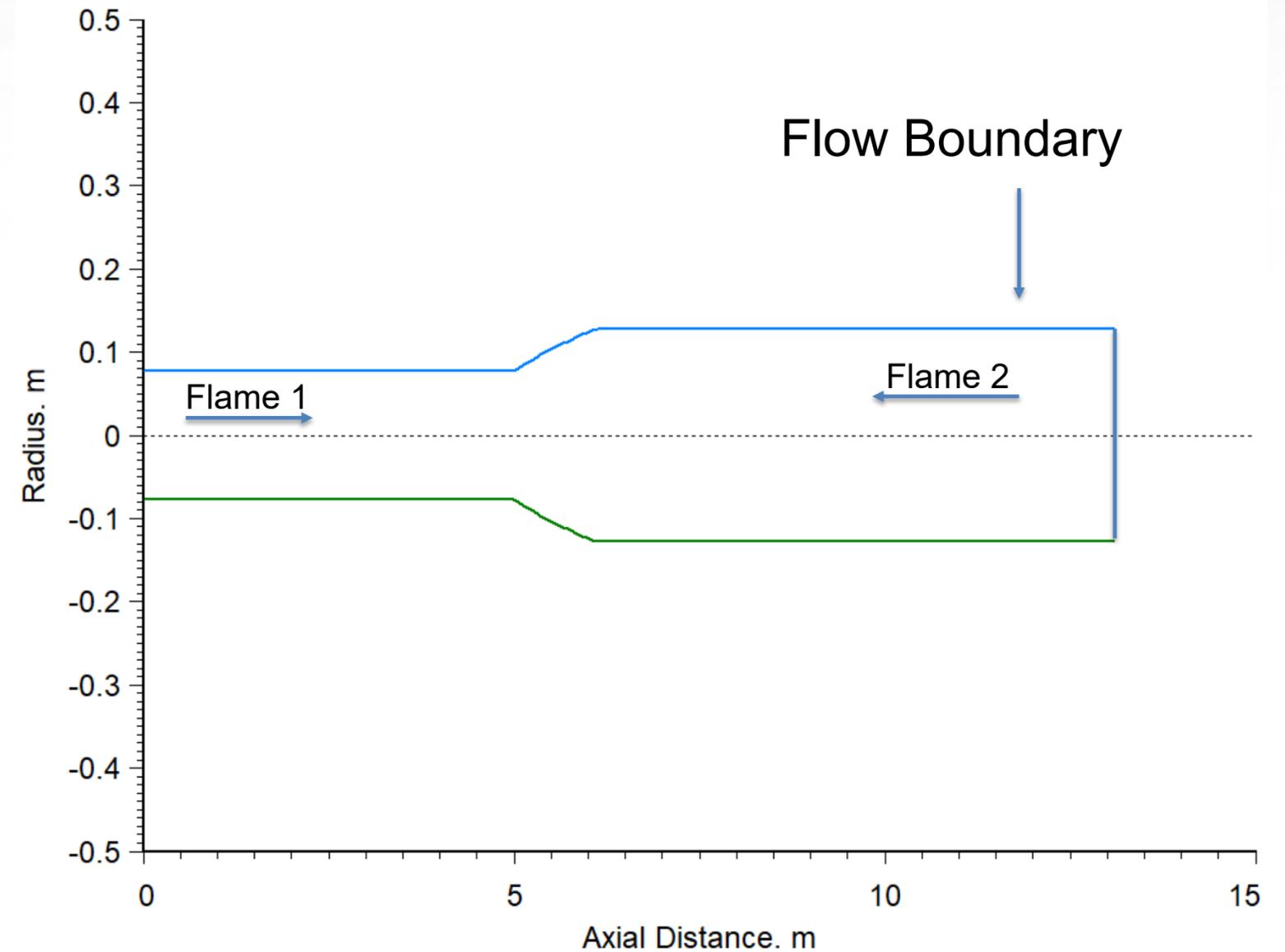
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# Case Study A – One Dimensional Explosion Dynamics

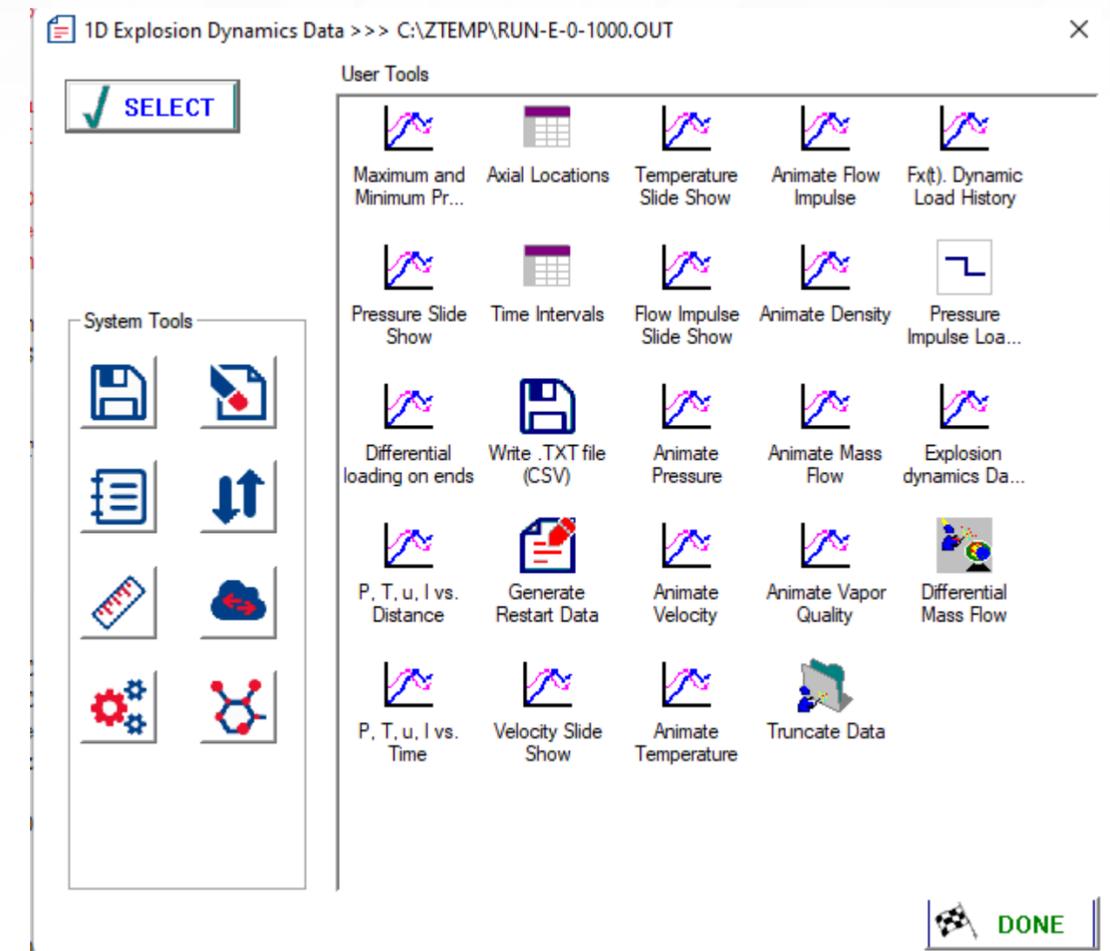
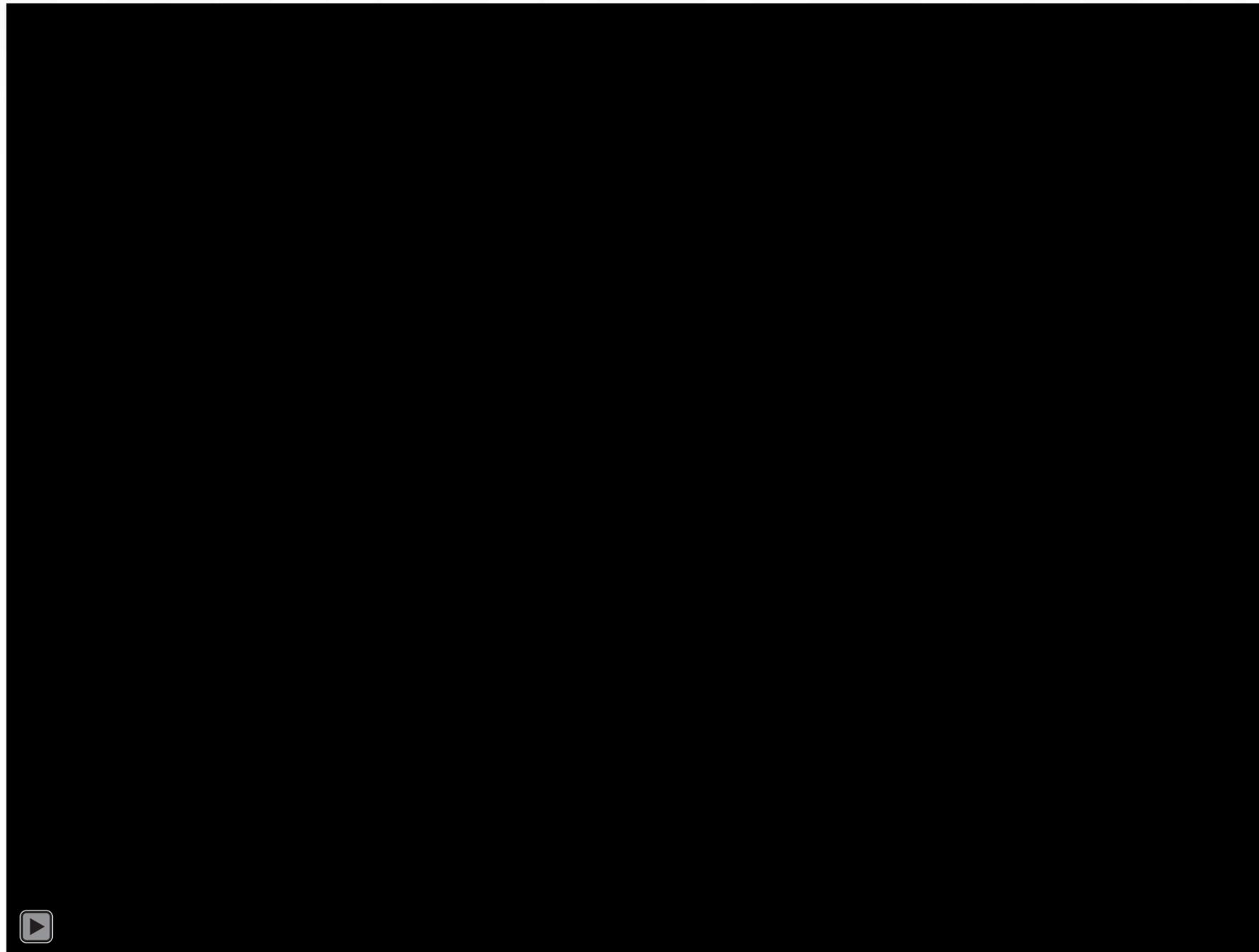


# It is best to illustrate the use of SuperChems one-dimensional (1D) explosion dynamics using an example

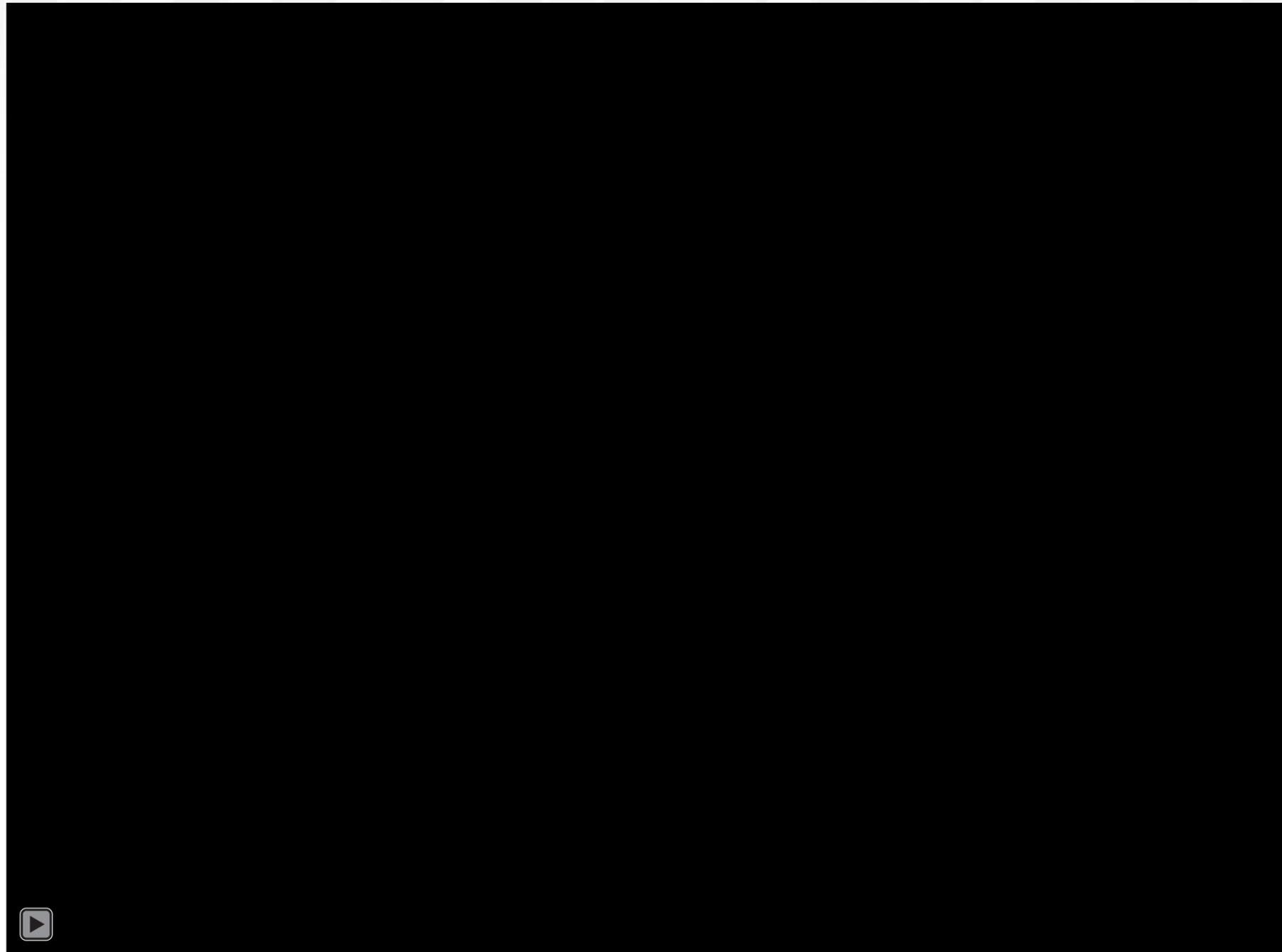
- ▶ Flow starts at the right boundary at 10 ms and is terminated at 100 ms
- ▶ Flame 1 ignites at 15 ms and starts at location 12.9 m and propagates to the left
- ▶ Flame 2 ignites at 25 ms and starts at location 0.1 m and propagates to the right
- ▶ Both flames are allowed to accelerate in the piping starting with laminar burning



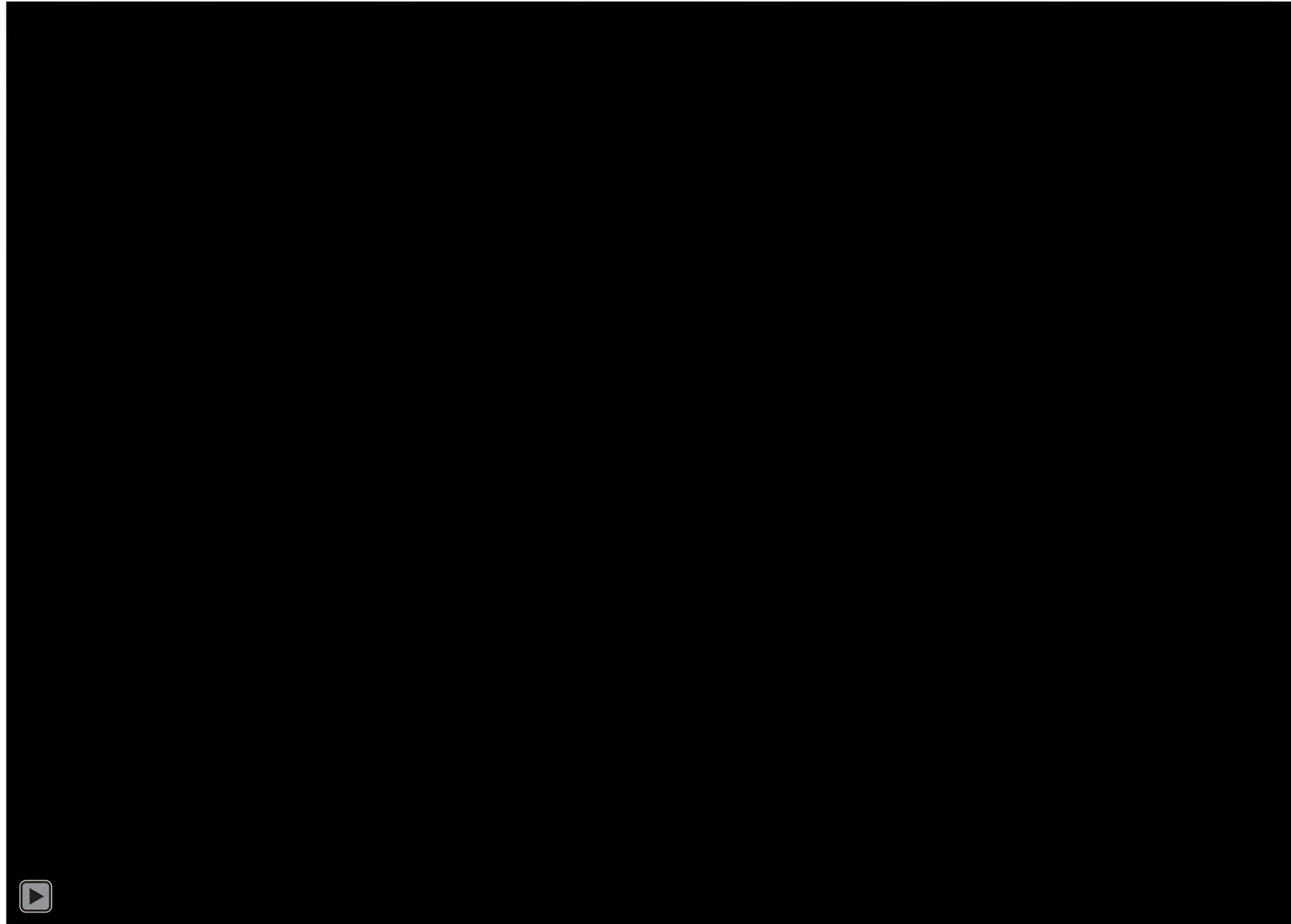
# We notice that one of the flames accelerates from a deflagration to a detonation (DDT)



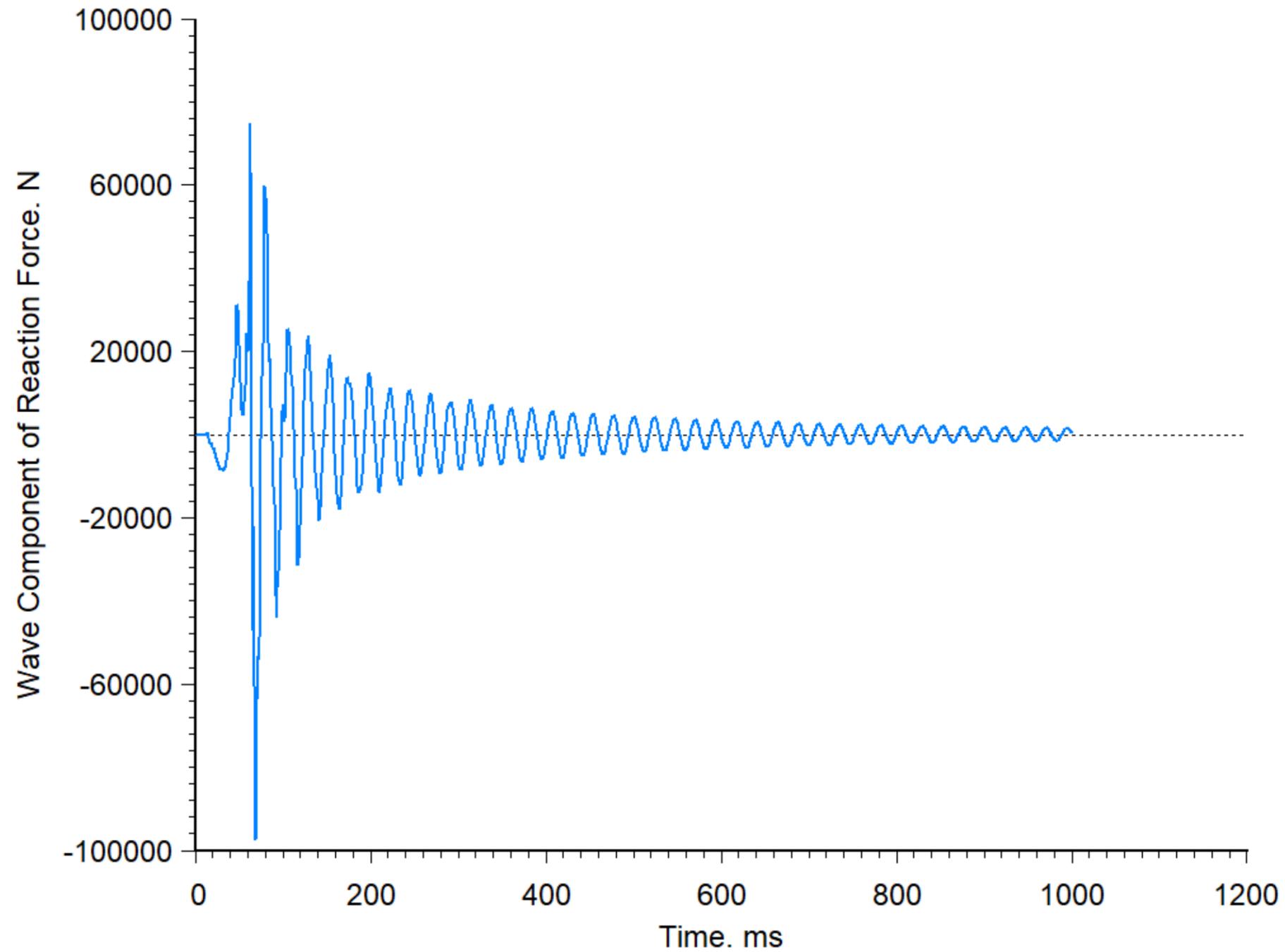
**Notice the flames proceeding towards the change in flow area**



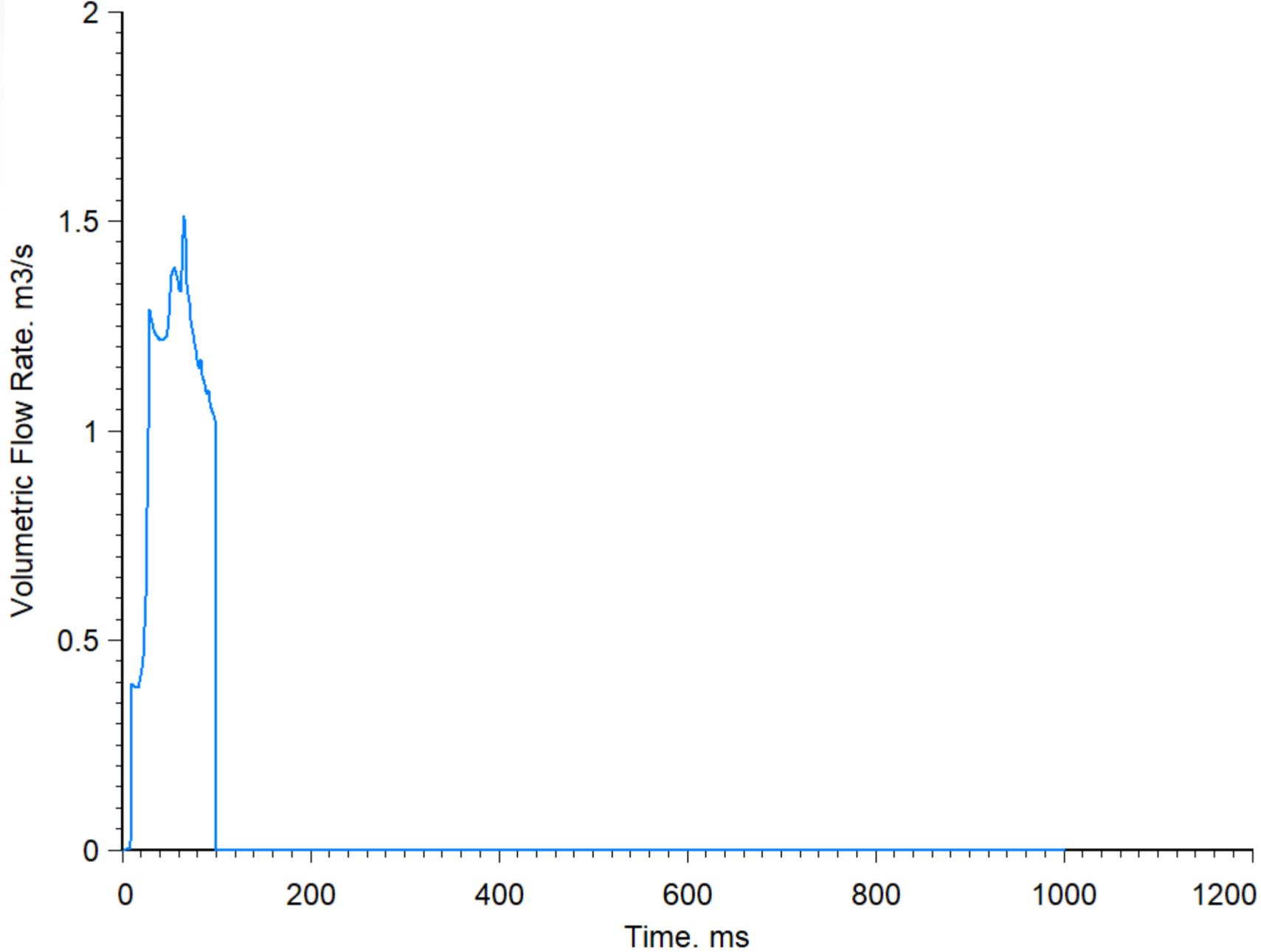
# There is nothing simple about what is happening inside this piping configuration during the explosion



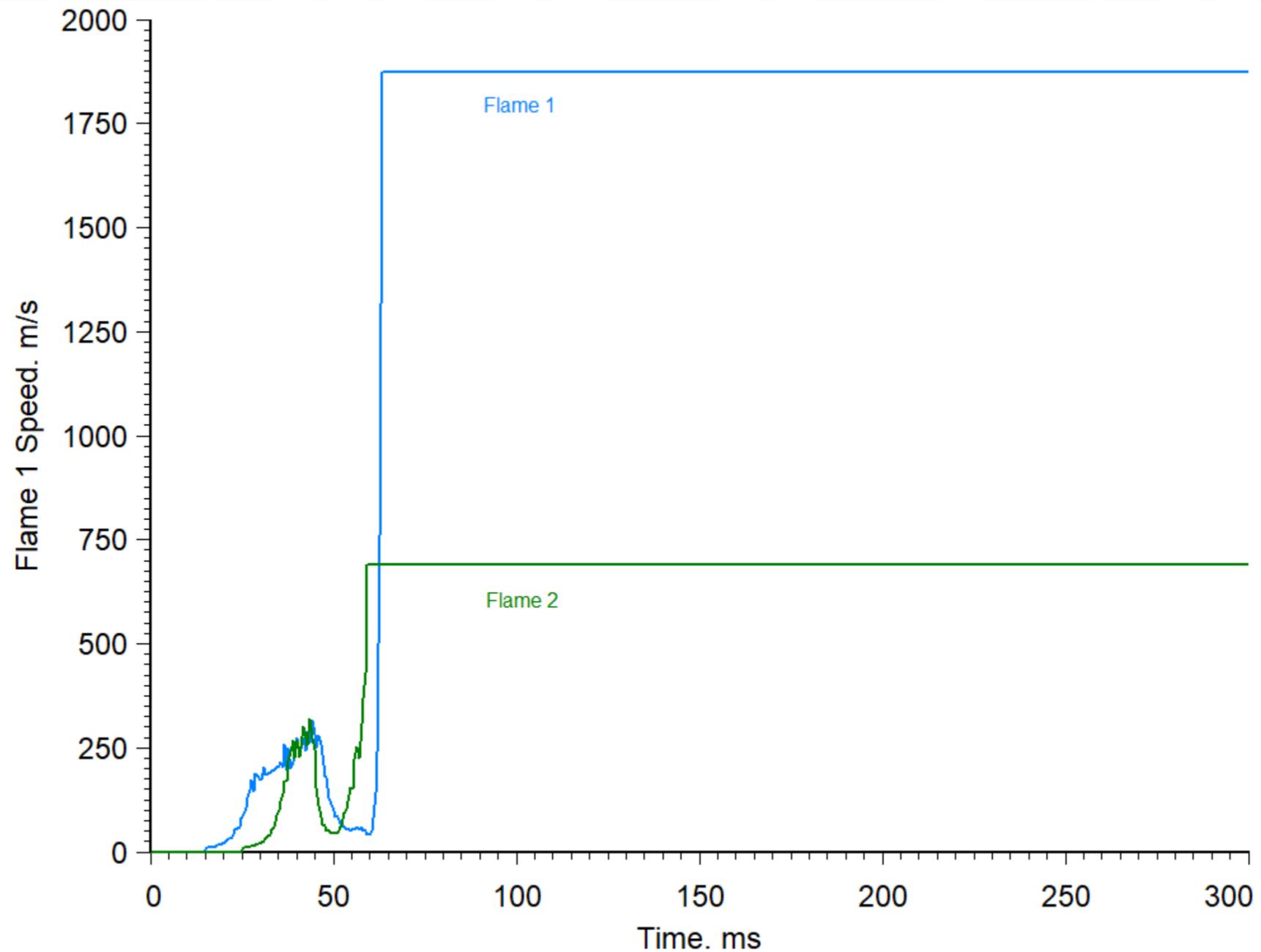
# The explosion imparts substantial dynamic loads on the piping



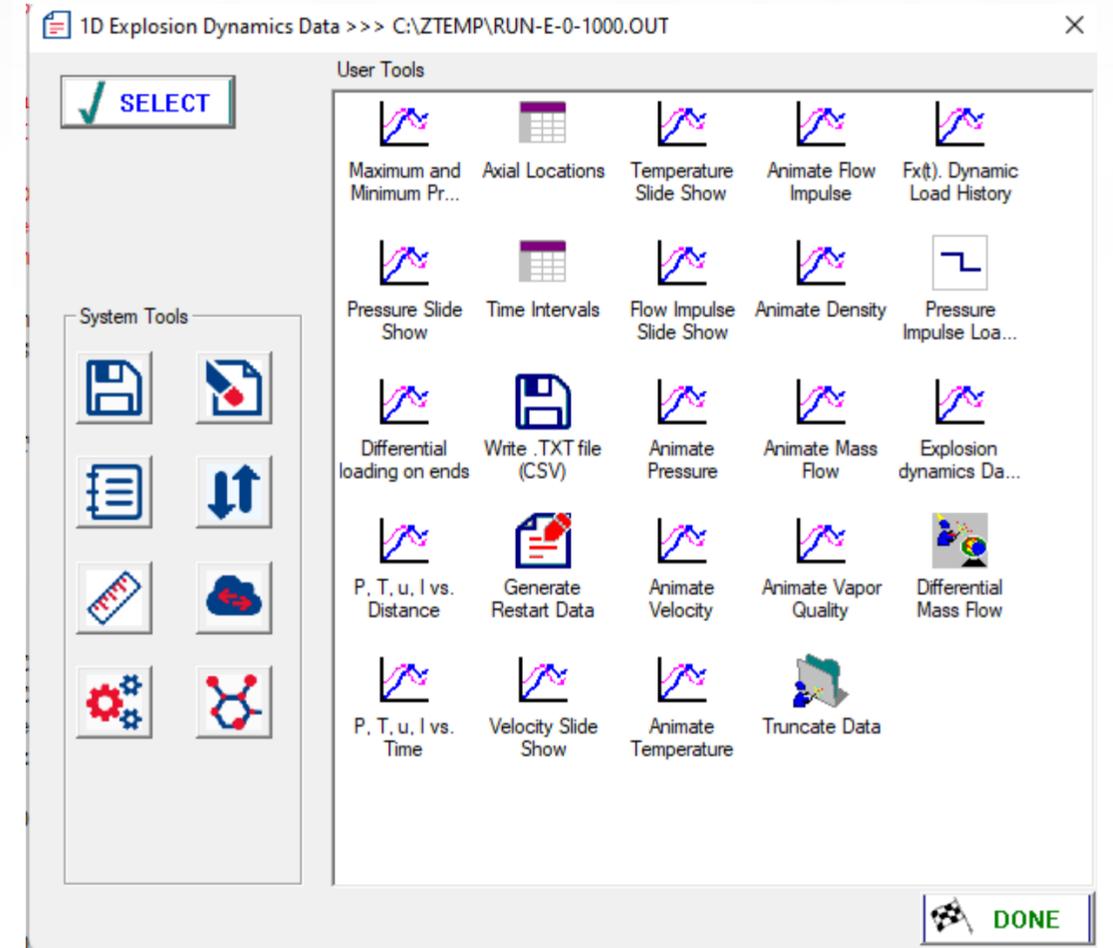
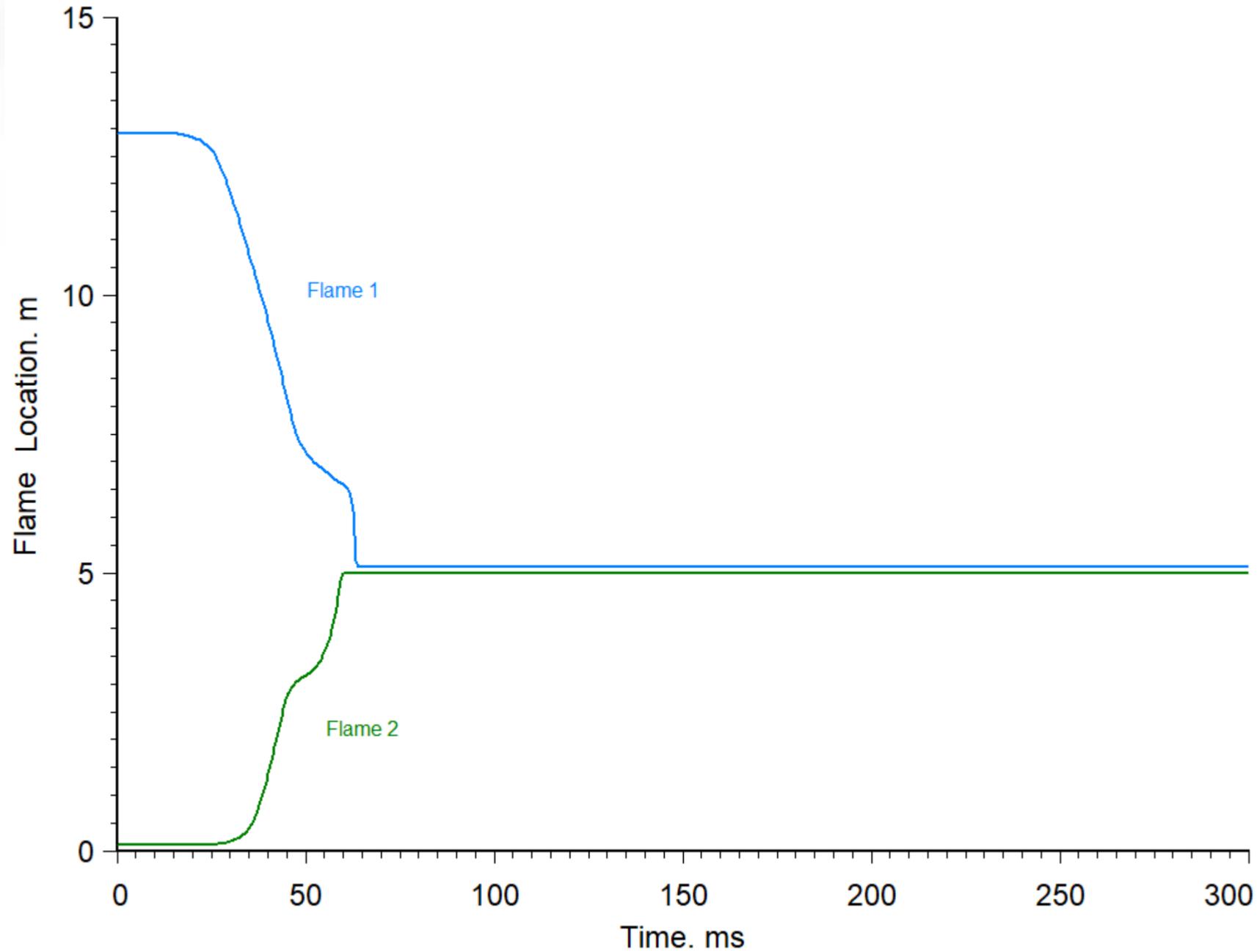
# The initial mass flow was not sufficient to provide any kind of meaningful venting or pressure relief



# The flame acceleration methods used are semi-empirical and based on actual measurements

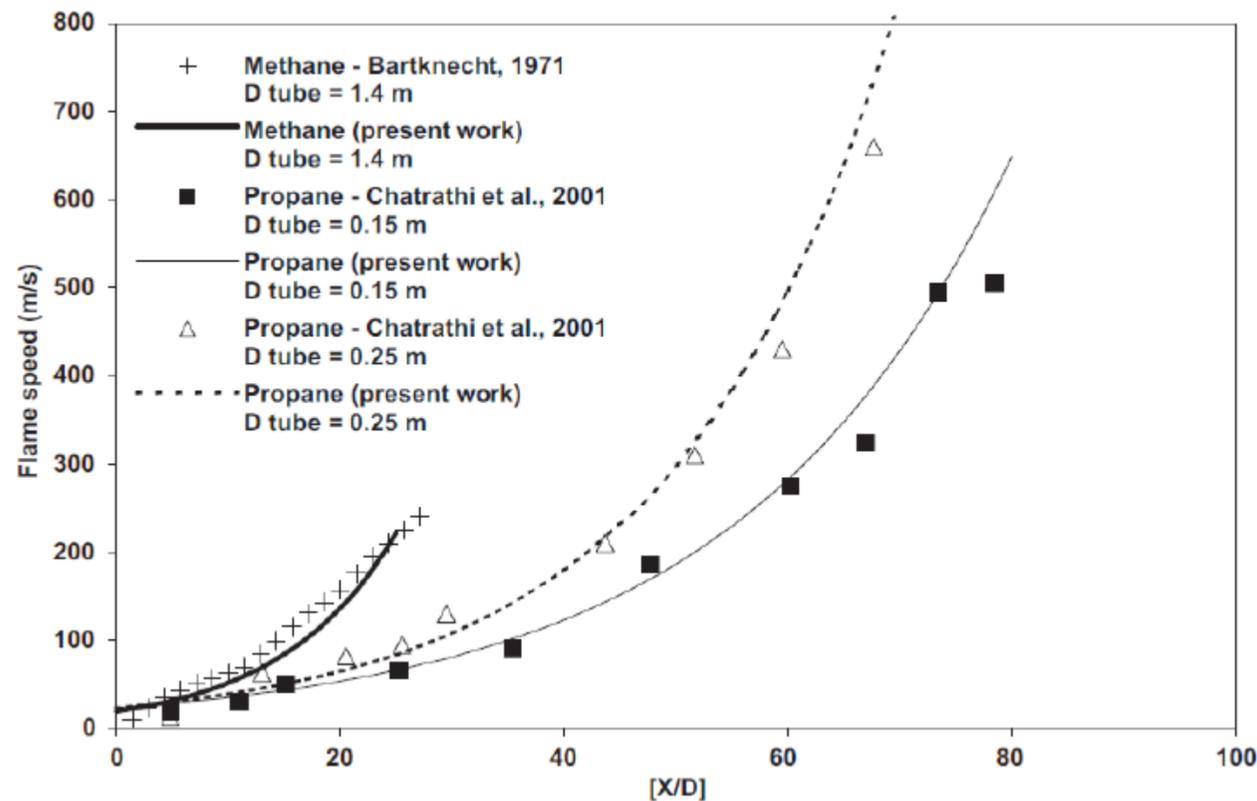


# Both flames proceed in opposite directions and meet at 5 m



# Flame acceleration is modeled based on a semi-empirical correlation

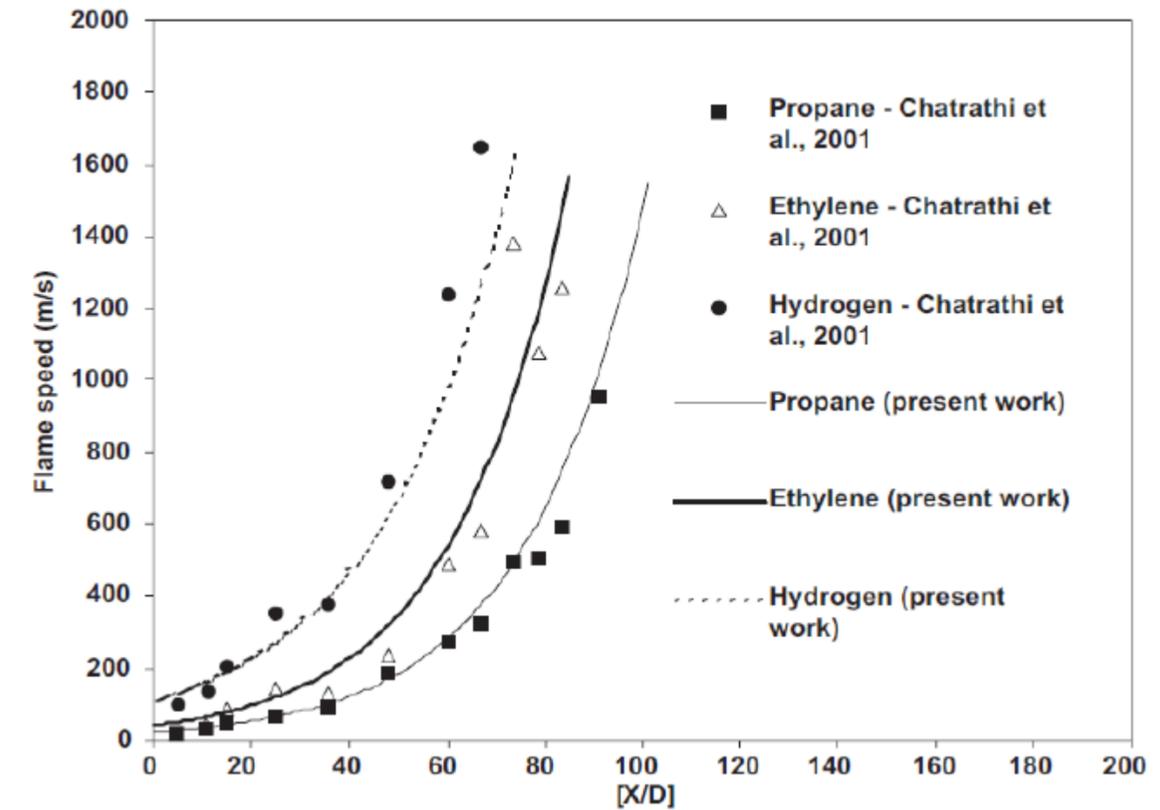
Figure 5: Comparison between measured and calculated flame speeds [18] using Equation 23



$$\frac{s_f(x)}{s_u} = 6.5\sigma \exp \left[ 0.0061 (\sigma - 1) \left( \frac{x}{D} \right) \left( \frac{D}{0.15} \right)^{0.4} \right]$$

$$\sigma = \frac{\rho_u}{\rho_b}$$

Figure 4: Flame speed of flammable materials in a 0.15 m diameter tube [18]



$$\frac{s_f(x)}{s_u} = 6.5\sigma \exp \left[ 0.0061 (\sigma - 1) (1 + 15BR) \left( \frac{x}{D} \right) \left( \frac{D}{0.15} \right)^{0.4} \right]$$

[18] M. Silvestrini, B. Genova, G. Parisi, and F. J. Leon Trujillo. Flame acceleration and ddt run-up distance for smooth and obstacle filled tubes. *Journal of Loss Prevention in the Process Industries*, 21:555–562, 2008.

# Case Study B – Single Volume Explosion Dynamics for an Energetic Dust

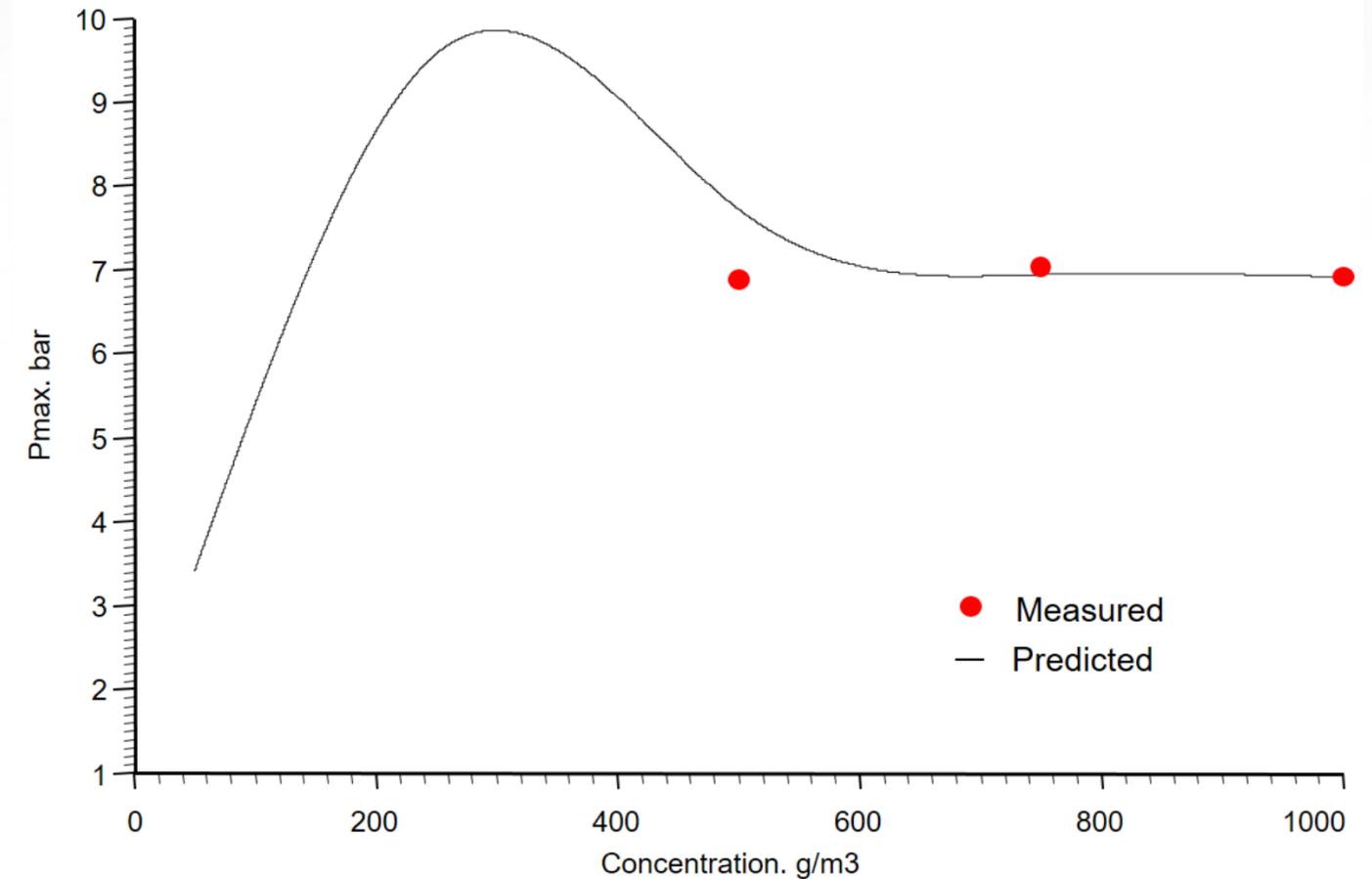
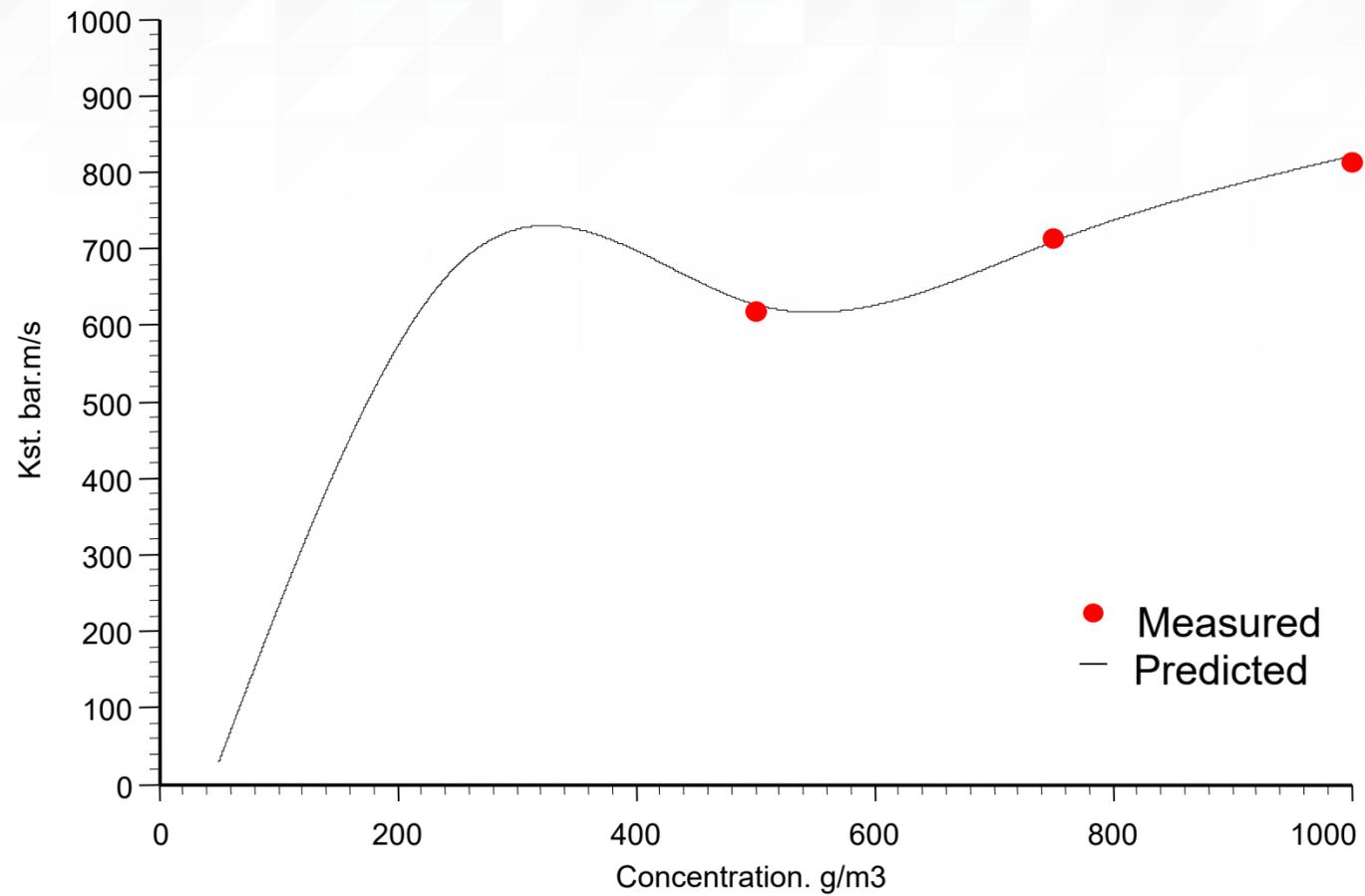


# We consider the explosion severity data for an energetic dust measured in a 20-liter sphere

- ▶ Dust contains an inert material
- ▶ Data reported included  $K_{st}$ ,  $P_{max}$ , and  $dP/dt_{max}$
- ▶ Data included tests for 500, 750, and 1000 g/m<sup>3</sup> dust concentrations
- ▶ Explosion severity parameters were established at an initial temperature of 25 C and an initial pressure of 1 bar

	Material A Concentration (g/m <sup>3</sup> )	Material B Concentration (g/m <sup>3</sup> )	Material B Mass (g)	$P_{max}$ (bar)	$dP/dt$ (bar/s)	$K_{st}$ (bar.m/s)	Equivalence Ratio	$S_{fo}$	Flame Temperature (C)
Measured	500	200	3.937	6.88	2274	617			
Predicted				7.73	2325	627	1.966	2.10	1383
Measured	750	300	5.905	7.04	2628	713			
Predicted				6.95	2623	709	2.946	2.75	1234
Mesured	1000	400	7.874	6.93	2995	813			
Predicted				6.92	3041	821	3.704	3.25	1158

# We simulated the 20-liter dust explosion dynamics for 500, 750, and 1000 g/m<sup>3</sup> concentrations

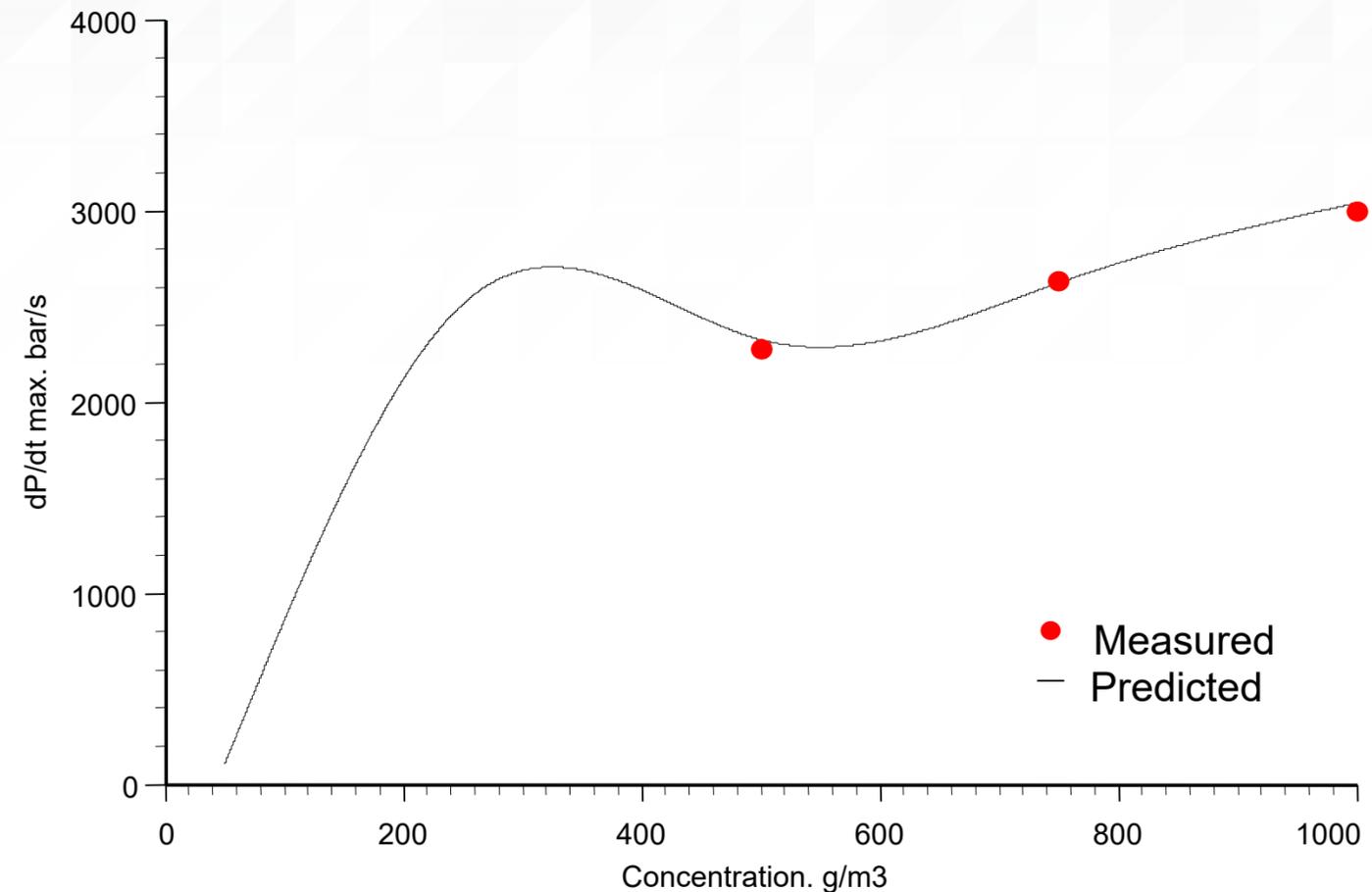


# Excellent agreement is obtained between measured and predicted data

- ▶ The estimated laminar burning velocity was found to have a linear dependence on equivalence ratio:

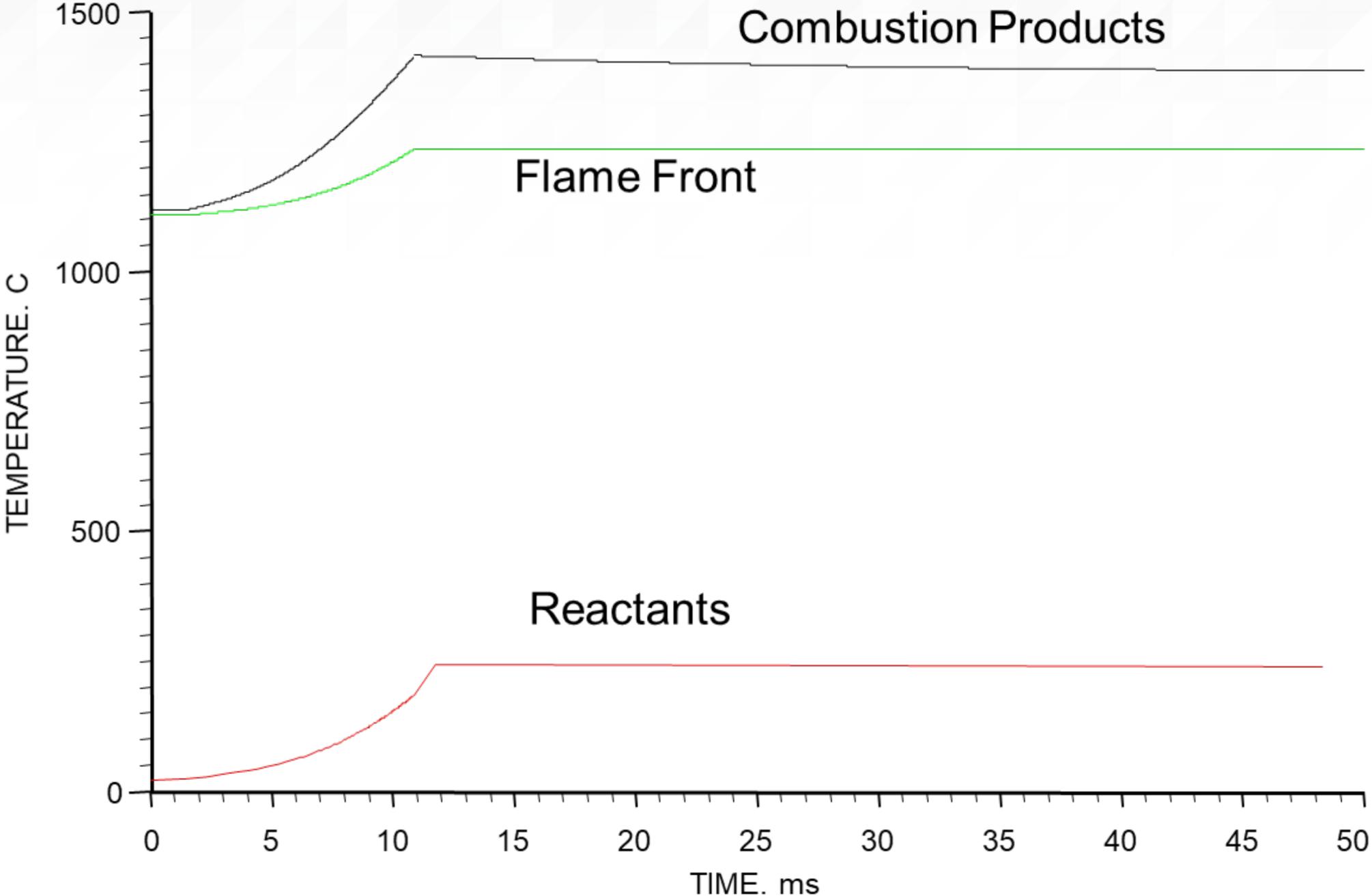
$$s_{uo} = 0.80 + 0.67 * \Phi$$

- ▶ The measured data contains fuel rich compositions (500, 750, and 1000 g/m<sup>3</sup>)



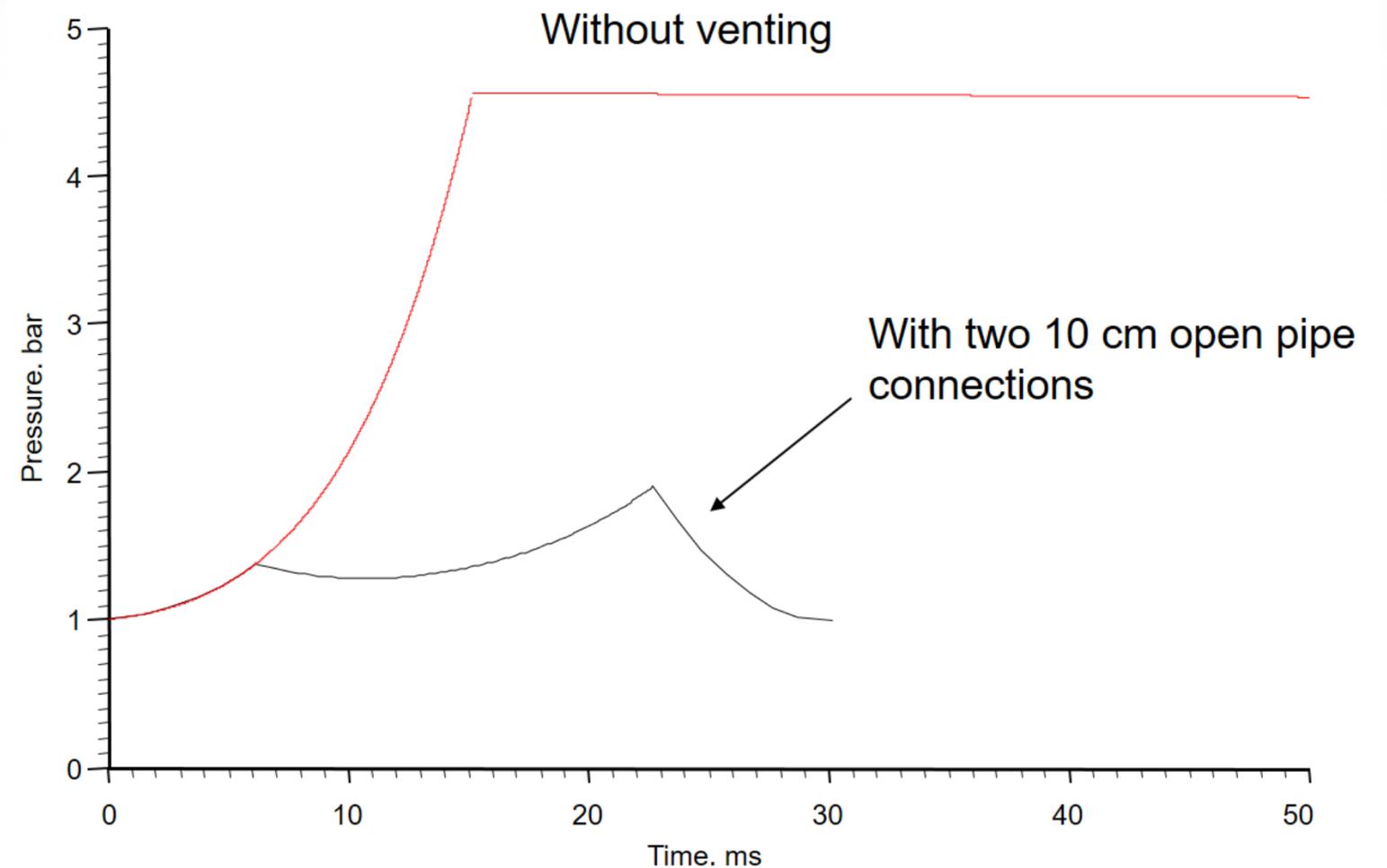
The average temperatures of interest in the process are > 300 C. As a result, the measured dust data can only be used for explosion venting using the temperature dependent burning velocity model established by the model above.

# This simulation of the explosion process in the 20-liter sphere with 750 g/m<sup>3</sup> shows the compression and flame acceleration



# The developed model is then used to obtain the maximum permissible equipment dust loading

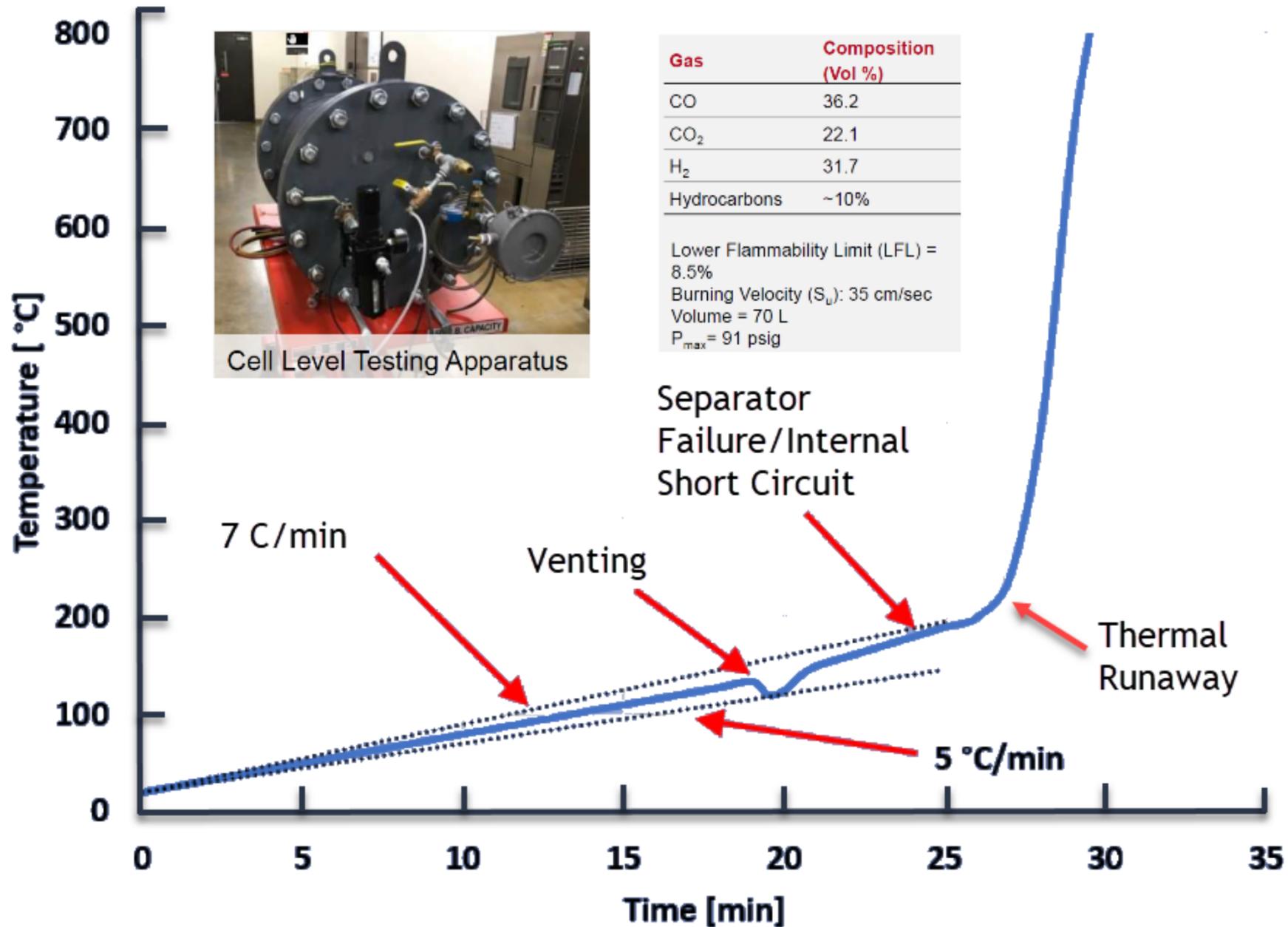
- ▶ Volume = 0.05 m<sup>3</sup>; T<sub>0</sub> = 300 C; P<sub>0</sub> = 1 bara;  
Two 10 cm OD open pipe connections
- ▶ The pressure built up during an explosion will be less than 1 barg with a dust concentration of 100 g/m<sup>3</sup>
- ▶ NFPA-68 allows a maximum deflagration pressure such that 2/3 of the ultimate tensile strength of the vessel metal is not exceeded



# Case Study C – Single Volume Explosion Dynamics for an Energy Storage System



# A runaway reaction in a lithium-ion battery can lead to the formation of flammable gas



$$s_{u_o} = 0.35$$

$$s_f = (\chi + \eta) s_{u_o} \left[ \frac{T_u}{T_o} \right]^{2.18} \left[ \frac{P}{P_o} \right]^{-0.17}$$

This burning rate model was obtained from published data (Tables provided in companion white paper)

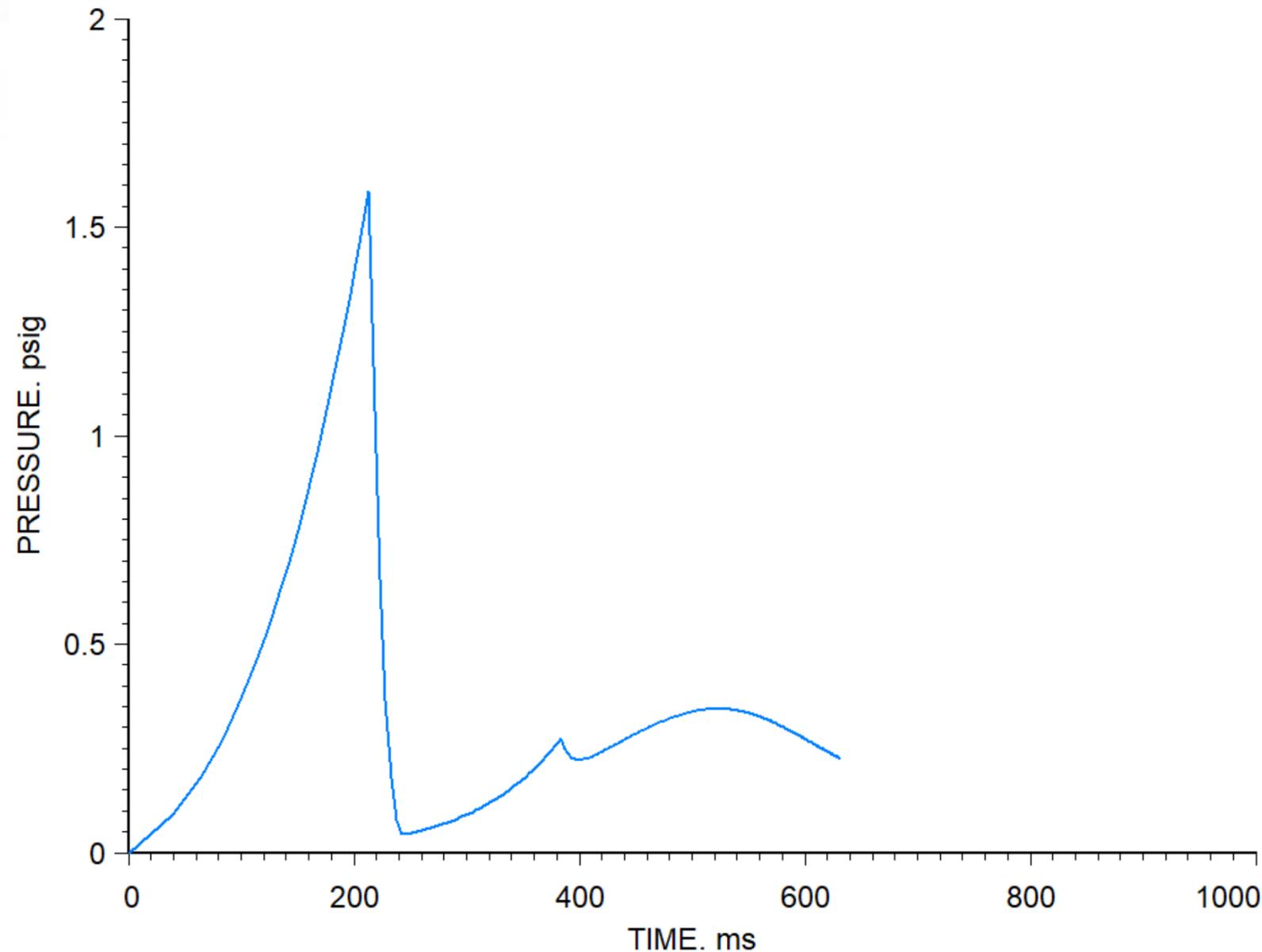
Source: Barowy A, "Large Scale Testing of Energy Storage Systems; Fire Protection and Response Considerations", March 2019

# Typical burning velocities of saturated hydrocarbons at 25 C air-fuel temperature and 1 atm in air

Chemical	Equivalence Ratio $\phi$								$S_u$ in cm/s		T and P Exponents	
	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	$S_{max}$	$\phi$ at $S_{max}$	$\alpha$	$\beta$
Ethane	30.60 22.00	36.00 29.00	40.60 36.50	44.50 42.50	47.30 43.00	47.30 42.50	44.40 40.00	37.40 27.50	47.60	1.14	2.07	-0.14
Propane	24.00 23.00	32.00 30.00	42.30 39.50 37.00	45.60 44.00 39.00	46.20 45.00 41.00	42.40 43.50 40.50	34.30 37.00 33.50	28.00 25.00	46.40	1.06	2.13	-0.16
n-Butane		38.00	42.60	44.80	44.20	41.20	34.40	25.00	44.90	1.03	2.16	-0.16
Methane	20.50 17.00	30.00 28.00 25.00	38.30 36.00 33.00	43.40 40.50 38.00	44.70 42.00 38.50	39.80 37.00 34.00	31.20 27.00 24.00	17.50 13.50	44.80	1.08	2.12	-0.15
n-Pentane		35.00	40.50	42.70	42.70	39.30	33.90		43.00	1.05	2.14	-0.16
n-Heptane		37.00	39.80	42.20	42.00	35.50	29.40		42.80	1.05	2.14	-0.16
2,2,4-Trimethylpentane		37.50	40.20	41.00	37.20	31.00	23.50		41.00	0.98	2.20	-0.17
2,2,3-Trimethylpentane		37.80	39.50	40.10	39.50	36.20			40.10	1.00	2.18	-0.17
2,2-Dimethylbutane		33.50	38.30	39.90	37.00	33.50			40.00	0.98	2.20	-0.17
Isopentane		33.00	37.60	39.80	38.40	33.40	24.80		39.90	1.01	2.17	-0.17
2,2-Dimethylpropane			31.00	34.80	36.00	35.20	33.50	31.20	36.00	1.10	2.10	-0.15

Exponents  $\alpha$  and  $\beta$  are calculated for  $\phi$  at  $S_{max}$  according to [10] and [11]

# Dynamic modeling of a deflagration in a 33 m<sup>3</sup> Energy Storage System (stoichiometric composition) provides an estimate of maximum expected pressure during venting



Fast acting rupture disk

$$C_d = 0.6$$

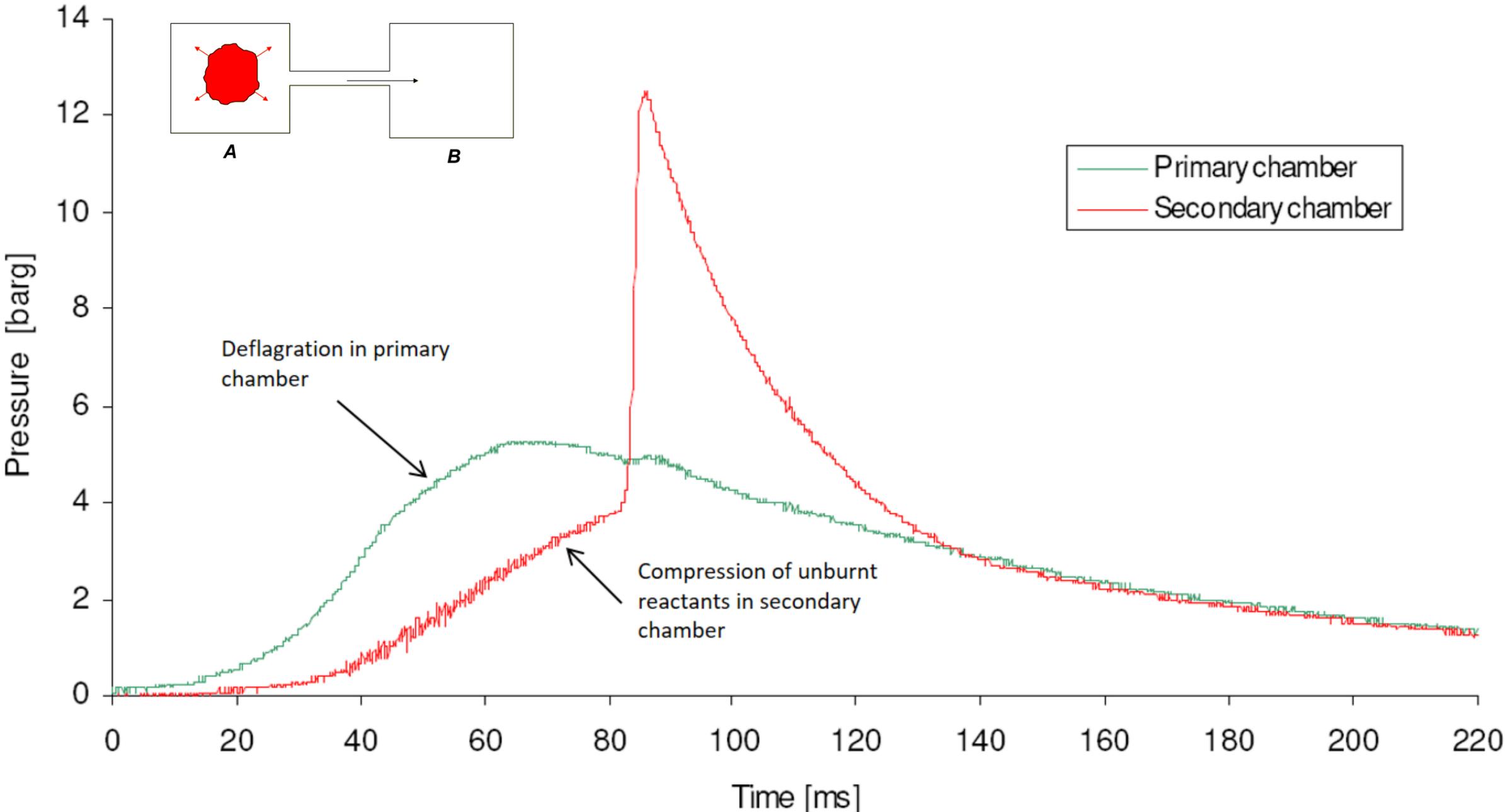
$$P_{set} = 1.5 \text{ psig}$$

$$\text{Vent area} = 22.5 \text{ ft}^2$$

# One Dimensional Explosion Dynamics with SuperChems



# When an explosion occurs in a vessel that is interconnected to another, pressure pileup can occur with significant severity



# Working fluid – heat addition reduced models can be derived from steady one-dimensional flow equations

## Steady One Dimensional Flow

**Mass:**

$$\rho_1 u_1 = \rho_2 u_2$$

**Momentum:**

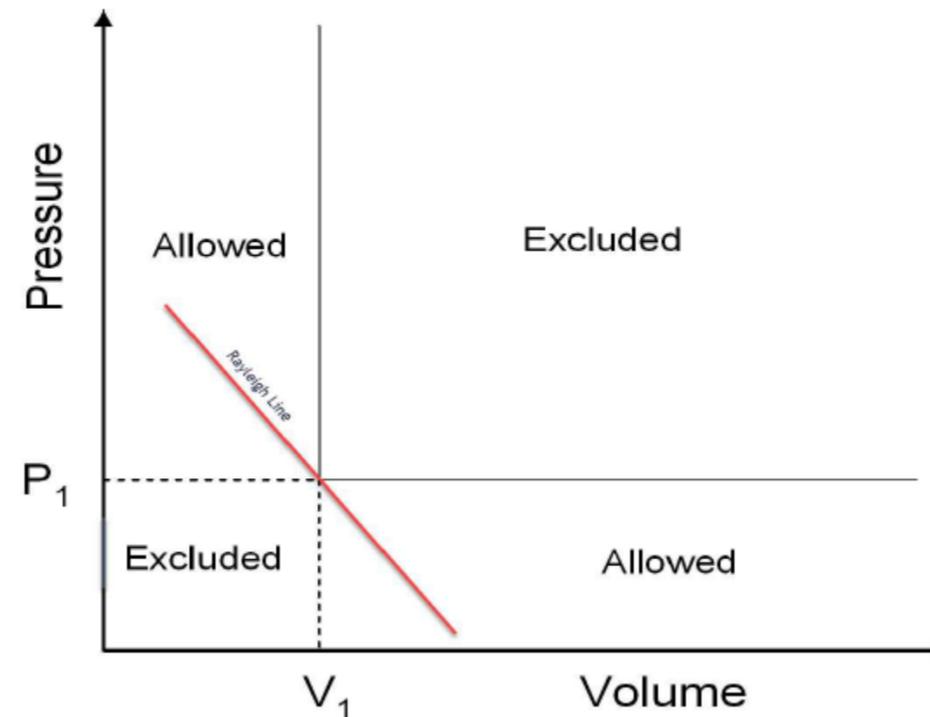
$$P_1 + \rho_1 u_1^2 = P_2 + \rho_2 u_2^2$$

**Energy:**

$$h_1 + \frac{1}{2}u_1^2 = h_2 + \frac{1}{2}u_2^2$$

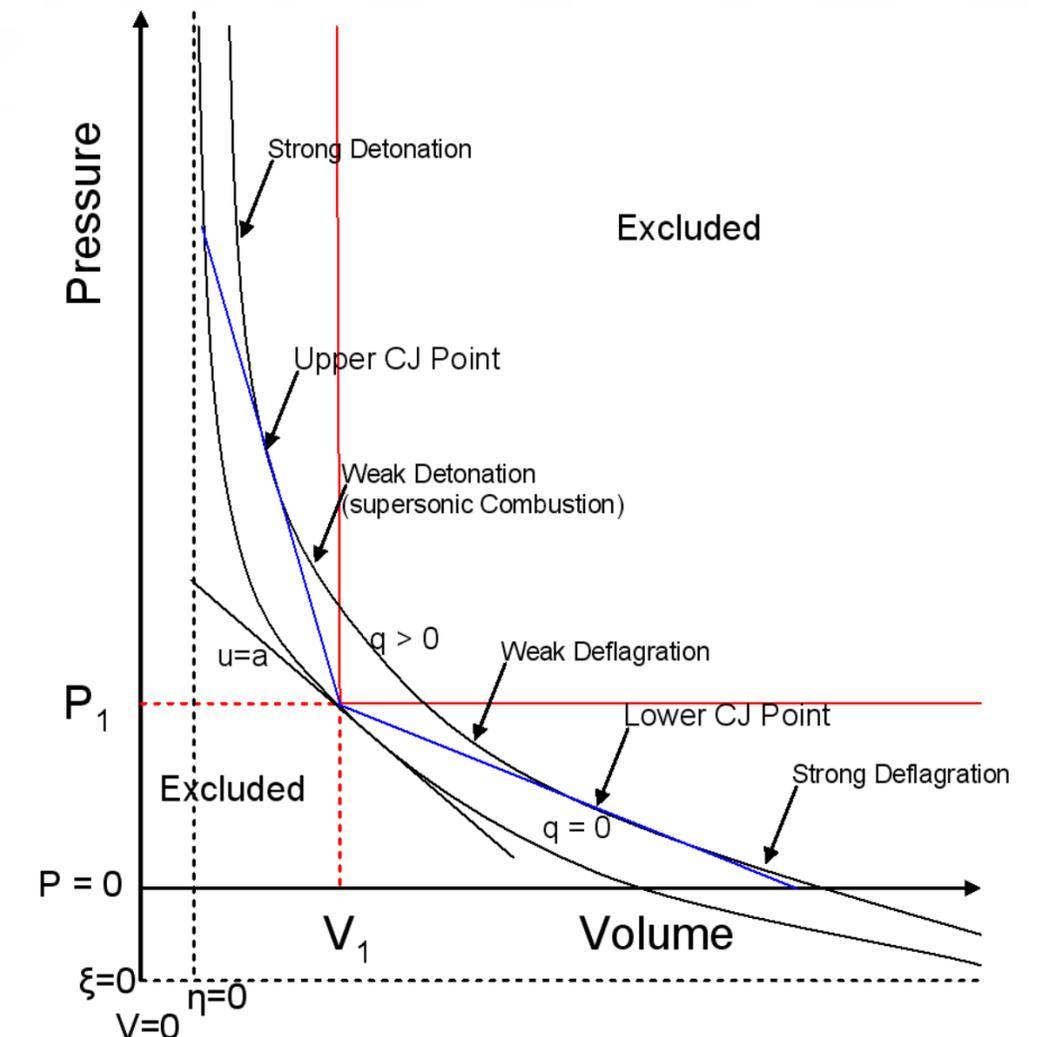
## The Rayleigh Line Equation

$$[\rho_1 u_1]^2 = [\rho_2 u_2]^2 = \frac{P_2 - P_1}{v_1 - v_2} \text{ which is always } > 0$$



## The Rankine-Hugoniot Equation

$$e_2 - e_1 = \frac{1}{2} (P_2 + P_1) (v_1 - v_2)$$



# Constant volume and CJ conditions can be estimated from these simple relationships

## CJ Conditions

$$\frac{P_{CJ}}{P_0} = \frac{1 + \gamma M_{CJ}^2}{\gamma + 1}$$

$$\frac{T_{CJ}}{T_0} = \left[ \frac{P_{CJ}}{P_0} \frac{1}{M_{CJ}} \right]^2$$

$$\frac{\rho_{CJ}}{\rho_0} = \frac{P_0}{P_{CJ}} M_{CJ}^2$$

$$\frac{u_{CJ}}{c_0} = M_{CJ} \text{ or } u_{CJ} = \left( \sqrt{\frac{\gamma P_0}{\rho_0}} \right) M_{CJ}$$

$$M_{CJ} = \sqrt{[\mathcal{H} + 1] \pm \sqrt{[\mathcal{H} + 1]^2 - 1}}$$

$$\mathcal{H} = \frac{\gamma^2 - 1}{\gamma} q$$

## Constant Volume Conditions

$$T_{max} = T_0 + \gamma (T_f - T_0) \simeq \gamma T_f$$

$$P_{max} = P_0 \left[ 1 + \gamma \left( \frac{T_f}{T_0} - 1 \right) \right] \simeq \gamma P_0 \left( \frac{T_f}{T_0} \right)$$

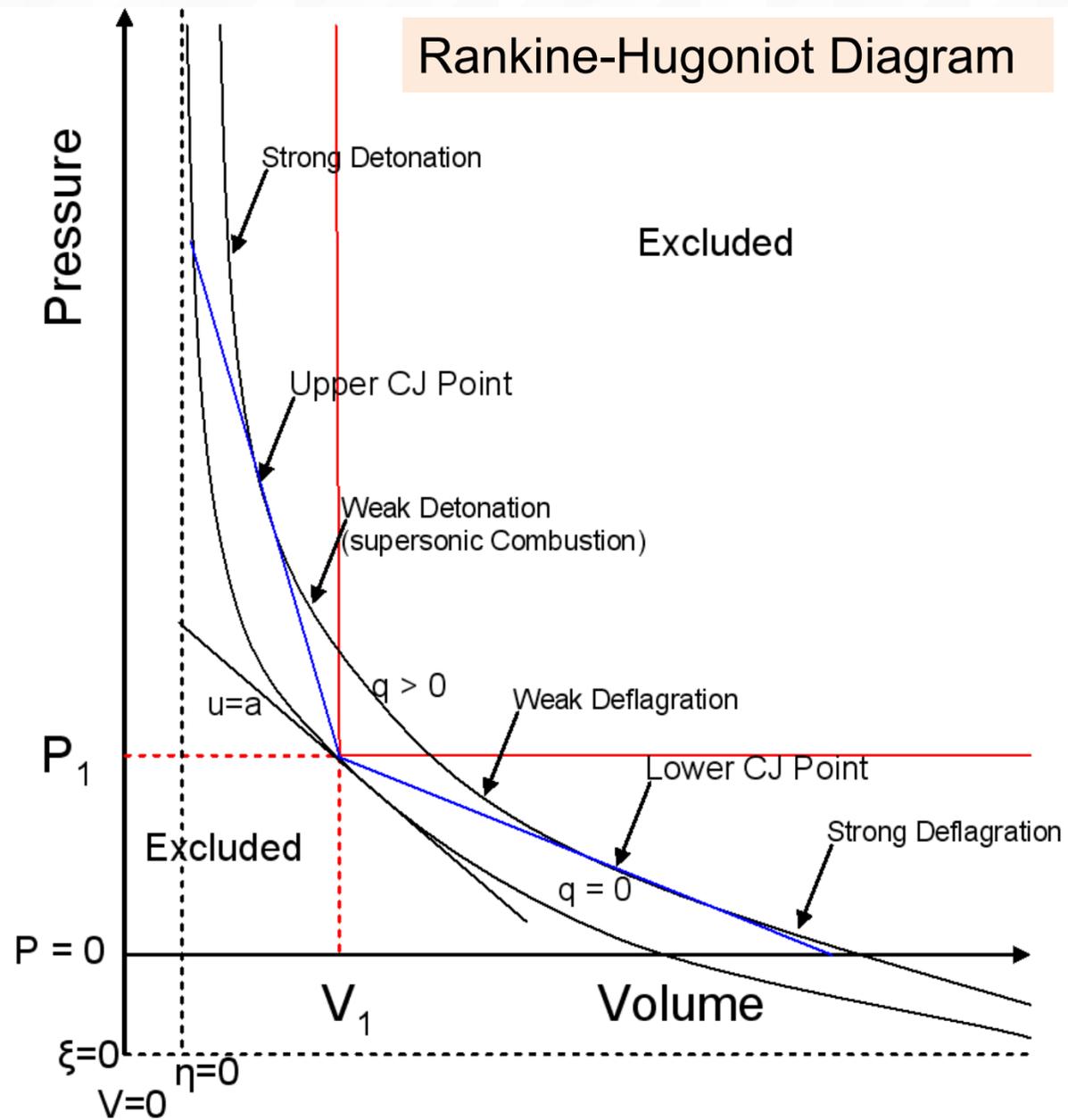
$$P_{CJ} \simeq 2P_{max}$$

$$T_{CJ} \simeq \left( \frac{2\gamma}{\gamma + 1} \right) T_{max}$$

Table 1: Rankine-Hugoniot Curves Regression Data (stoichiometric combustion)

Fuel	Heat of Combustion MJ/kg fuel	Heat of Combustion h. MJ/kg mixture	Best Fit for h/ P <sub>1</sub> V <sub>1</sub>	Best Fit for q <sub>rxn</sub> =Q <sub>rxn</sub> /P <sub>1</sub> V <sub>1</sub>	γ
H <sub>2</sub>	120.00	3.40	28.86	33.89	1.173
CH <sub>4</sub>	50.01	2.74	30.90	39.27	1.202
C <sub>2</sub> H <sub>2</sub>	48.22	3.38	39.12	44.79	1.195
C <sub>2</sub> H <sub>4</sub>	47.16	2.99	34.91	43.29	1.199
C <sub>2</sub> H <sub>4</sub> O	28.69	3.24	40.78	47.27	1.203
C <sub>3</sub> H <sub>8</sub>	46.35	2.78	35.68	47.42	1.208

# Useful data can be derived from chemical equilibrium estimates before any testing and/or dynamic modeling is performed

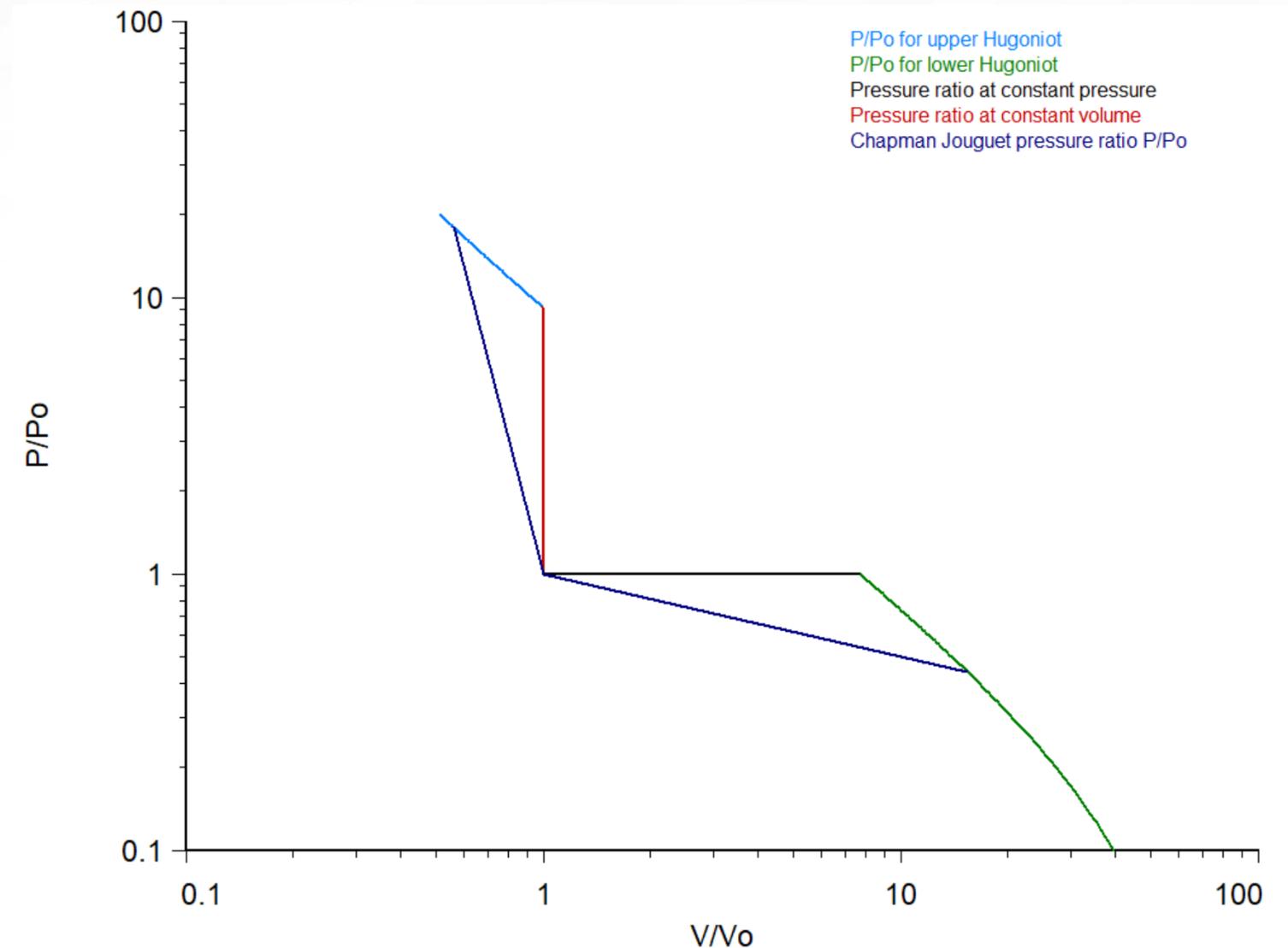


Hugoniot							
Summary Profiles							
	A	B	C	D	E	F	G
1	**Hugoniot / METHANE COMBUSTION						
2							
3		Initial Conditions	Constant Pressure	Constant Volume	Upper CJ	Lower CJ	Mw
4	METHANE. kmol	10.0000	0.0000	0.0000	0.0000	0.0000	16.0428
5	OXYGEN. kmol	18.9000	0.0464	0.1994	0.3698	0.0040	31.9988
6	NITROGEN. kmol	71.1000	71.0658	70.9463	70.8086	71.0945	28.0135
7	CARBON MONOXIDE. kmol		0.9091	0.9091	0.9091	0.9091	28.0104
8	CARBON DIOXIDE. kmol		9.0909	9.0909	9.0909	9.0909	44.0098
9	WATER. kmol		18.5481	18.0029	17.3865	18.6902	18.0153
10	NITRIC OXIDE. kmol		0.0683	0.3072	0.5825	0.0108	30.0061
11	NITROGEN DIOXIDE. kmol		0.0000	0.0001	0.0002	0.0000	46.0055
12	AMMONIA. kmol		0.0000	0.0000	0.0000	0.0000	17.0306
13	NITRIC ACID. kmol		0.0000	0.0000	0.0000	0.0000	63.0129
14	HYDROGEN. kmol		1.4519	1.9971	2.6134	1.3098	2.0159
15							
16	CARBON-REF. kmol		0.0000	0.0000	0.0000	0.0000	12.0110
17							
18	Temperature. K	298.0000	2263.6497	2704.5169	2953.1210	2003.4541	
19	Pressure. bara	1.0132	1.0132	9.3294	18.2150	0.4487	
20							
21	T/To		7.5961	9.0756	9.9098	6.7230	
22	P/Po		1.0000	9.2074	17.9768	0.4429	
23	Expansion Ratio at Po		7.6858				
24							
25	Total mass. kg	2756.9652	2756.9652	2756.9652	2756.9652	2756.9652	
26	Total moles. kg-mol	100.0000	101.1805	101.4530	101.7611	101.1094	
27	Average Molecular Weight. kg/kg-mol	27.5697	27.2480	27.1748	27.0925	27.2671	
28	Total volume. m3	2445.2688	18793.8689	2445.2688	1371.7047	37533.1144	
29	Total enthalpy. MJ	-748.9470	-748.4574	1284.6269	2533.8720	-1877.4722	
30	Total entropy. MJ/K	-0.8075	6.5246	5.4429	5.2886	6.6898	
31							
32	Speed of sound in gas. m/s	353.0483	929.0435	1015.0350	1061.7637	875.2958	
33	Particle velocity. m/s				1045.7250	906.6945	
34	Shock velocity. m/s				1864.1612	59.0708	
35							

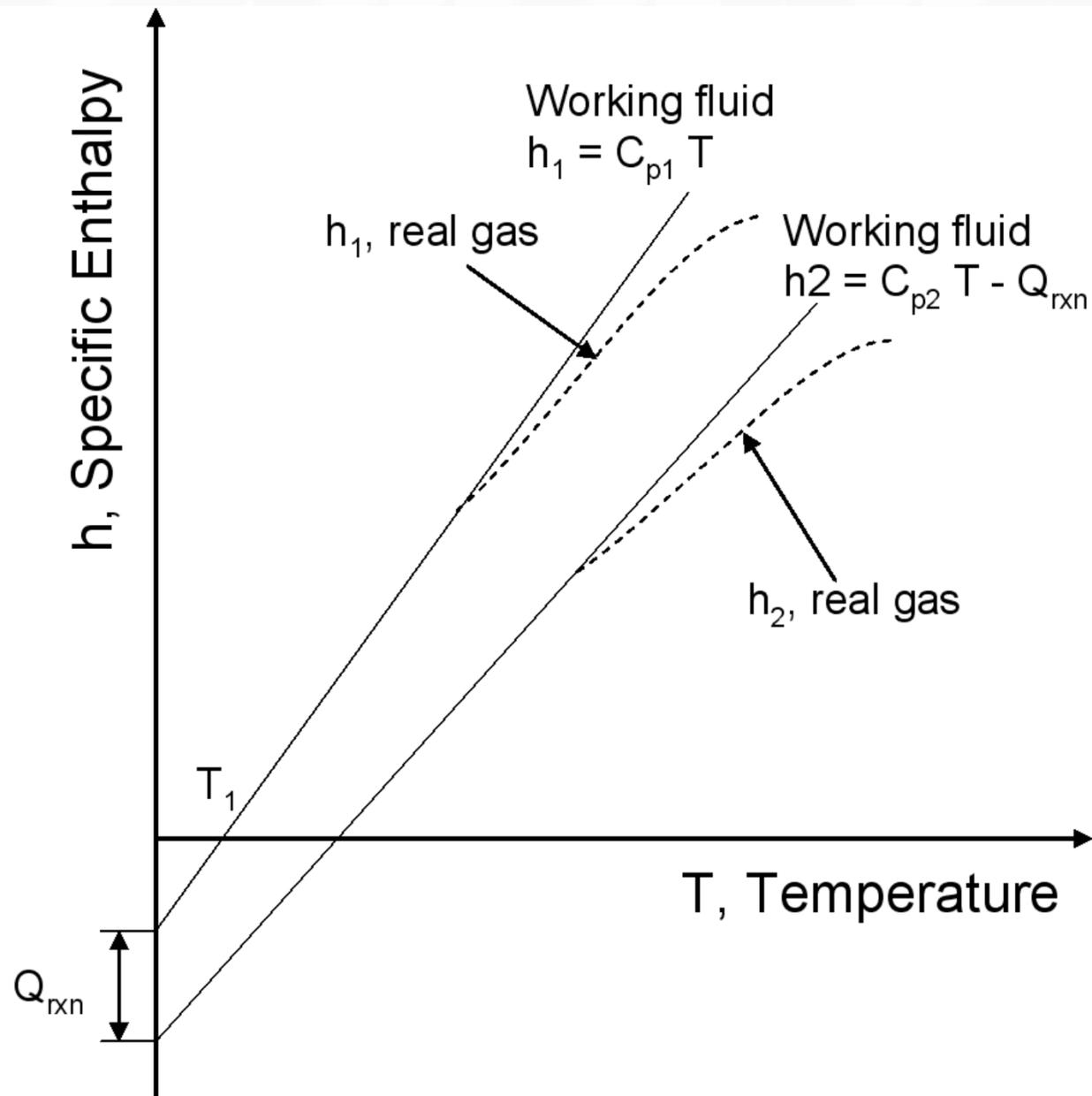


# It has been observed that steady premixed gas detonations tend to propagate at the upper CJ conditions

- ▶ Deflagration waves are influenced by finite reaction and transport rates and are not as reliable as CJ detonation velocities
- ▶ A CJ detonation corresponds to an increase in pressure and a decrease in specific volume and is a compression wave
- ▶ A CJ deflagration corresponds to a decrease in pressure and an increase in specific volume and is an expansion wave

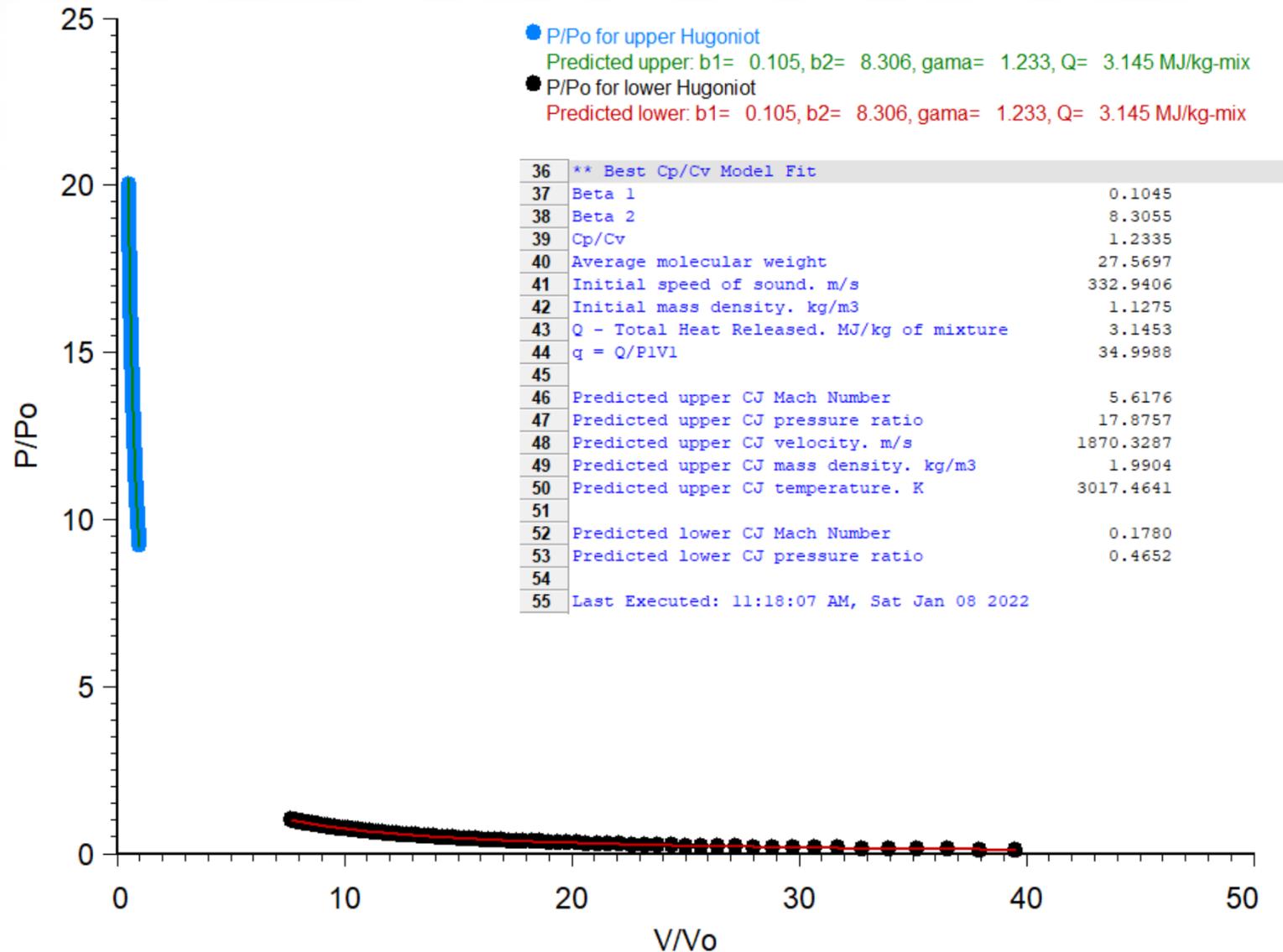


# The Rankine-Hugoniot data is used to develop simple working fluid models for explosion dynamics



$$\gamma = \frac{1+\beta_1}{1-\beta_1}$$

$$q_{rxn} = \frac{Q_{rxn}}{P_1 v_1} = \frac{1}{2} \left[ \beta_2 - \frac{4\gamma}{(\gamma+1)^2} \right] \left( \frac{\gamma+1}{\gamma-1} \right)$$



# We should notice some unique 1D fluid dynamics features of the partial differential equations shown below

## Continuity

$$\frac{\partial \tilde{\rho}}{\partial \tilde{t}} = -\frac{1}{\tilde{A}} \frac{\partial}{\partial \tilde{x}} [\tilde{\rho} \tilde{u} \tilde{A}] + \left[ \frac{\dot{m}_{in} - \dot{m}_{out}}{A(x) \Delta x} \right] \frac{t_o}{\rho_o}$$

## Momentum

$$\begin{aligned} \frac{\partial \tilde{u}}{\partial \tilde{t}} = & -\frac{1}{\tilde{\rho}} \frac{\partial \tilde{P}}{\partial \tilde{x}} - \tilde{u} \frac{\partial \tilde{u}}{\partial \tilde{x}} - \tilde{g} \sin \theta - \frac{f \tilde{u} |\tilde{u}|}{\sqrt{\frac{\tilde{A}}{\pi}}} - \frac{\tilde{u} |\tilde{u}|}{2} \frac{\partial K}{\partial \tilde{x}} + \nu \frac{\partial^2 \tilde{u}}{\partial \tilde{x}^2} \\ & + \left[ \frac{\dot{m}_{in} u_{in} - \dot{m}_{out} u_{out}}{A(x) \Delta x \rho(x)} \right] \frac{t_o}{c_o} \end{aligned}$$

## Equation of state

$$\tilde{P} = \frac{\tilde{\rho} R g \tilde{T}}{M_w}$$

or

$$\frac{\partial \tilde{P}}{\partial \tilde{t}} \simeq \left( -\frac{\rho u c^2}{A} \frac{\partial A}{\partial x} - u c^2 \frac{\partial \rho}{\partial x} - \rho c^2 \frac{\partial u}{\partial x} + c^2 \left[ \frac{\dot{m}_{in} - \dot{m}_{out}}{A(x) \Delta x} \right] \right) \frac{t_o}{P_o}$$

## Energy

$$\begin{aligned} \frac{\partial \tilde{T}}{\partial \tilde{t}} = & -\tilde{u} \frac{\partial \tilde{T}}{\partial \tilde{x}} + Q \frac{S_u}{dx \tilde{C}_v} \frac{x_o}{c_o^3} - \frac{\tilde{P}}{\tilde{C}_v \tilde{\rho} \tilde{A}} \frac{\partial}{\partial \tilde{x}} [A u] + \frac{f u^3}{\sqrt{\frac{\tilde{A}}{\pi}} \tilde{C}_v} + \frac{\tilde{u}^3}{2 \tilde{C}_v} \frac{\partial K}{\partial \tilde{x}} + \nu \frac{\partial^2 \tilde{T}}{\partial \tilde{x}^2} \\ & + \left[ \frac{\dot{m}_{in} \left( h_{in} + \frac{u_{in}^2}{2} + g z_{in} \right) - \dot{m}_{out} \left( h_{out} + \frac{u_{out}^2}{2} + g z_{out} \right)}{A(x) \Delta x \rho(x) c_v} \right] \frac{t_o}{T_o} \\ & - \left[ \frac{\pi D(x)}{A(x) \rho(x) c_v} 5.67 \times 10^{-8} \left( \frac{\epsilon_b \alpha_w}{\alpha_w + \epsilon_b \alpha_w \epsilon_b} \right) (T^4 - T_s^4) \right] \frac{x_o}{c_o T_o} \\ & + \left[ \frac{\pi \tilde{D}(x) U (\tilde{T}_s - \tilde{T})}{\rho(x) c_v \tilde{A}(x)} \right] \frac{x_o^2}{A_o c_o} \\ & + \left[ \frac{k}{\rho(x) c_v} \right] \left[ \frac{\partial^2 \tilde{T}}{\partial \tilde{x}^2} + \frac{1}{\tilde{A}(x)} \frac{\partial \tilde{A}(x)}{\partial \tilde{x}} \frac{\partial \tilde{T}}{\partial \tilde{x}} \right] \frac{1}{x_o c_o} \end{aligned}$$

# SuperChems Single Volume Explosion Dynamics



# SuperChems includes several fundamental building blocks for explosion dynamics

SuperChems Enterprise, Sc= METHANE COMBUSTION, Ch= METHANE COMB, Im= C:\ztemp\methane combustion.cor - []

Files Define Apply Flow NetFlow Control Disperse Burn Explode Report BatchQ Properties VLE Tools QRA Scripts

loaded project file:  
 C:\ztemp\methane combustion.cor  
 2 processors allocated

METHANE COMB. Maximum Number of Independent Reactions and Stoichiometry:  
 5 atoms x 12 components

Atom Matrix (Input): H,C,O,N, c1

0.0000	1.0000	0.0000	0.0000	0.0000	C, CARBON-REF
4.0000	1.0000	0.0000	0.0000	0.0000	CH4, METHANE
0.0000	0.0000	2.0000	0.0000	0.0000	O2, OXYGEN
0.0000	0.0000	0.0000	2.0000	0.0000	N2, NITROGEN
0.0000	1.0000	1.0000	0.0000	1.0000	CO, CARBON MONOXIDE
0.0000	1.0000	2.0000	0.0000	-0.1000	CO2, CARBON DIOXIDE
2.0000	0.0000	1.0000	0.0000	0.0000	H2O, WATER
0.0000	0.0000	1.0000	1.0000	0.0000	NO, NITRIC OXIDE
0.0000	0.0000	2.0000	1.0000	0.0000	NO2, NITROGEN DIOXIDE
3.0000	0.0000	0.0000	1.0000	0.0000	H3N, AMMONIA
1.0000	0.0000	3.0000	1.0000	0.0000	HNO3, NITRIC ACID
2.0000	0.0000	0.0000	0.0000	0.0000	H2, HYDROGEN

Method 1 - LU Decomposition  
 Atom Matrix Rank = 5  
 Maximum Number of Independent Chemical Reactions = 7

```

+0.013 CO +0.131 CO2 +0.575 HNO3 <----> +0.144 CH4 +1.000 O2 +0.288 N2
+0.359 CH4 +0.562 HNO3 <----> +0.281 N2 +0.033 CO +0.327 CO2 +1.000 H2O
+0.356 N2 +0.007 CO +0.065 CO2 +0.288 HNO3 <----> +0.072 CH4 +1.000 NO
+0.212 N2 +0.013 CO +0.131 CO2 +0.575 HNO3 <----> +0.144 CH4 +1.000 NO2
+0.647 CH4 +0.294 N2 +0.412 HNO3 <----> +0.059 CO +0.588 CO2 +1.000 H3N
+0.137 CH4 +0.275 N2 +0.078 CO +0.784 CO2 <----> +1.000 C +0.549 HNO3
+0.431 CH4 +0.275 HNO3 <----> +0.137 N2 +0.039 CO +0.392 CO2 +1.000 H2
  
```

Method 2 - Singular Value Decomposition  
 Atom Matrix Rank = 5  
 Maximum Number of Independent Chemical Reactions = 7

```

+1.000 C +0.147 O2 +0.234 H2O +0.052 NO2 +0.145 H3N +0.206 HNO3 +0.160 H2 <----> +0.357 CH4 +0.190 N2 +0.058 CO +0.585 CO2 +0.022 NO
+0.192 N2 +0.022 CO +0.225 CO2 +1.000 H2O +0.003 NO <----> +0.247 CH4 +0.450 O2 +0.042 NO2 +0.180 H3N +0.164 HNO3 +0.153 H2
+0.095 CH4 +1.000 NO +0.000 H2 <----> +0.163 O2 +0.356 N2 +0.009 CO +0.086 CO2 +0.002 H2O +0.097 NO2 +0.092 H3N +0.099 HNO3
+0.397 O2 +0.268 N2 +0.016 CO +0.164 CO2 +0.062 H2O +0.128 NO +0.112 H3N +0.224 HNO3 +0.019 H2 <----> +0.180 CH4 +1.000 NO2
+0.049 CO +0.495 CO2 +0.005 NO2 +1.000 H3N <----> +0.544 CH4 +0.332 O2 +0.455 N2 +0.170 H2O +0.035 NO +0.060 HNO3 +0.211 H2
+0.900 O2 +0.146 N2 +0.011 CO +0.111 CO2 +0.234 H2O +0.172 NO +0.280 NO2 +0.255 H3N +0.127 H2 <----> +0.122 CH4 +1.000 HNO3
+0.071 N2 +0.028 CO +0.280 CO2 +0.029 NO +0.026 NO2 +1.000 H2 <----> +0.308 CH4 +0.209 O2 +0.129 H2O +0.157 H3N +0.040 HNO3
  
```

FILTER \* [36/36]

User selected dynamic tools

- Select Tools
- Atom Matrix Independ...
- Reactivity Expert
- Update Mixture Reactivity a...
- Select potential reaction pro...
- Specify atom matrix con...

# The deflagration dynamics process can be modeled in detail using transient chemical equilibrium estimates

- ▶ The gas and/or dust mixture is uniform in composition and the thickness of the flame in the reaction zone is negligible
- ▶ The burning rate accelerates when the flame front becomes wrinkled at a critical expansion ratio corresponding to a critical Reynolds number
- ▶ Burnt and unburnt gases are treated assuming non-ideal gas behavior using a modified cubic equation of state
- ▶ When venting occurs and depending on the location of the vent relative to the flame front, unburnt, burnt, or a mixture of burnt and unburnt materials can be vented
- ▶ The burnt and unburnt materials are compressed during the deflagration

# Transient chemical equilibrium estimates yield stoichiometry of the reactions as temperature and pressure change

- ▶ The pressure is uniform in the vessel
- ▶ Materials are incrementally reacted using direct minimization of the Gibbs free energy
- ▶ The deflagration process is rapid, and therefore the only heat loss mechanism considered is radiation to the vessel walls from combustion
- ▶ The final conditions are determined by solving for the pressure and temperatures that satisfy the energy and mass balance constraints at constant volume

```

+0.857 CO2 +0.143 CH4 +0.286 N2 <----> + C +0.571 HNO3
+0.929 CO2 +0.0714 CH4 +0.143 N2 <----> + CO +0.286 HNO3
+0.143 CO2 +0.571 HNO3 <----> +0.143 CH4 +0.286 N2 + O2
+0.357 CH4 +0.571 HNO3 <----> +0.357 CO2 +0.286 N2 + H2O
+0.643 CH4 +0.286 N2 +0.429 HNO3 <----> +0.643 CO2 + H3N
+0.0714 CO2 +0.357 N2 +0.286 HNO3 <----> +0.0714 CH4 + NO
+0.143 CO2 +0.214 N2 +0.571 HNO3 <----> +0.143 CH4 + NO2
+0.143 CH4 +0.429 HNO3 <----> +0.143 CO2 +0.214 N2 + OH
+0.214 CH4 +0.143 HNO3 <----> +0.214 CO2 +0.0714 N2 + H
+0.0714 CO2 +0.286 HNO3 <----> +0.0714 CH4 +0.143 N2 + O
+0.5 N2 <----> + N
+0.429 CH4 +0.286 HNO3 <----> + H2 +0.429 CO2 +0.143 N2
    
```

$$\frac{dm_T}{dt} = A_f \rho_u s_f = A_f \rho_u s_u (\eta + \chi)$$

$$\frac{dQ_r}{dt} = - \frac{\sigma A_f [T_b^4 - T_w^4]}{\frac{1}{\epsilon_b} + \left(\frac{A_f}{A_w}\right) \left(\frac{1}{\alpha_w} - 1\right)}$$

$$V_u \beta_u \frac{dT_u}{dt} + V_b \beta_b \frac{dT_b}{dt} - (V_u \kappa_u + V_b \kappa_b) \frac{dP}{dt} + \sum_i^r \bar{V}_{u_i} \frac{dN_i}{dt} + \sum_i^p \bar{V}_{b_i} \frac{dn_i}{dt} = 0$$

**In addition to measured explosion severity data, formation energies may be necessary and can be measured as needed**

<b>Chemical</b>	<b>Measured Heat of Combustion (MJ/kg) [BTU/lb]</b>	<b>CAS #</b>
Benzoic Acid	26.53 [11419.8]	65-85-0
Nicotinic Acid	22.09 [9506.43]	59-67-6
Lycopodium	30.64 [13183.1]	8023-70-9

The heat of formation can be calculated from a measured heat of combustion using an instrument such as the Parr 6200 calorimeter

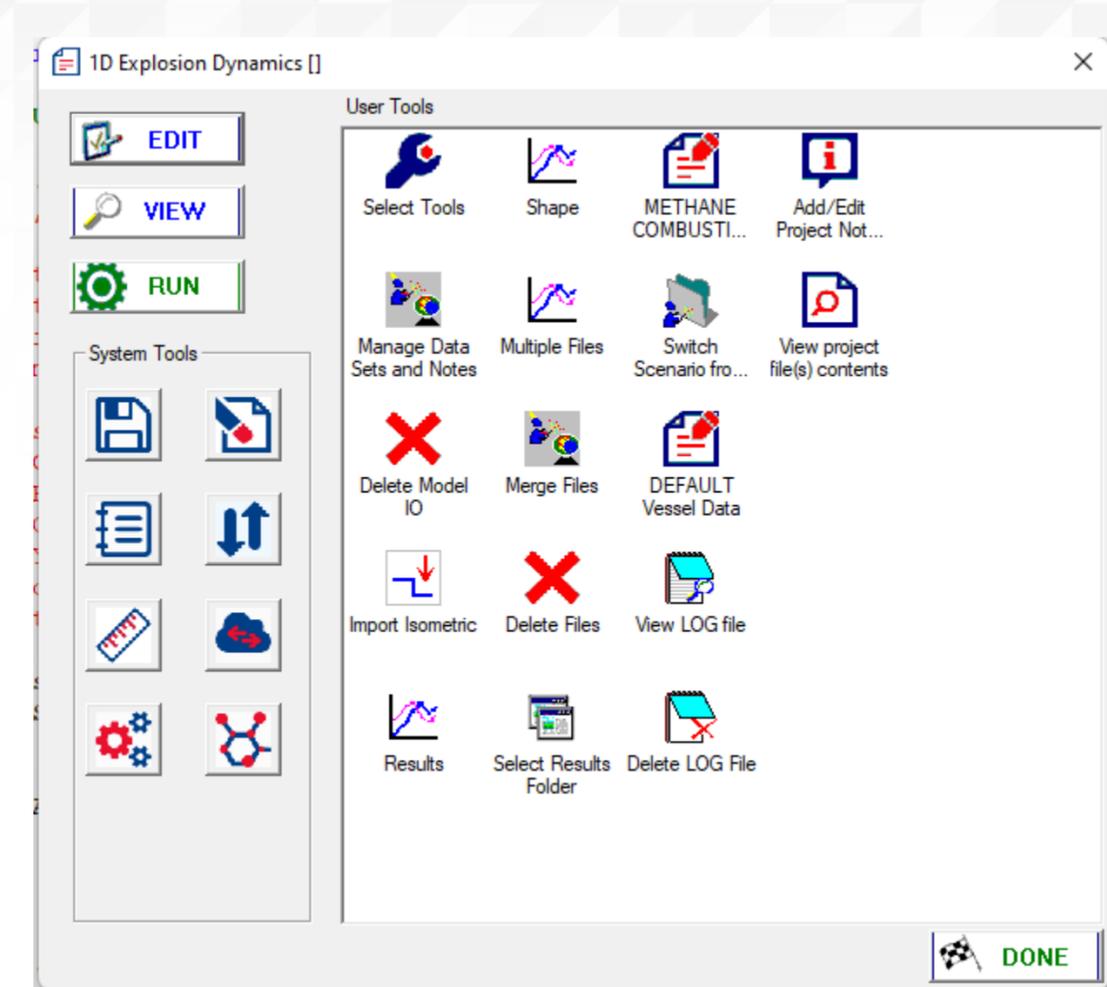


# Deflagration Dynamics Explosion Severity Data and Burning Rate Model Development



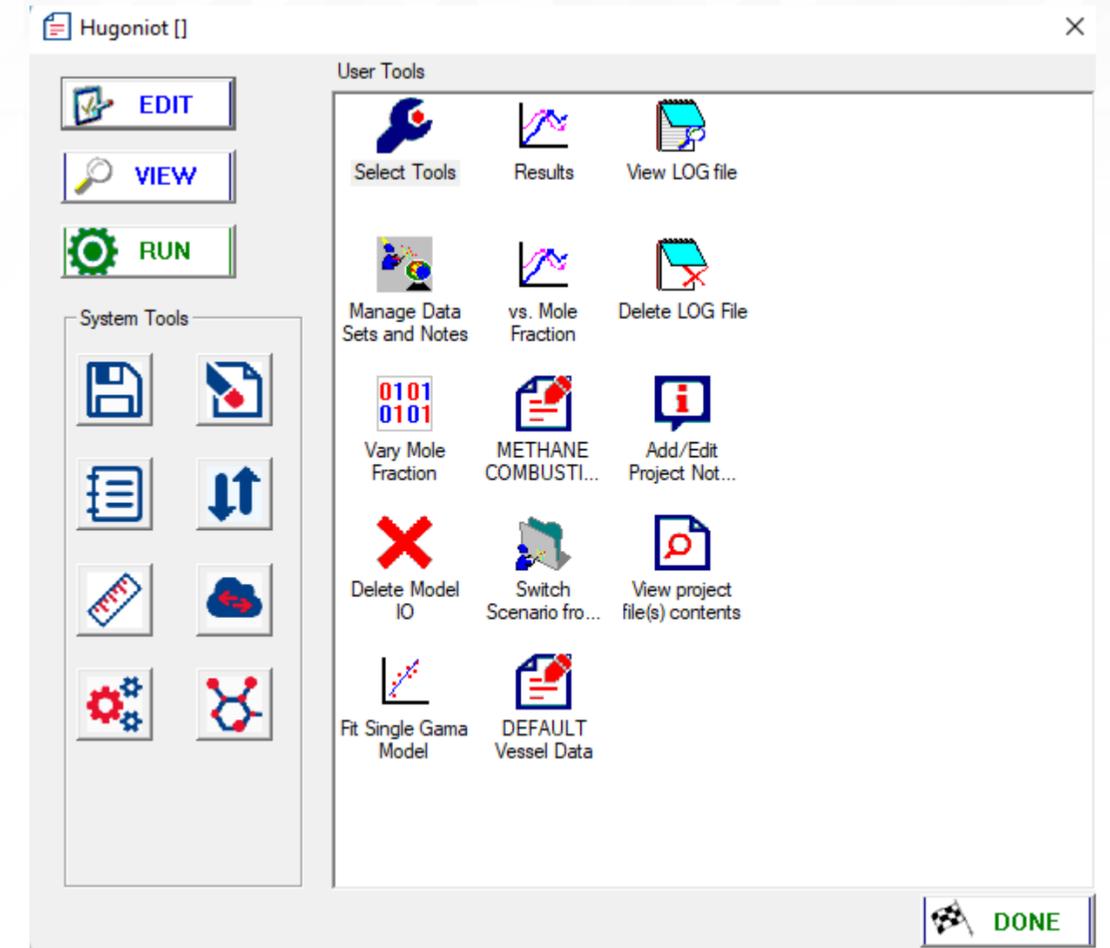
# Proper modeling of deflagration dynamics requires explosion severity data

- ▶ What is an explosion severity index?
- ▶ How do we measure the explosion severity index?
- ▶ How do we correlate explosion severity with burning rate?
- ▶ Explosion severity index testing apparatus
- ▶ Understanding Dust Explosions and Hazards
- ▶ Anatomy of deflagration venting dynamics
- ▶ Detailed modeling of deflagration venting dynamics
- ▶ Burning rate model development and fitting

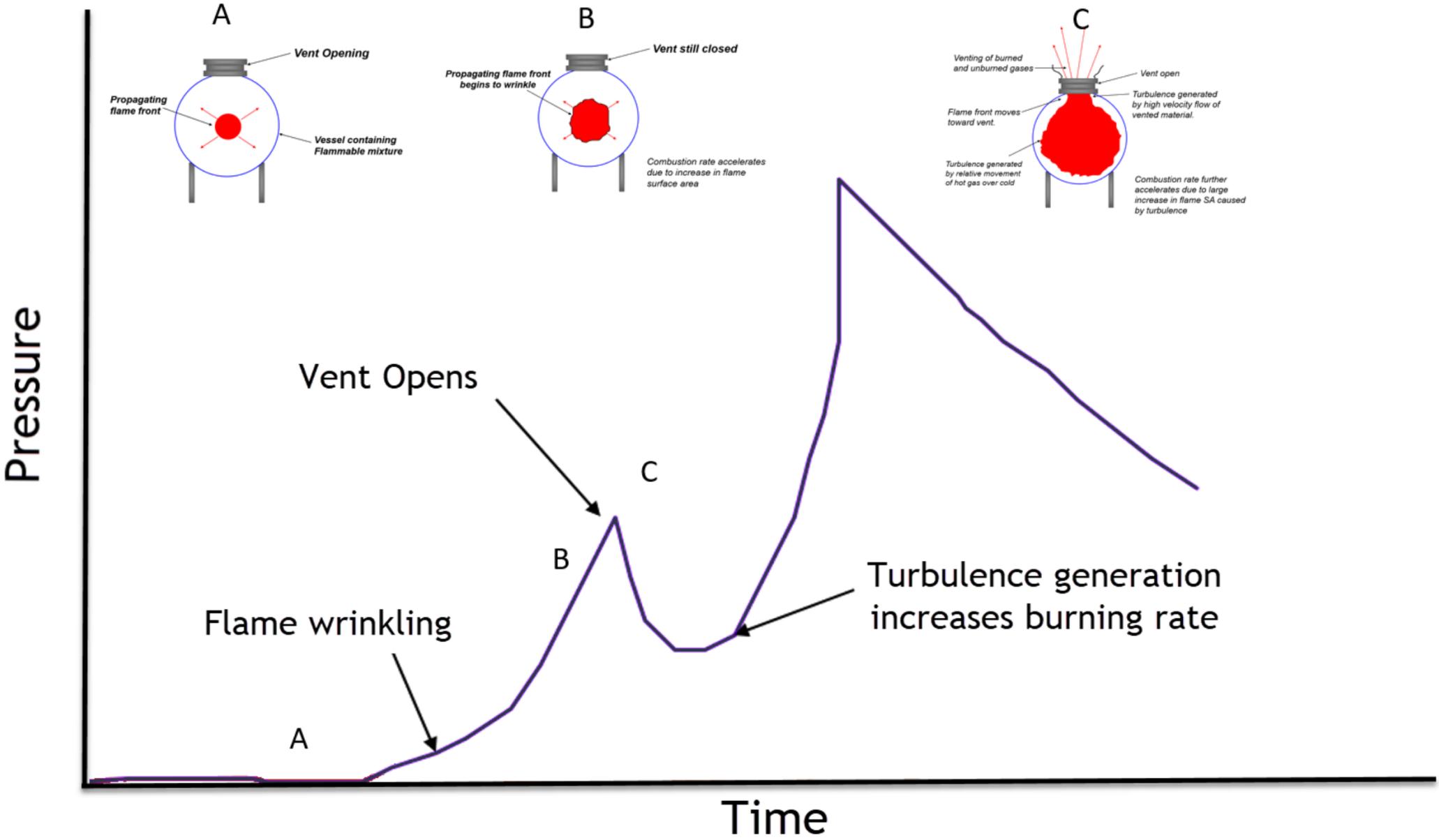
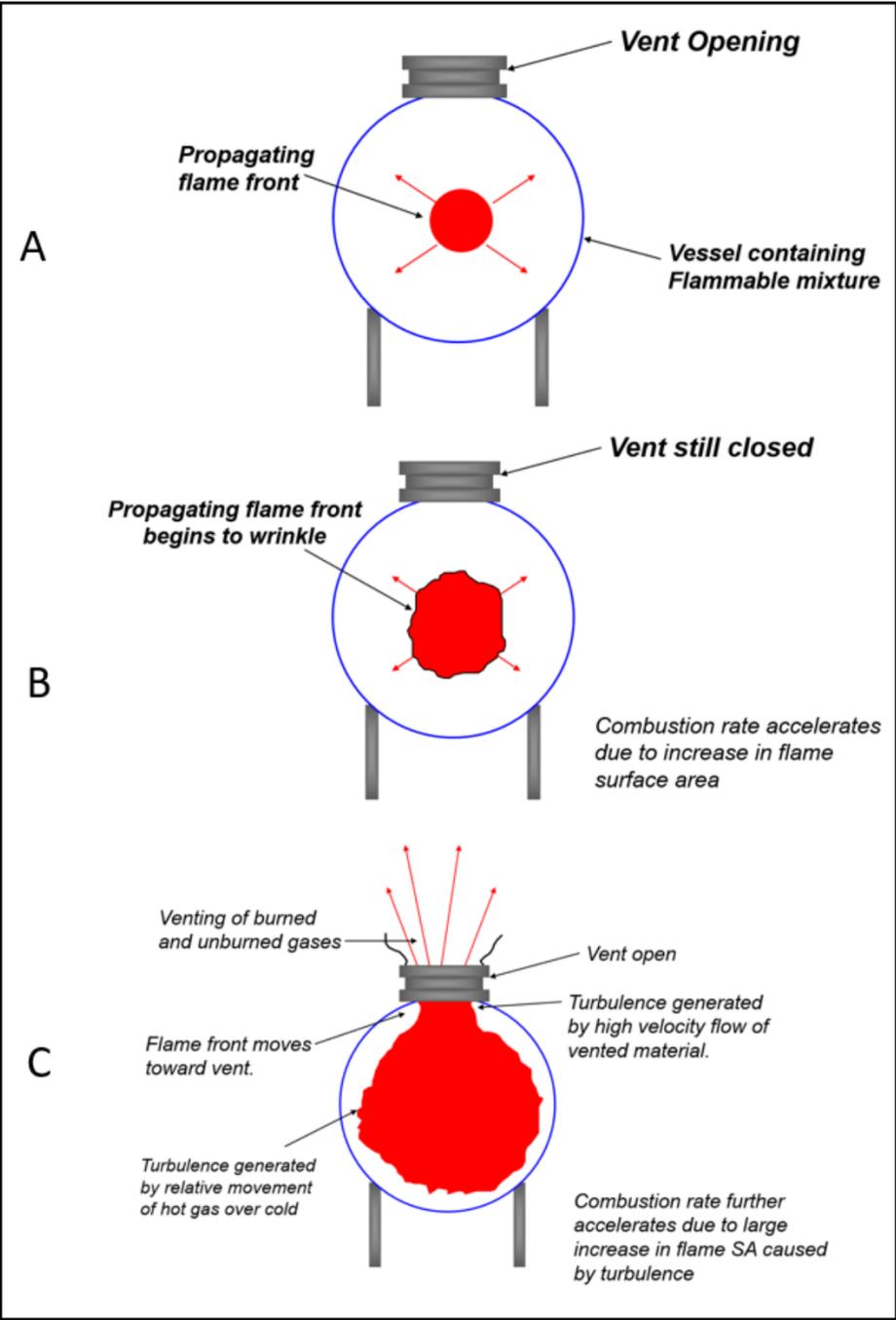


# Deflagration vent sizing is usually based on simple, semi-empirical formulas such as those provided by NFPA 68

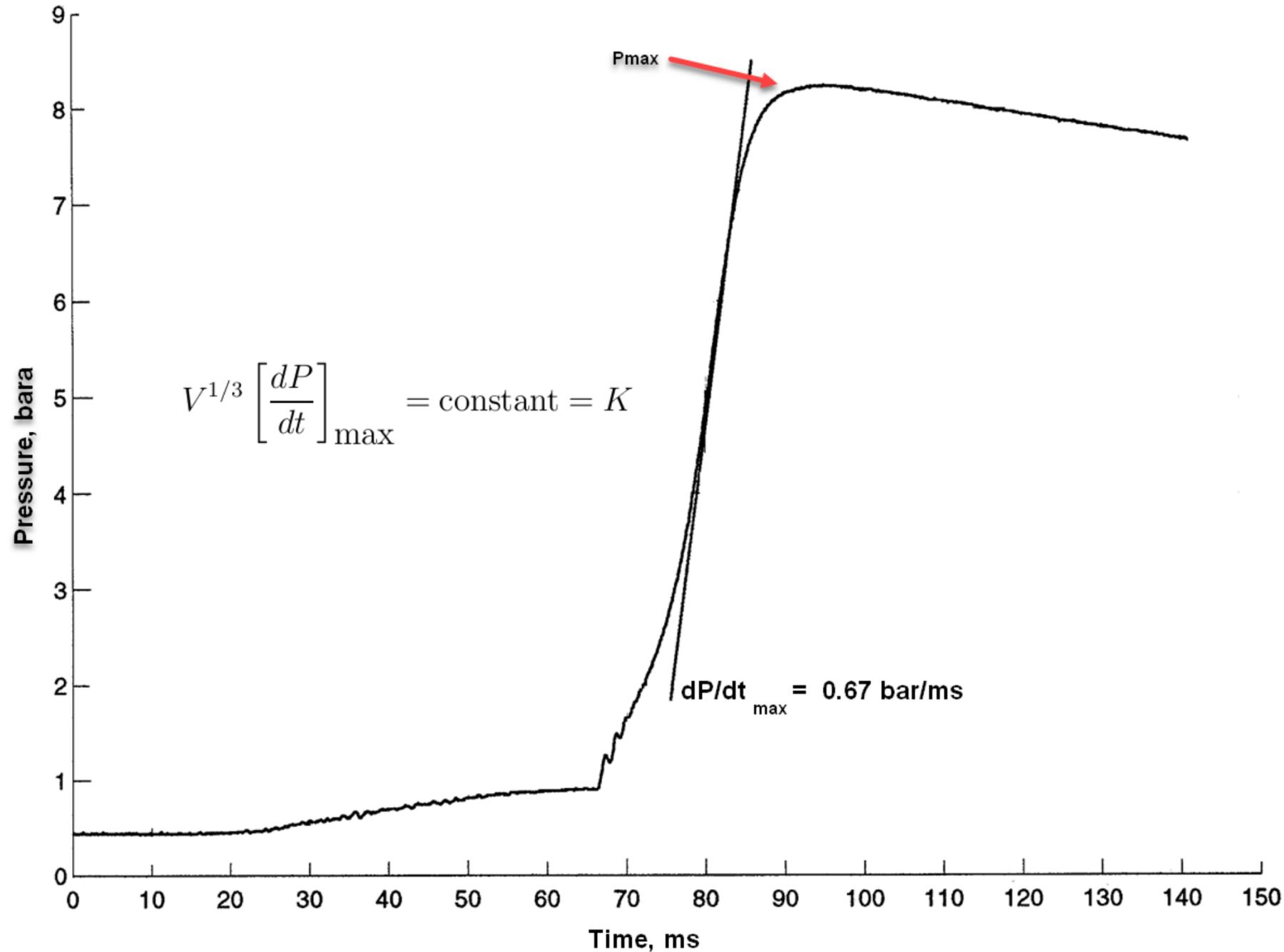
- ▶ Used by US and International Standards
- ▶ Applies to simple geometries with  $L/D < 5$
- ▶ Additional vent area is required for  $L/D > 5$
- ▶ Care must be exercised to avoid deflagration to detonation transitions (DDT)
- ▶ Methods exist for addressing vent panel inertia, reaction forces, safe discharge location, etc.
- ▶ One must read the fine print regarding applicability and limitations which makes these equations complex to apply at times



# The propagation of a deflagration depends on ignition location, strength of ignition/explosion, vent location, and overall geometry



# What is an explosion severity index?



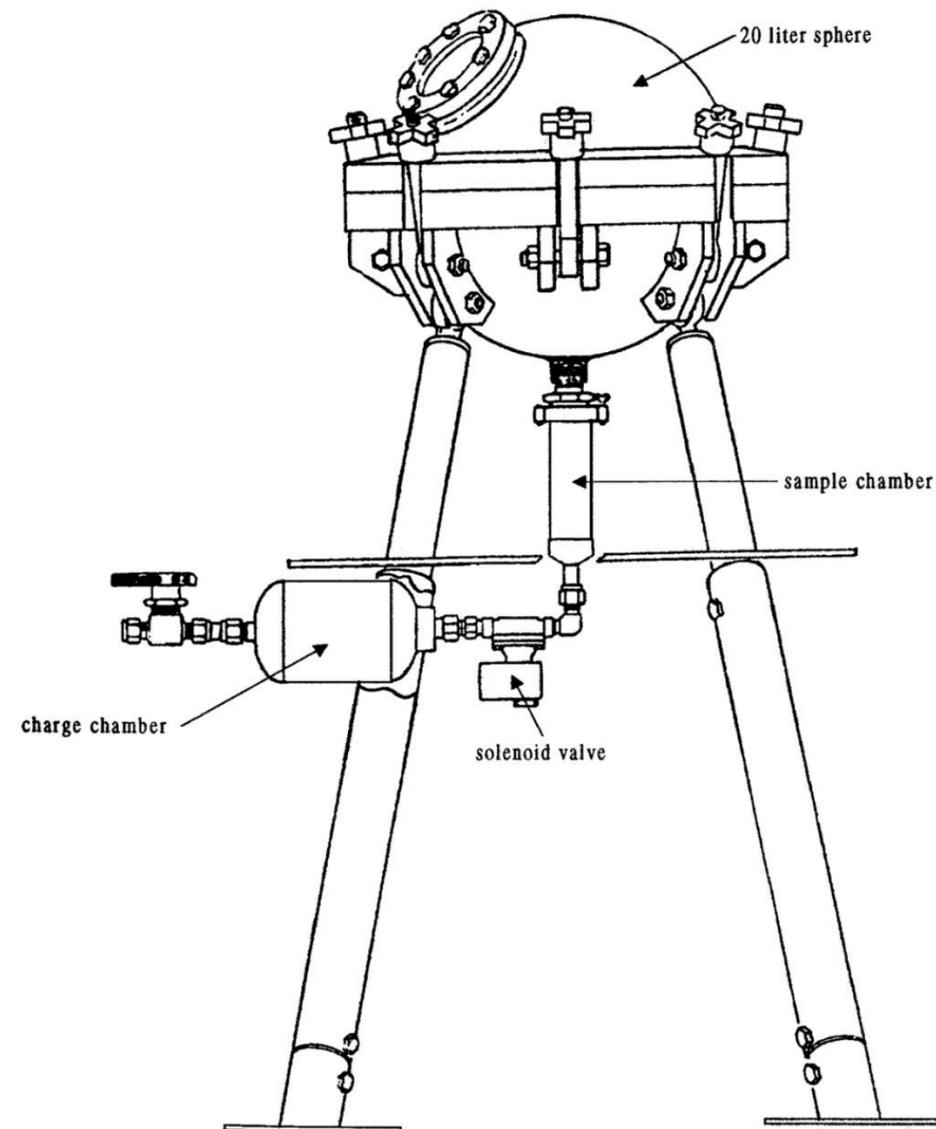
For many hydrocarbon fuel – air and dust – air deflagrations in vessels with low L/D ratios, the maximum deflagration pressure rise rate correlates with volume raised to the 1/3 power

$$\left[ \frac{dP}{dt} \right]_{\max} = \frac{K}{V^{1/3}}$$

# How do we measure the explosion severity index?

- ▶  $K_g$  or  $K_{st}$
- ▶  $P_{max}$ ,  $dP/dt_{max}$
- ▶ LEL, UEL
- ▶ LOC
- ▶ MIE
- ▶ Tests usually conducted with chemical igniters
- ▶ Starting pressure and temperature are usually 1 bar and 25 C

Deflagration explosion severity is usually measured in a 20-liter sphere



# The explosion severity index can also be measured in a 1 m<sup>3</sup> vessel

- ▶ The 20-liter sphere can overdrive the explosion due to the strength of the igniters, i.e., burns materials without flame propagation
- ▶ In some cases, the 100-liter sphere can underdrive the explosion due to heat loss to the walls of the sphere which can quench/temper the intensity of the deflagration
- ▶ Note that 7 to 15 kgs of sample is required for 1 m<sup>3</sup> testing
- ▶ Cost and availability of materials?
- ▶ Toxicity of combustion products?

CA 1M3 chamber



# How do we correlate the explosion severity index with burning rate?

The explosion severity index is directly related to the burning rate or rate of reaction

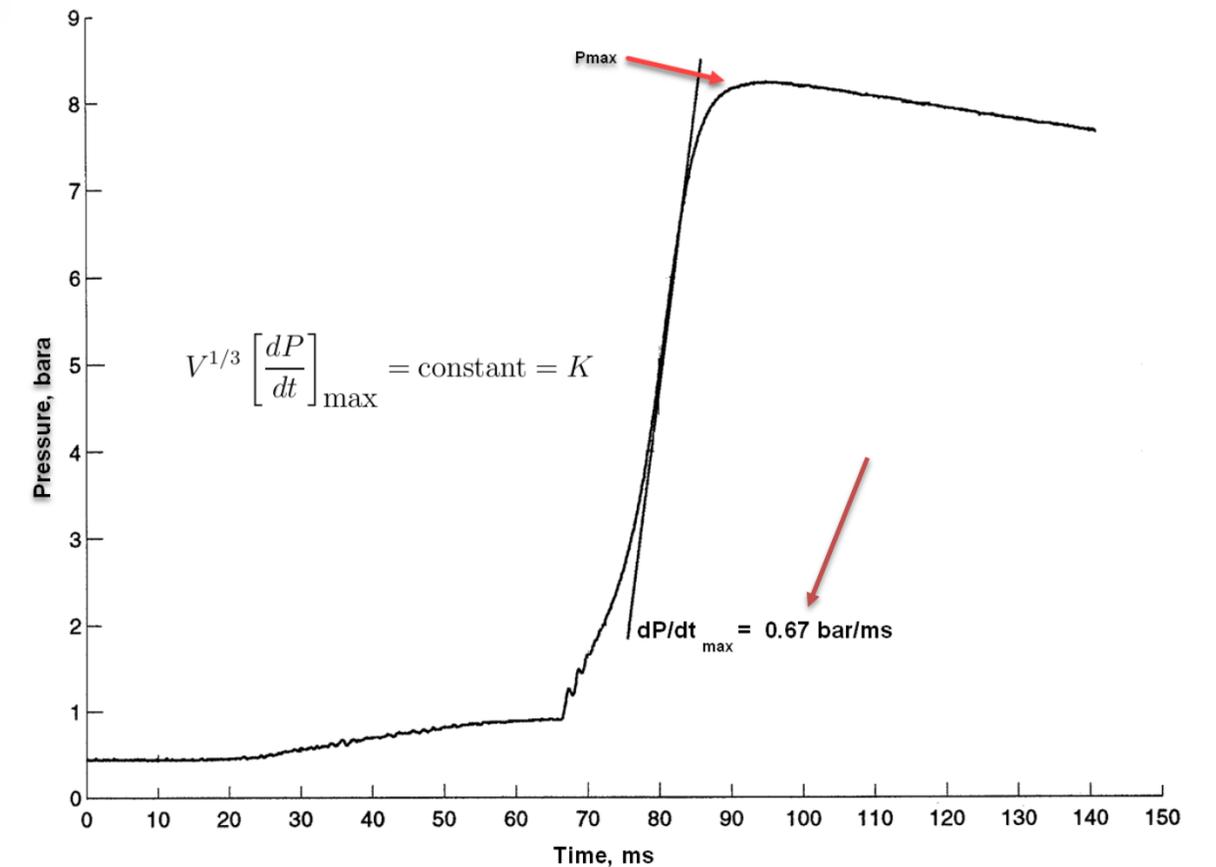
$$K = \left[ \frac{dP}{dt} \right]_{\max} V^{1/3} = (36\pi)^{1/3} (P_{max} - P_0) \left( \frac{P_{max}}{P_0} \right)^{1/\gamma_u} s_f$$

$$s_f = \left( \frac{20 \times 10^{-3}}{36\pi} \right)^{1/3} \left( \frac{1}{8.5} \right)^{1/1.4} \left( \frac{1}{8.5 - 1} \right) [670]$$

$$= 5.61 \times 10^{-2} \times 0.216 \times 0.133 \times 670 = 1.09 \text{ m/s}$$

$$s_{f2} = s_{f1} \left[ \frac{K_2}{K_1} \right] \left[ \frac{P_{max1} - P_0}{P_{max2} - P_0} \right] \left[ \frac{\left( \frac{P_{max1}}{P_0} \right)^{1/\gamma_{u1}}}{\left( \frac{P_{max2}}{P_0} \right)^{1/\gamma_{u2}}} \right]$$

$$\approx s_{f1} \left[ \frac{K_2}{K_1} \right]$$



The measured pressure-time data in a 20-liter sphere or 1 m<sup>3</sup> vessel can be used to develop a burning rate model

$$s_f = (\chi + \eta) s_u = (\chi + \eta) s_{u_o} \left[ \frac{T_u}{T_o} \right]^\alpha \left[ \frac{P}{P_o} \right]^\beta$$

$$\eta = \left( \frac{N_{Pr} N_{Re}}{N_{Pr_c} N_{Re_c}} \right)^\theta$$

Chemical	$s_{u_o}$ , m/s	$\alpha$	$\beta$	$\theta$
Methane	0.33	2.00	-0.25	0.40
Propane	0.32	2.13	-0.17	0.25
Pentane	0.50	1.60	-0.25	0.39
Acetylene	1.58	2.00	-0.06	0.39
Hydrogen	3.50	1.26	0.26	0.39
Methanol	0.37	2.18	-0.16	0.39
isoOctane	0.26	2.18	-0.16	0.39

# Final Thoughts and Conclusions



# The SuperChems dynamic explosion models provide significant advantages over static and simplified methods

- The explosion models' updates are available in SuperChems Expert v11.0
- Extend the use of limited measured data to elevated temperatures, elevated pressures, different compositions, hybrid systems, and systems with diluents and/or chemical oxidizers
- Determine the composition of the vented material(s)
- Reduce venting requirements with lower relief device set points
- Consider flame acceleration, pressure pileup, and complex geometries

# Contact us to learn more about how we can help

**Georges A. Melhem, Ph.D., FAIChE**

President and CEO

[melhem@iomosaic.com](mailto:melhem@iomosaic.com)



# Suggested Additional Reading

1. G. A. Melhem, “Quantify explosion venting dynamics in vessels, enclosures, and energy storage systems”, ioMosaic Corporation White Paper, December 2021.
2. G. A. Melhem, “Development of reduced analytical models for explosion dynamics”, ioMosaic Corporation White Paper, January 2022.
3. G. A. Melhem, “Proper calculations of pipe and vessel wall temperatures during relief and/or depressurization”, In 78th API Fall Refining and Equipment Standards Meeting, pages 221–226, November 2013.
4. G. A. Melhem, “Get the most out of your deflagration test data - dusts, gases, and hybrid systems”, In DIERS Users Group Meeting, AIChE, Spring 2007.
5. G. A. Melhem, “Calculate phase and chemical equilibria using Process Safety Office® Superchems Expert™. ioMosaic Corporation White Paper, 2021.
6. J. Shepherd, G. A. Melhem, and P. Athens, “Unconfined vapor cloud explosions: A new perspective”, In International Conference and Workshop on Modeling. AIChE/CCPS, 1991.
7. G. A. Melhem, “An overview of explosion modeling for facility siting”, In DIERS Users Group Meeting, AIChE, October 2010.
8. G. A. Melhem, R. Saini, and B. M. Goodwin, “Computation of complex equilibria by direct minimization of the Gibbs free energy”, AIChE, 1989 Spring National Meeting and Petrochemical Expo, 1989.
9. G. A. Melhem, “A detailed method for the estimation of mixture flammability limits using chemical equilibrium”, Process Safety Progress, 16(4), 1997.

# 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.

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.

For more information on ioMosaic, please visit: [www.ioMosaic.com](http://www.ioMosaic.com)