JOINT EUROPEAN SUMMER SCHOOL ON FUEL CELL
AND HYDROGEN TECHNOLOGIES

THE SAFETY OF HYDROGEN TECHNOLOGIES

MITIGATION OF HYDROGEN DEFLAGRATIONS

Dr A.E. Dahoe

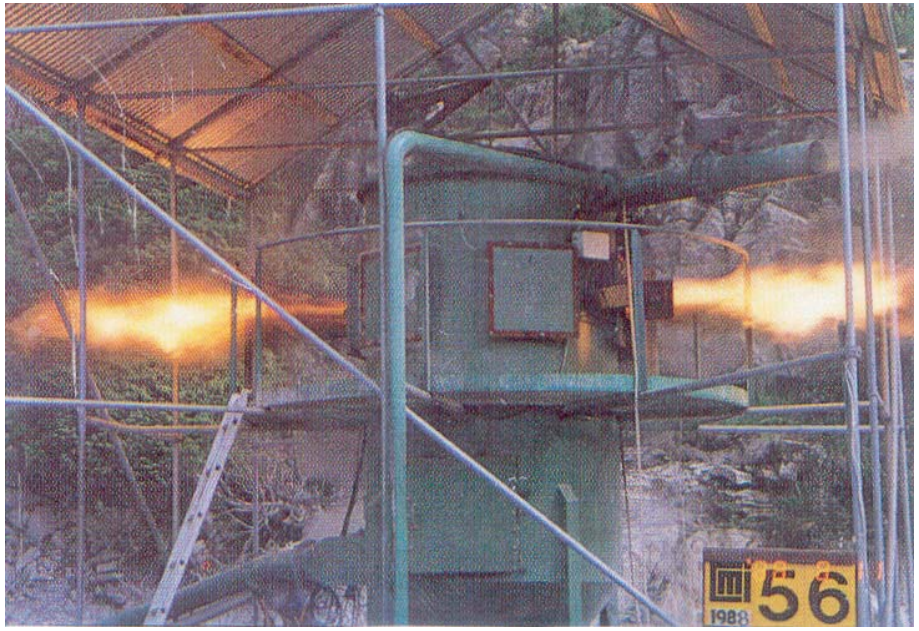
University of Ulster, United Kingdom

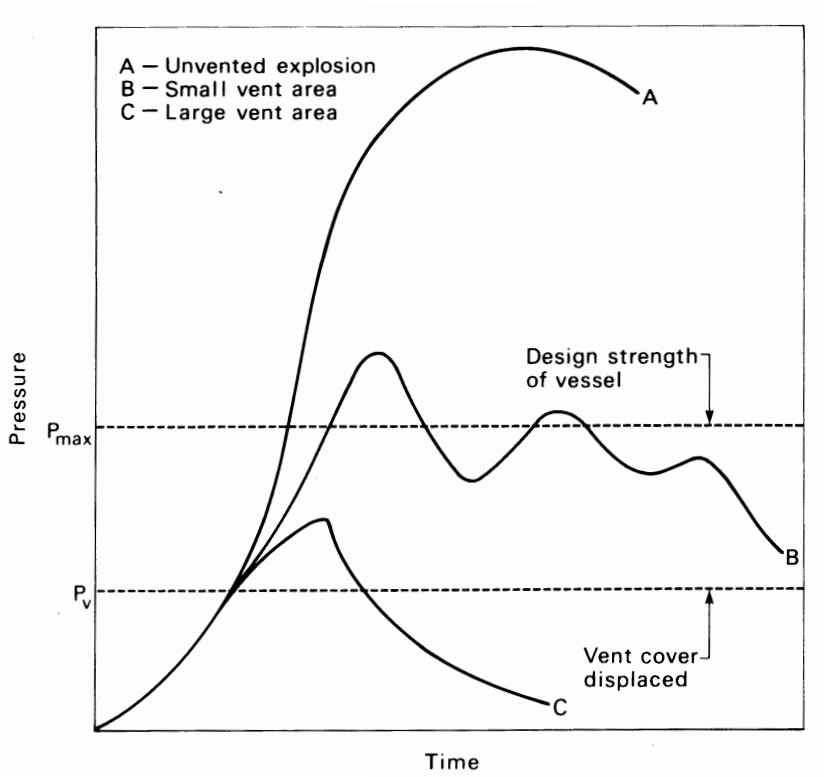
MITIGATION STRATEGIES

- **INERTISATION**
- **FLAME QUENCHING**

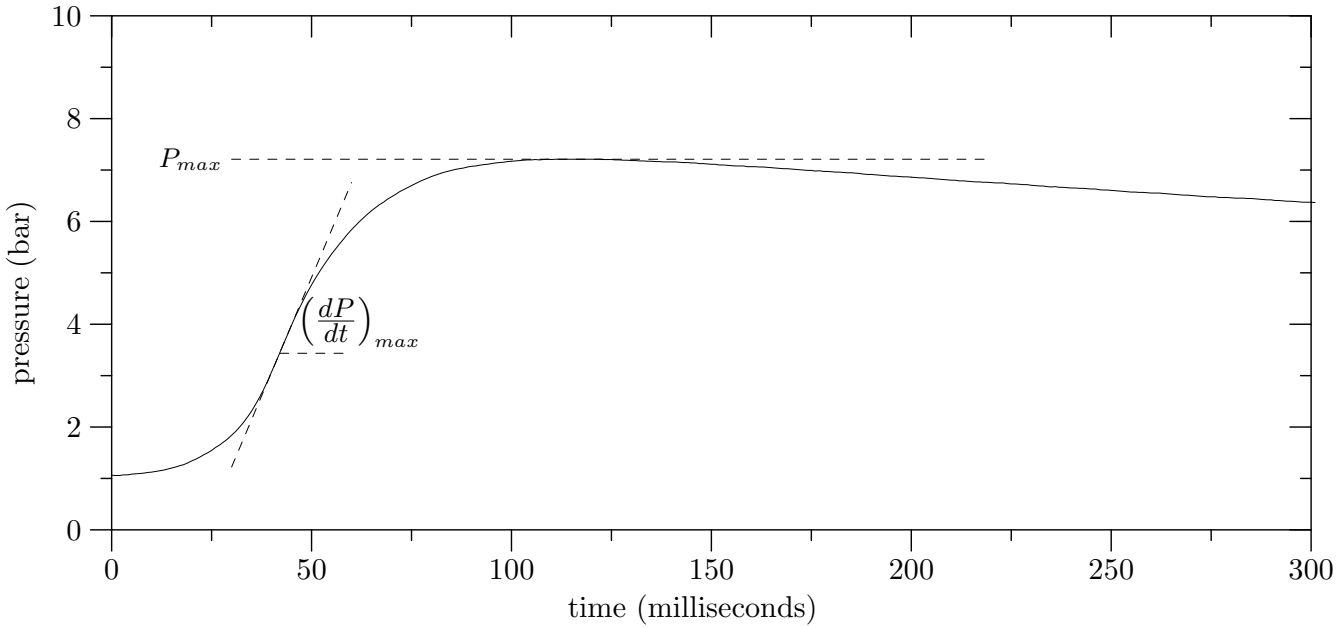
$\Longrightarrow$ **PRESSURE RELIEF VENTING**

The basic idea behind pressure relief venting



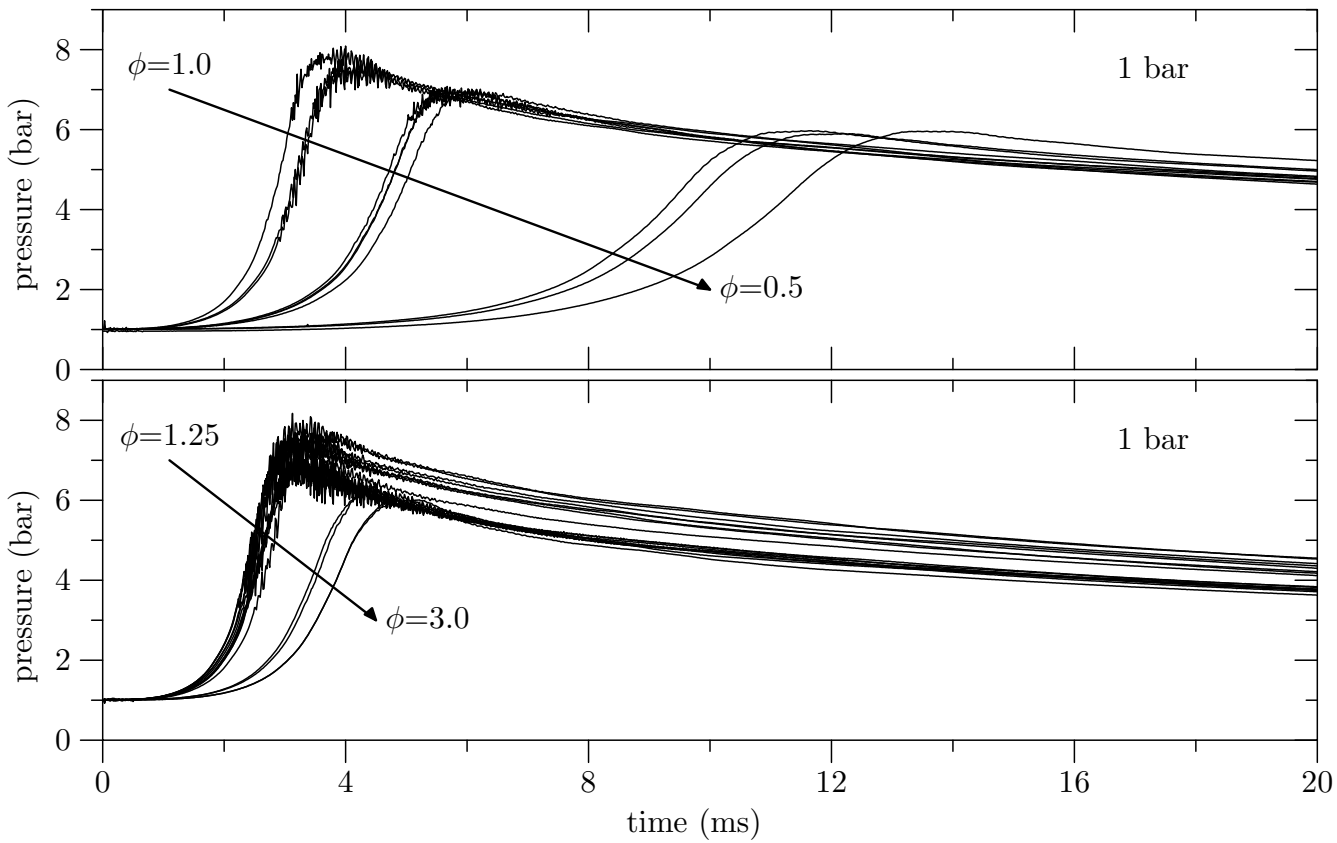


Deflagration parameters



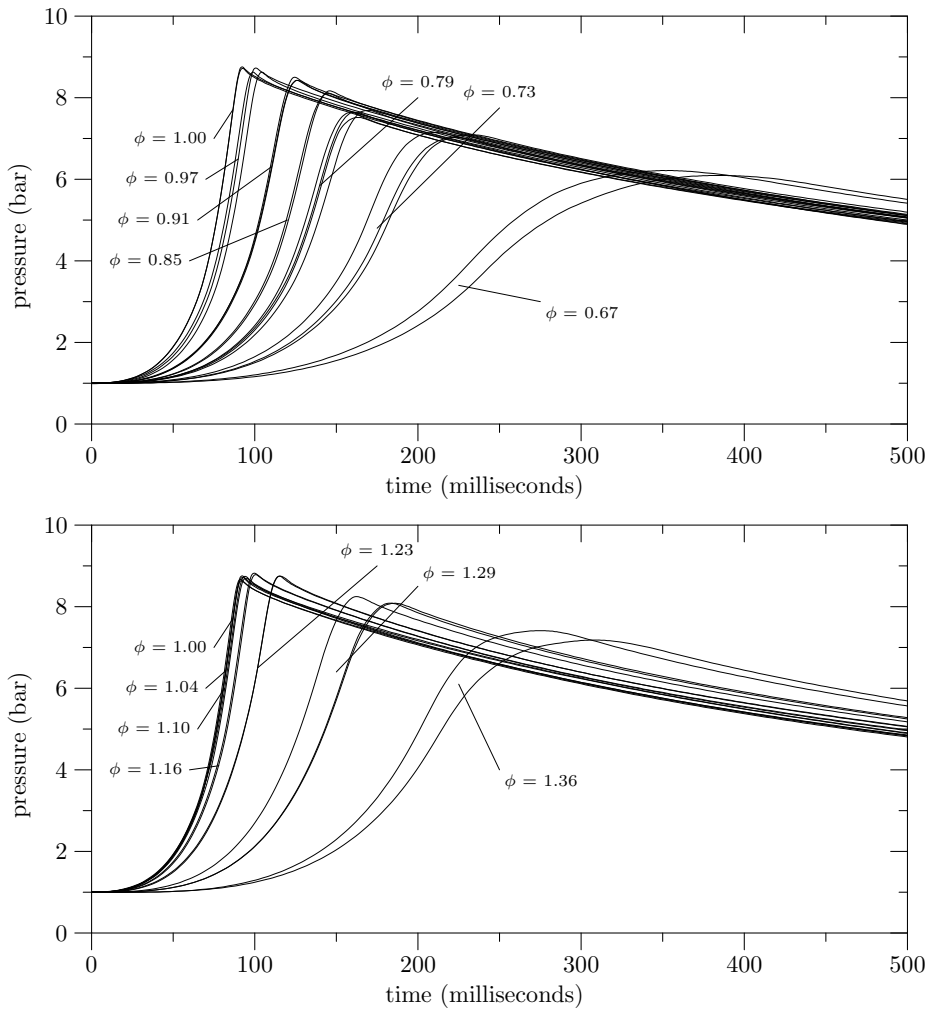
$$n_0\text{Reactants} \longrightarrow n_p\text{Products} \qquad \Longrightarrow \qquad P_{\max} = \frac{n_p}{n_0}\frac{T_f}{T_0}P_0$$

Deflagration parameters



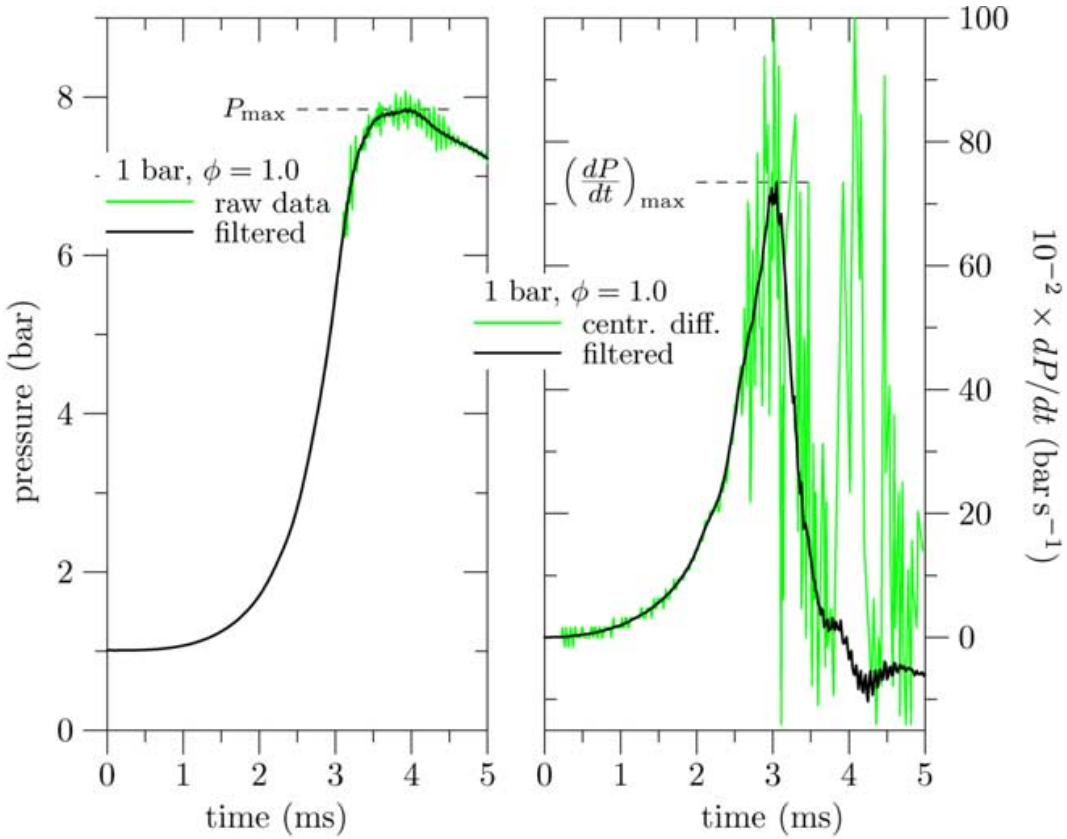
Experimental deflagration pressure curves of hydrogen-air mixtures at initial conditions T_0=298.15 K and P_0=1 bar.

Deflagration parameters



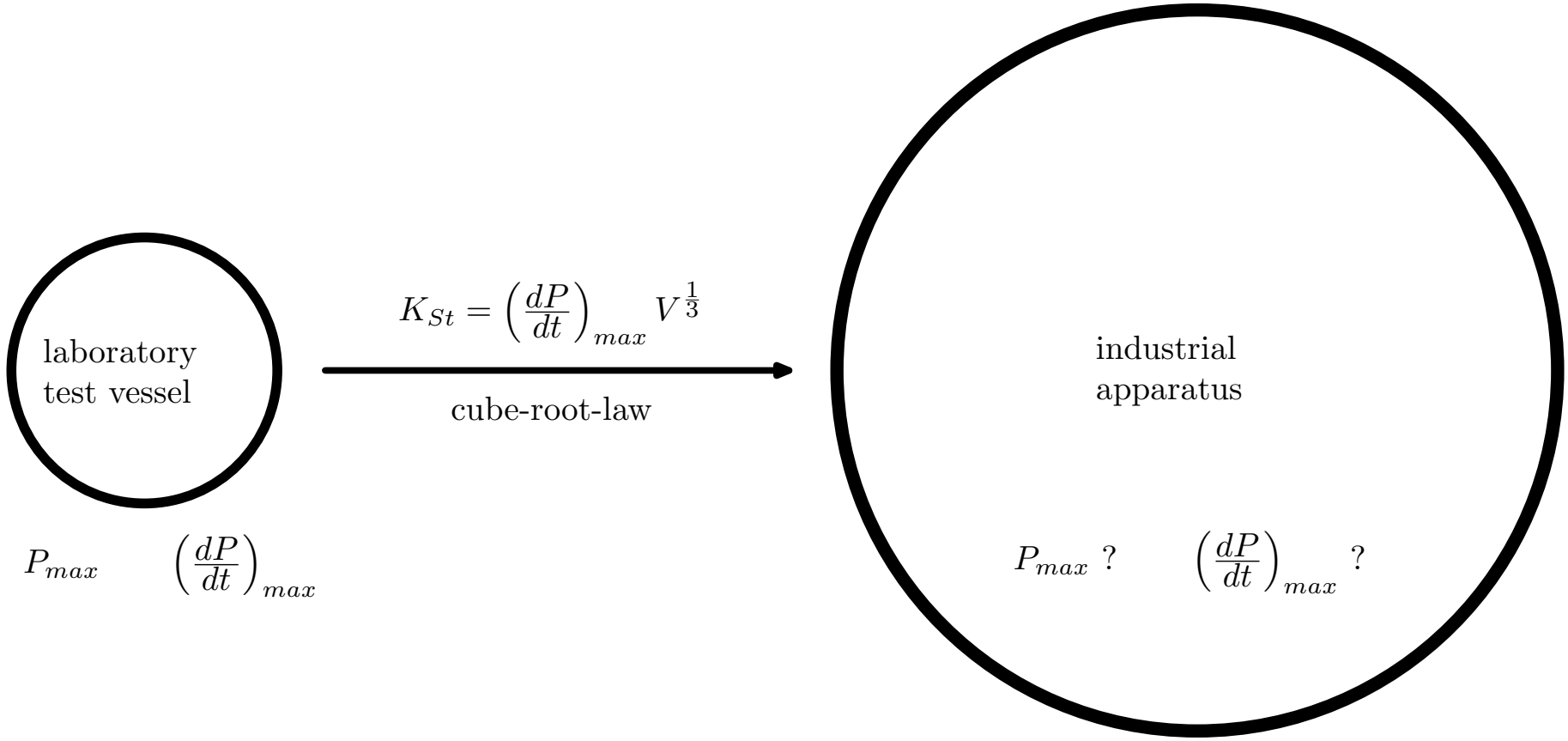
Experimental deflagration pressure curves of methane-air mixtures at initial conditions T_0=298.15 K and P_0=1 bar.

Deflagration parameters

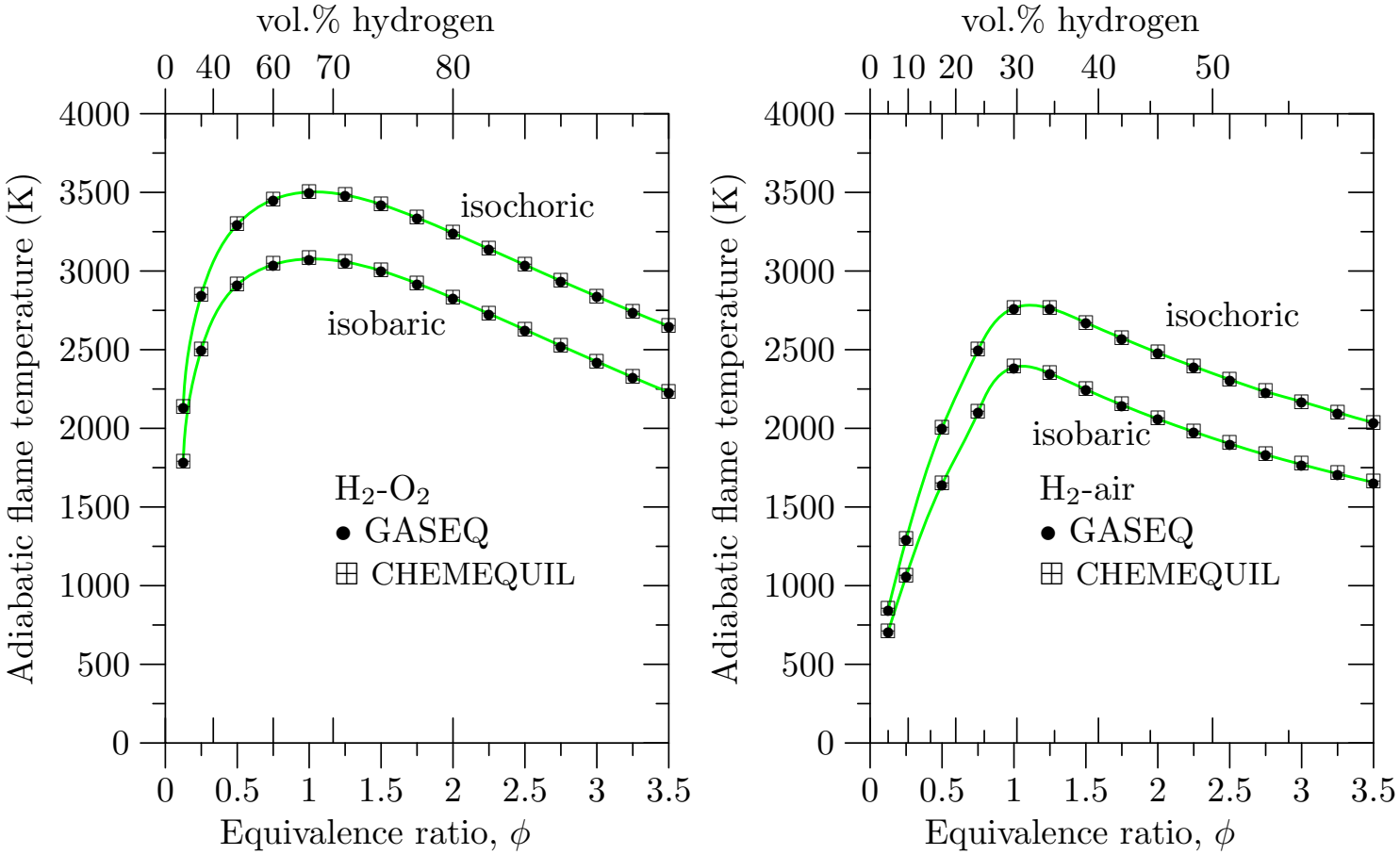


Determination of explosion parameters from experimental deflagration pressure curves.

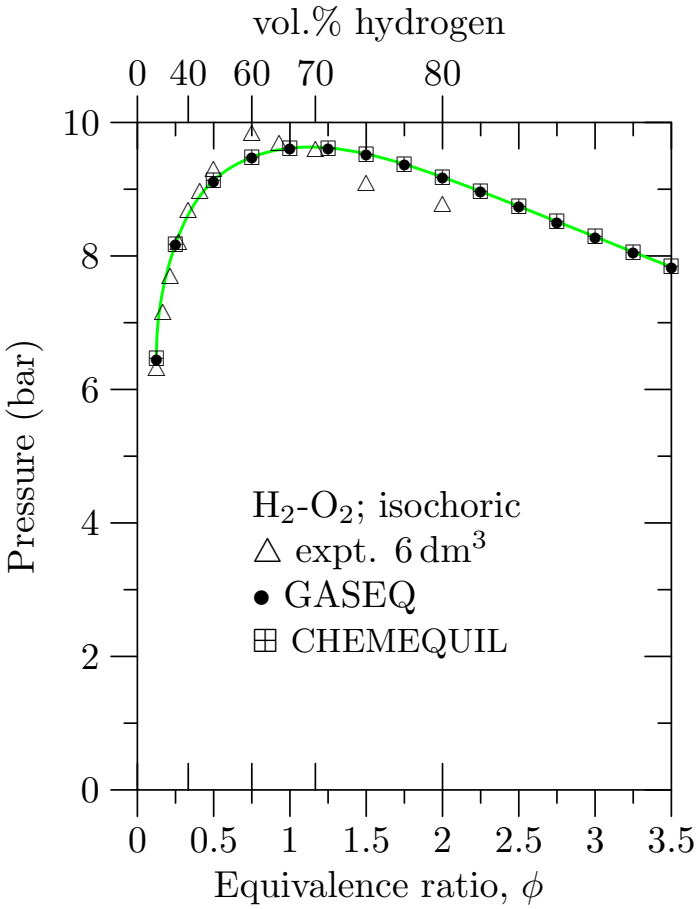
Scaling an explosion: a matter of invariance across size?

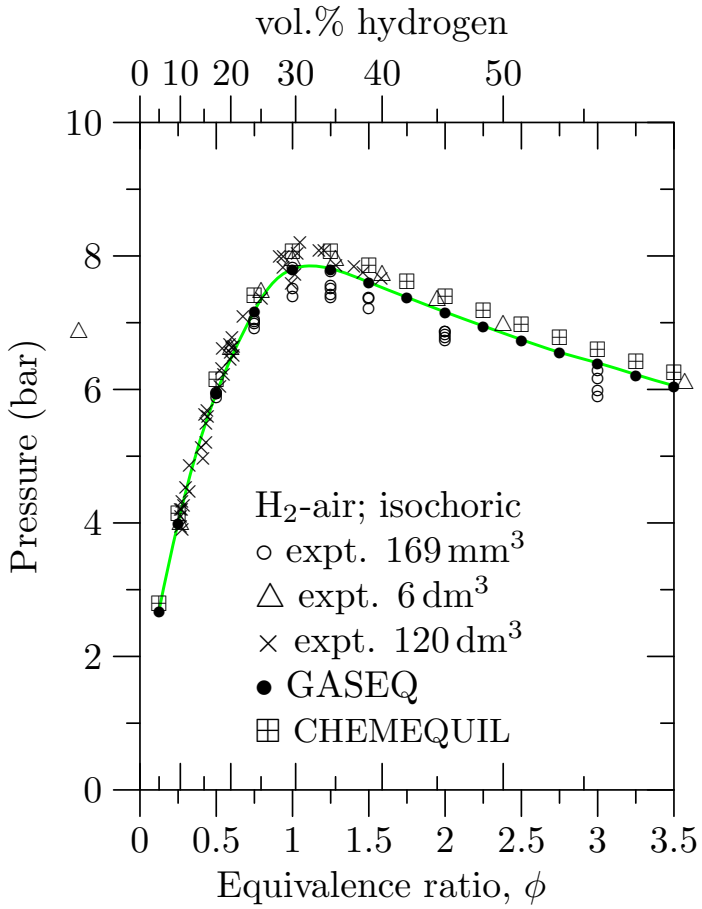


Scaling an explosion: a matter of invariance across size?

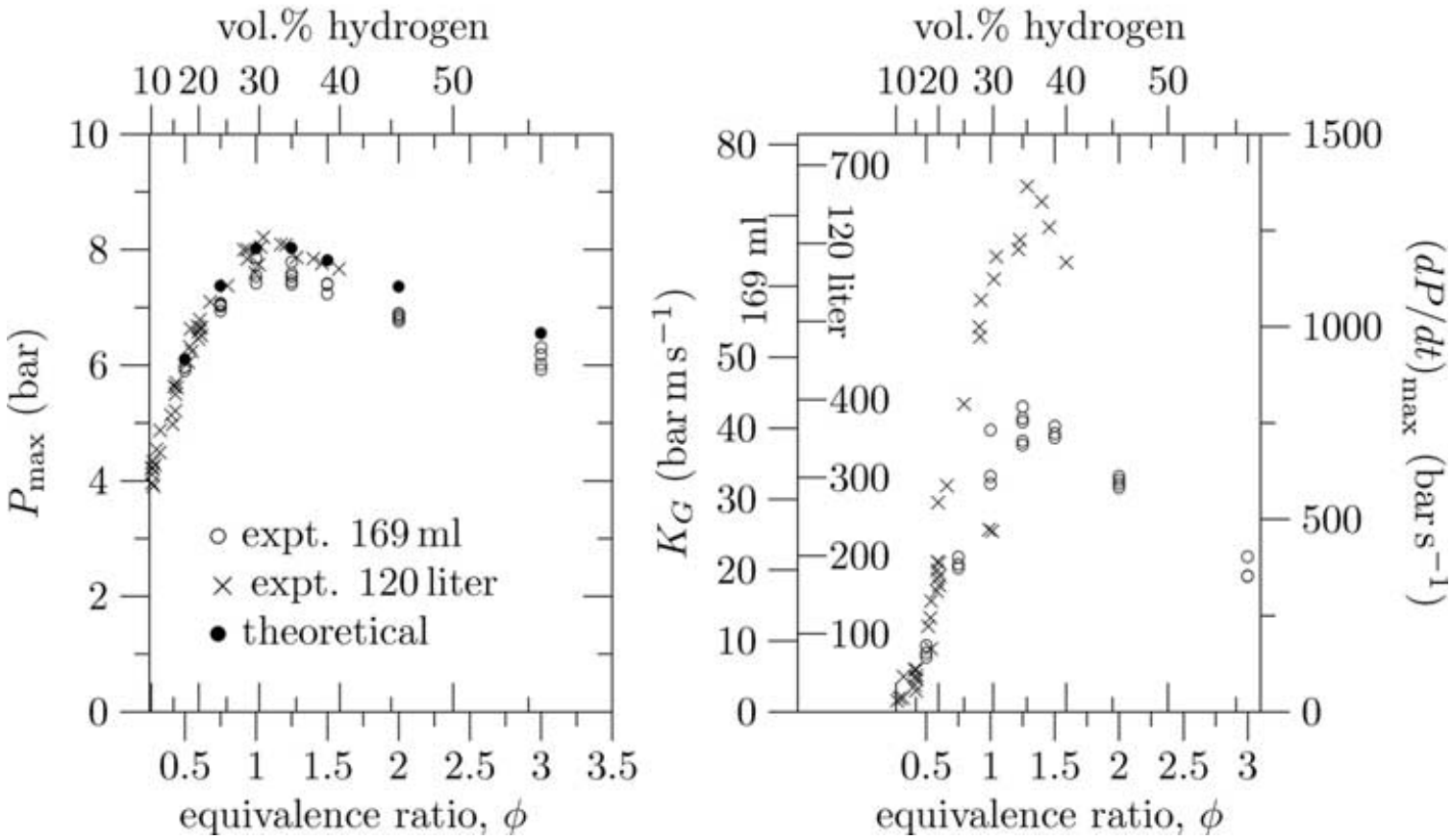


Scaling an explosion: a matter of invariance across size?





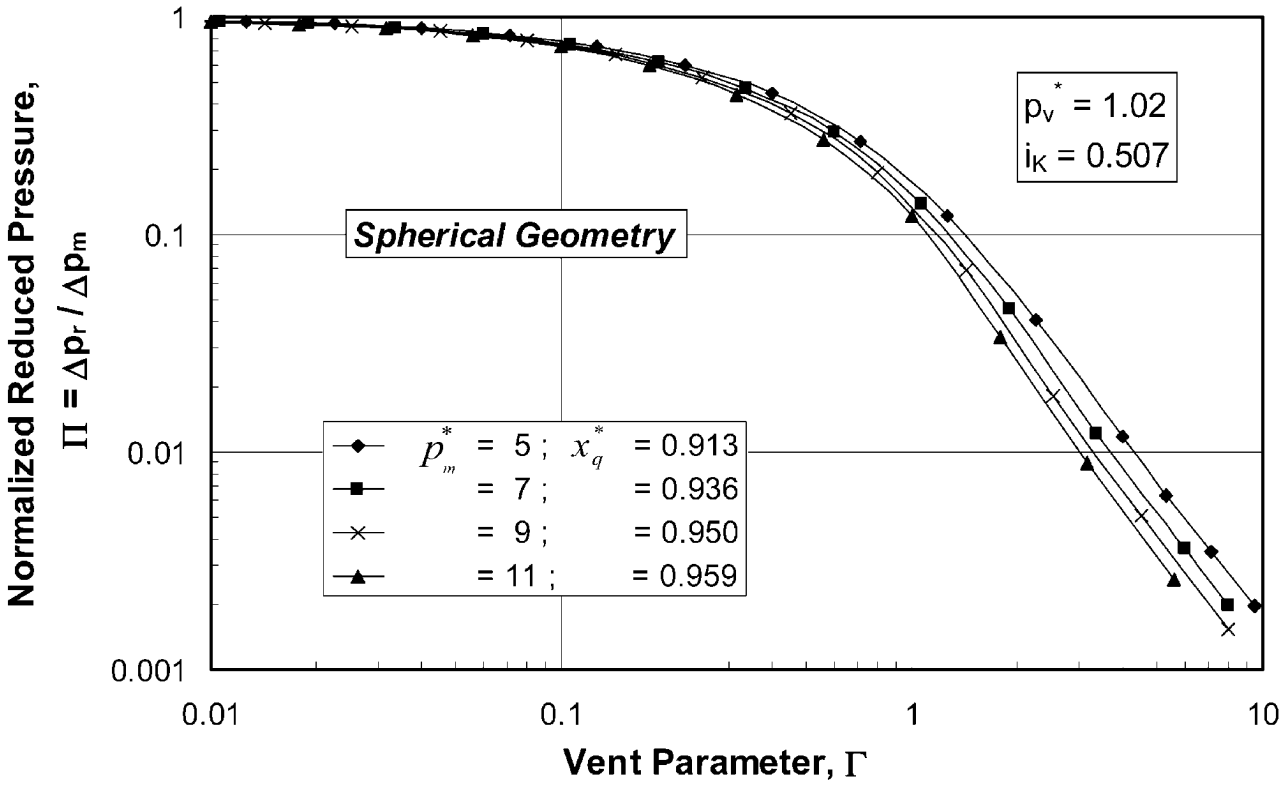
Scaling an explosion: a matter of invariance across size?



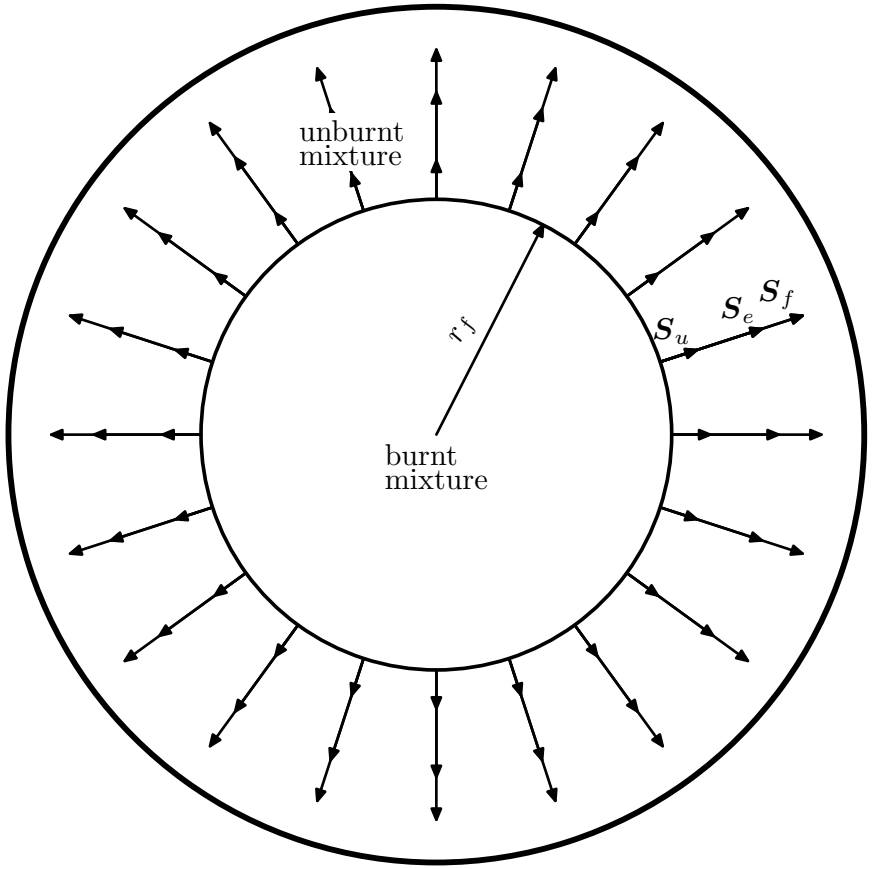
Application of deflagration parameters to vented explosions

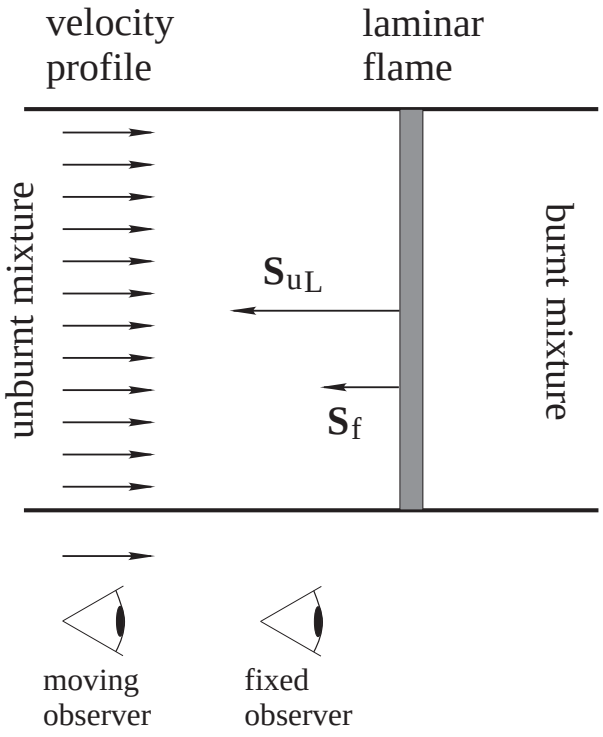
Tamanini H. Scaling parameters for vented gas and dust explosions. Journal of Loss Prevention in the Process Industries, 14:455–461, 2001.

$$\text{Define} \qquad \Pi = \frac{P - P_0}{P_{max} - P_0} \qquad \text{and} \qquad \Gamma = C_d c_u \sqrt{\frac{\gamma + 1}{2}} \frac{A_v}{V^{2/3}} \frac{P_{max} - P_0}{K_G}$$



Derivation of a simple deflagration model





Derivation of a simple deflagration model

Objective:
Find a dynamic equation to predict the pressure evolution

Approximate expression Lewis and von Elbe which relates the mass fraction of burnt mixture in the vessel to the fractional pressure rise:

$$\frac{m_u}{m_{u0}} = \frac{P_{max} - P}{P_{max} - P_0} \tag{1}$$

Differentiation with respect to time:

$$\frac{dP}{dt} = -\frac{P_{max} - P_0}{m_{u0}} \frac{dm_u}{dt} \tag{2}$$

The mass consumption rate of the unburnt mixture can be expressed as

$$\frac{dm_u}{dt} = -4\pi r_f^2 \rho_u S_u \tag{3}$$

The combustion wave moves with a velocity that is the sum of the expansion velocity, S_e, the conversion velocity, S_n, and the burning velocity S_u. Since the unburnt mixture immediately ahead of the flame front moves with velocity $S_e + S_n$, the velocity at which the unburnt mixture enters the combustion wave is minus the burning velocity. Therefore, the mass consumption rate of the unburnt mixture can be expressed as

$$\frac{dm_u}{dt} = -4\pi r_f^2 \rho_u S_u \tag{4}$$

A relationship can be established between the rate of pressure rise and the burning velocity. By substitution of equation (4) into equation (2):

$$\frac{dP}{dt} = 4\pi \frac{P_{max} - P_0}{m_{u0}} r_f^2 \rho_u S_u \tag{5}$$

Derivation of a simple deflagration model

The next step is to express the density of the unburnt mixture, ρ_u, and the location of the flame front, r_f, in terms of known variables. For adiabatic compression of the unburnt mixture, $P\rho^{-\gamma} =$ constant and hence

$$\frac{\rho_{u0}}{\rho_u} = \left(\frac{P_0}{P}\right)^{\frac{1}{\gamma}} \tag{6}$$

Furthermore, $V_b = V_{vessel} - V_u$, which can be rewritten as

$$\frac{4}{3}\pi r_f^3 = V_{vessel} - \frac{m_u R T_u}{P} \tag{7}$$

Since $\rho^{-1} = \hat{\mathrm{R}}T/P$ where $\hat{\mathrm{R}}$ denotes the specific gas constant in $\mathrm{J\,kg^{-1}\,K^{-1}}$, the volume of the unburnt mixture can be expressed as

$$\begin{aligned} \frac{m_u \hat{\mathrm{R}} T_u}{P} &= V_{vessel}\rho_{u0}\frac{P_{max} - P}{P_{max} - P_0}\rho_u^{-1} = V_{vessel}\left(\frac{\rho_{u0}}{\rho_u}\right)\frac{P_{max} - P}{P_{max} - P_0} \\ &= V_{vessel}\left(\frac{P_0}{P}\right)^{\frac{1}{\gamma}}\frac{P_{max} - P}{P_{max} - P_0} \end{aligned} \tag{8}$$

and equation (7) yields the following expression for the location of the flame front:

$$r_f = R_{vessel}\left[1 - \left(\frac{P_0}{P}\right)^{\frac{1}{\gamma}}\frac{P_{max} - P}{P_{max} - P_0}\right]^{\frac{1}{3}} \tag{9}$$

Derivation of a simple deflagration model

By inserting equations (9) and (6) into equation (5) and by noting that $m_{u0} = \rho_{u0} V_{vessel}$, the following ordinary differential equation is obtained for the rate of pressure rise:

$$\frac{dP}{dt} = \frac{3\left(P_{max} - P_0\right)}{R_{vessel}} \left[1 - \left(\frac{P_0}{P}\right)^{\frac{1}{\gamma}} \frac{P_{max} - P}{P_{max} - P_0}\right]^{\frac{2}{3}} \left(\frac{P}{P_0}\right)^{\frac{1}{\gamma}} S_u \tag{10}$$

From equation (10) it can be seen that (dP/dt) increases monotonically with P and hence the maximum rate of pressure rise is attained when $P = P_{max}$. By substituting $P = P_{max}$ into equation (10) and multiplying both sides by the cube root of the vessel volume, the following expression is found for the K_G-value:

$$\boxed{K_G = \left(\frac{dP}{dt}\right) V^{1/3} = (36\pi)^{1/3}(P_{max} - P_0)\left(\frac{P_{max}}{P_0}\right)^{\frac{1}{\gamma}} S_u} \tag{11}$$

which is a normalization of the maximum rate of pressure rise with respect to the vessel volume.

Derivation of a vented deflagration model

Bradley D. and Mitcheson A. The venting of gaseous explosions in spherical vessels. I - Theory. Combustion and Flame, 32:221-236, 1978.
Bradley D. and Mitcheson A. The venting of gaseous explosions in spherical vessels. II - Theory and experiment. Combustion and Flame, 32:237-255, 1978.

Model developed for centrally ignited fuel-air mixtures in a spherical vessel with vent flow expressions for the rate of change in the mass of unburnt mixture:

$$\frac{dm_u}{dt} = \begin{cases} -4\pi r_f^2 \rho_u S_u - C_d A_v \rho \left[\frac{\gamma P}{\rho} \left(\frac{\gamma+1}{2} \right)^{\frac{1+\gamma}{1-\gamma}} \right]^{1/2} & \text{if} \quad \frac{P_a}{P} \leq \left(\frac{2}{\gamma+1} \right)^{\frac{\gamma}{\gamma-1}} \quad \text{(sonic)} \\ -4\pi r_f^2 \rho_u S_u - C_d A_v \left\{ \frac{2\gamma P \rho}{\gamma-1} \left(\frac{P_a}{P} \right)^{\frac{2}{\gamma}} \left[1 - \left(\frac{P_a}{P} \right)^{\frac{\gamma-1}{\gamma}} \right]^{\frac{1+\gamma}{1-\gamma}} \right\}^{1/2} & \text{if} \quad \frac{P_a}{P} > \left(\frac{2}{\gamma+1} \right)^{\frac{\gamma}{\gamma-1}} \quad \text{(sub-sonic)} \end{cases} \tag{12}$$

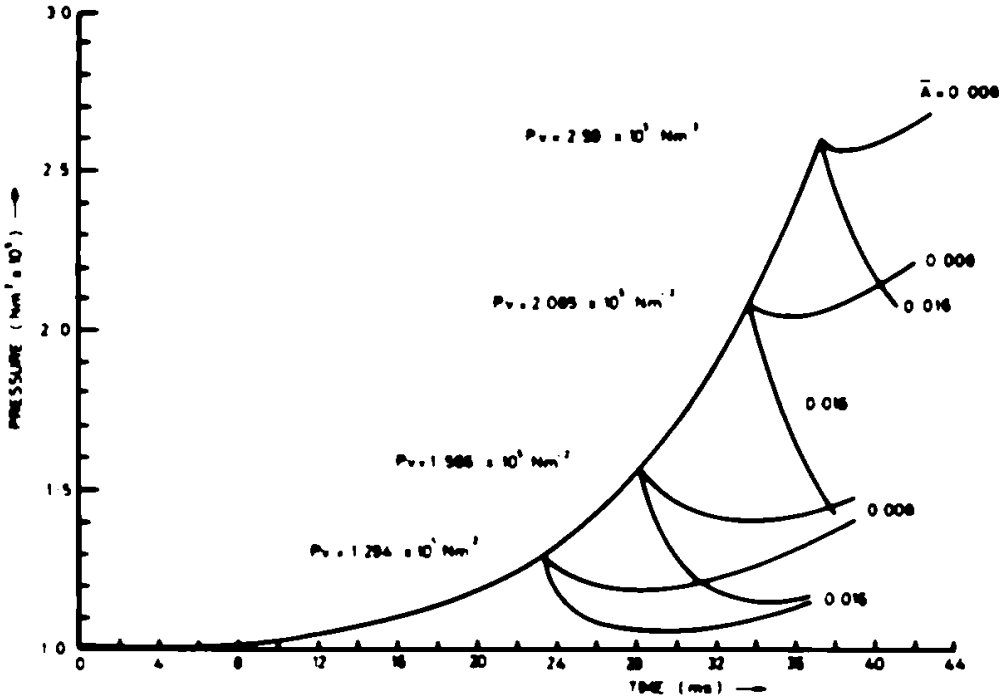
where ρ is the density of the vented mixture, P_a the ambient pressure, C_d a discharge coefficient and A_v the vent area. Substitution into (2), and repeating steps (4) to (10) results in

$$\frac{dP}{dt} = \begin{cases} \frac{3\left(P_{max} - P_0\right)}{R_{vessel}} \left[1 - \left(\frac{P_0}{P} \right)^{\frac{1}{\gamma}} \frac{P_{max} - P}{P_{max} - P_0} \right]^{\frac{2}{3}} \left(\frac{P}{P_0} \right)^{\frac{1}{\gamma}} S_u + C_d A_v \rho \left[\frac{\gamma P}{\rho} \left(\frac{\gamma+1}{2} \right)^{\frac{1+\gamma}{1-\gamma}} \right]^{1/2} \\ \frac{3\left(P_{max} - P_0\right)}{R_{vessel}} \left[1 - \left(\frac{P_0}{P} \right)^{\frac{1}{\gamma}} \frac{P_{max} - P}{P_{max} - P_0} \right]^{\frac{2}{3}} \left(\frac{P}{P_0} \right)^{\frac{1}{\gamma}} S_u + C_d A_v \left\{ \frac{2\gamma P \rho}{\gamma-1} \left(\frac{P_a}{P} \right)^{\frac{2}{\gamma}} \left[1 - \left(\frac{P_a}{P} \right)^{\frac{\gamma-1}{\gamma}} \right]^{\frac{1+\gamma}{1-\gamma}} \right\}^{1/2} \end{cases} \tag{13}$$

Derivation of a vented deflagration model

Assume that the density of the vented mixture, ρ, is equal to that of the burnt mixture, ρ_b. With this assumption, the density of the vented mixture, ρ, in equation (13) can be computed from

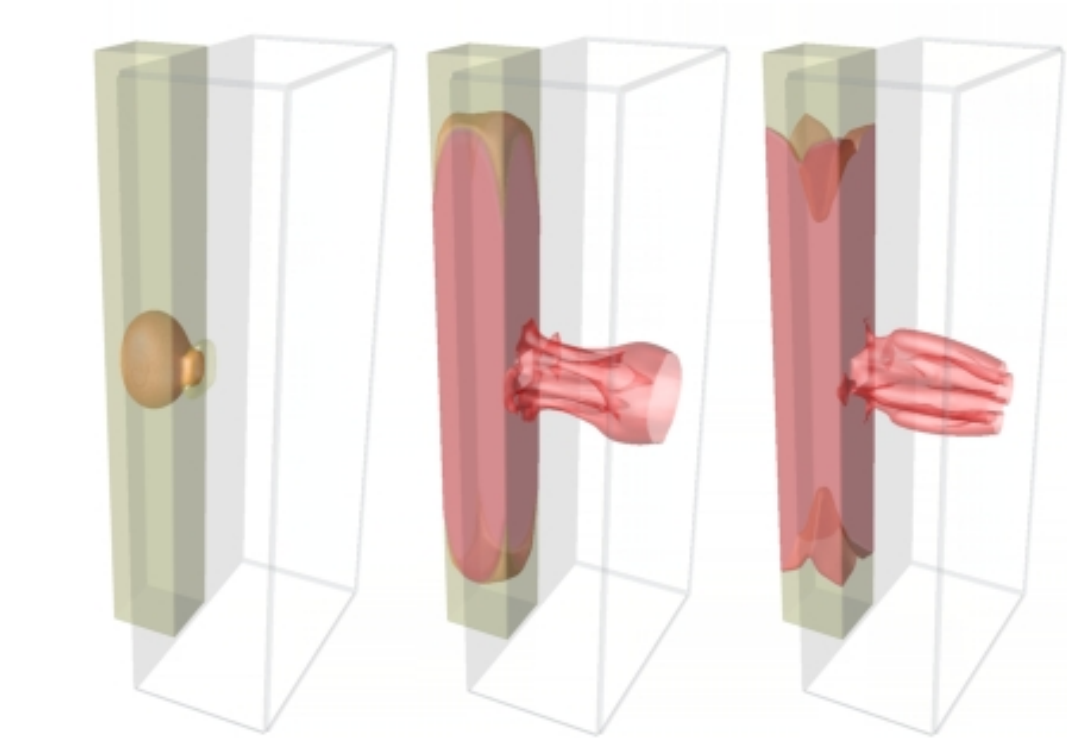
$$\rho \equiv \rho_b = \frac{T_u}{T_f}\rho_u = \rho_{u0}\frac{T_{u0}}{T_f}\left(\frac{P}{P_0}\right)^{\frac{\gamma-1}{\gamma}}\left(\frac{P}{P_0}\right)^{\frac{1}{\gamma}} \tag{14}$$



The figure shows the solution of equations (13) and (14) for two area ratios (vent area divided by total surface area of enclosure) and four different vent opening pressures.

From: Bradley D. and Mitcheson A. The venting of gaseous explosions in spherical vessels. I - Theory. Combustion and Flame, 32:221-236, 1978.

Peculiarities of vented deflagrations

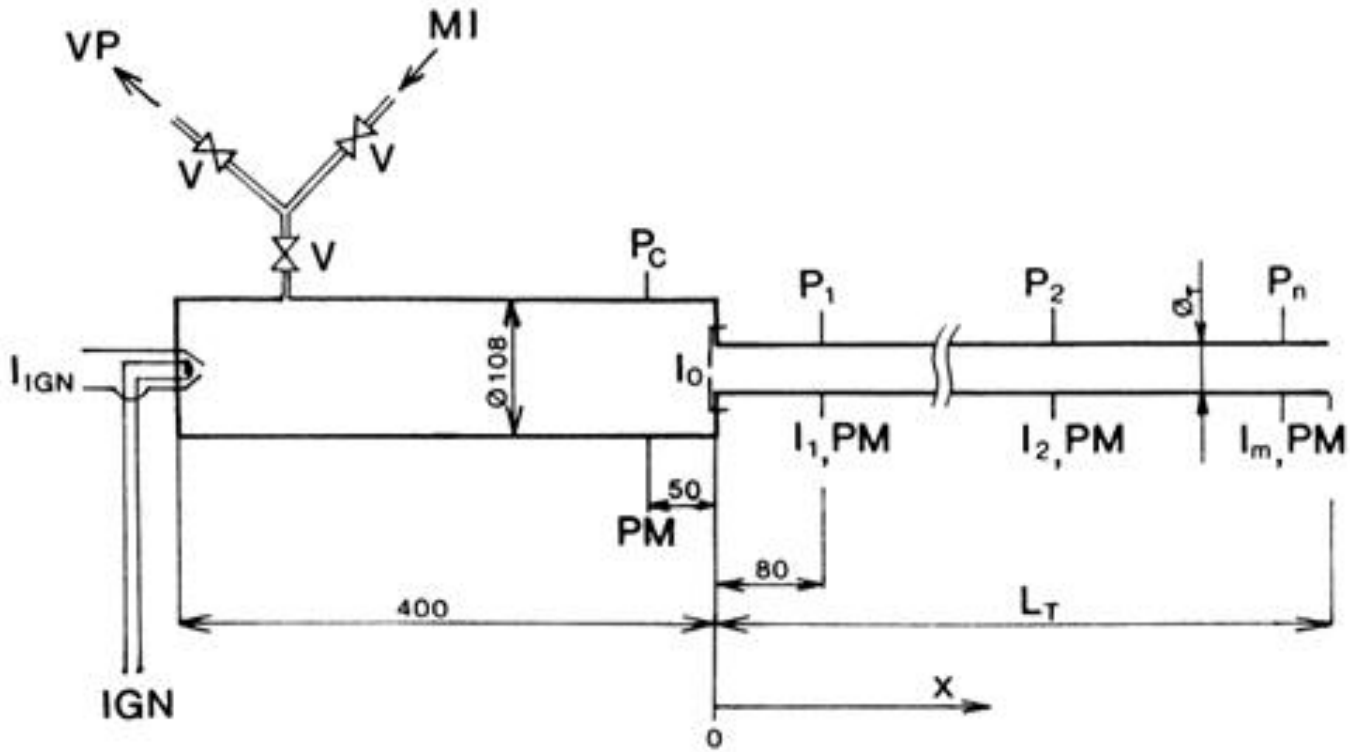


From: Bauwens C.R., Dorofeev S. and Tamanini F. Effects of aspect ratio and ignition location on vented explosion pressures. Proceedings of the 5th International Seminar on Fire and Explosion Hazards, Edinburgh, UK, 23–27 April 2007

- **Enclosure geometry/aspect ratio**
- **Ignition location**
- **Varying pressure and temperature**
- **Varying turbulence**
- **Changes in flame shape**
- **Flame stretch and flame curvature**
- **Darrieu-Landau instability**
- **Hydrodynamic instability**
- **Raleigh-Taylor instability**
- **Richtmeyer-Meshkov instability**
- **Flame distortion at outflow boundaries**
- **Vent cover inertia**

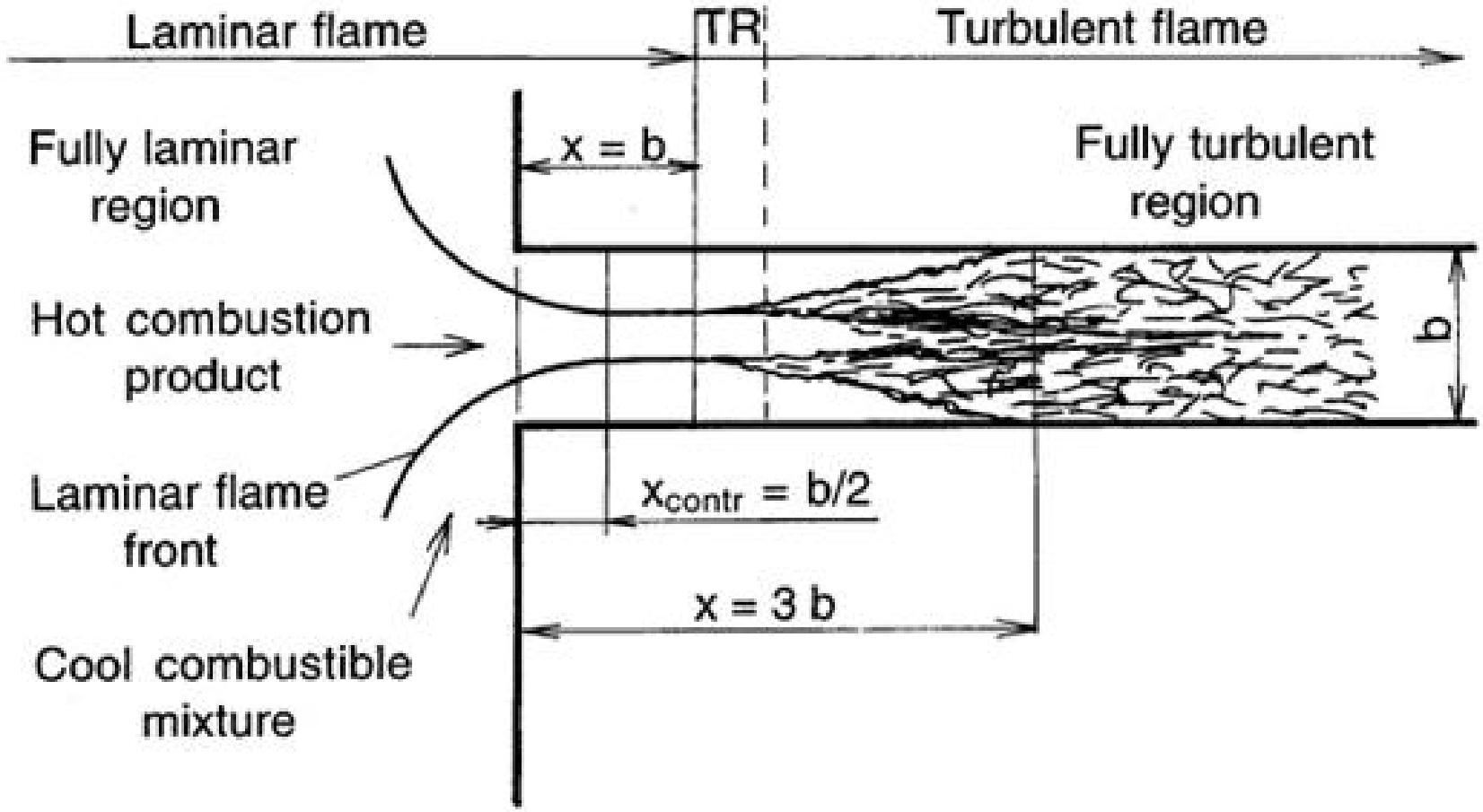
Peculiarities of vented deflagrations: flame distortion by vent ducts

Ponizy B. and Leyer J.C. Flame dynamics in a vented vessel connected to a duct: I. Mechanism of vessel-duct interaction. Combustion and Flame, 116:259-271, 1999.
Ponizy B. and Leyer J.C. Flame dynamics in a vented vessel connected to a duct: II. Influence of ignition site, membrane rupture, and turbulence. Combustion and Flame, 116:272-281, 1999.



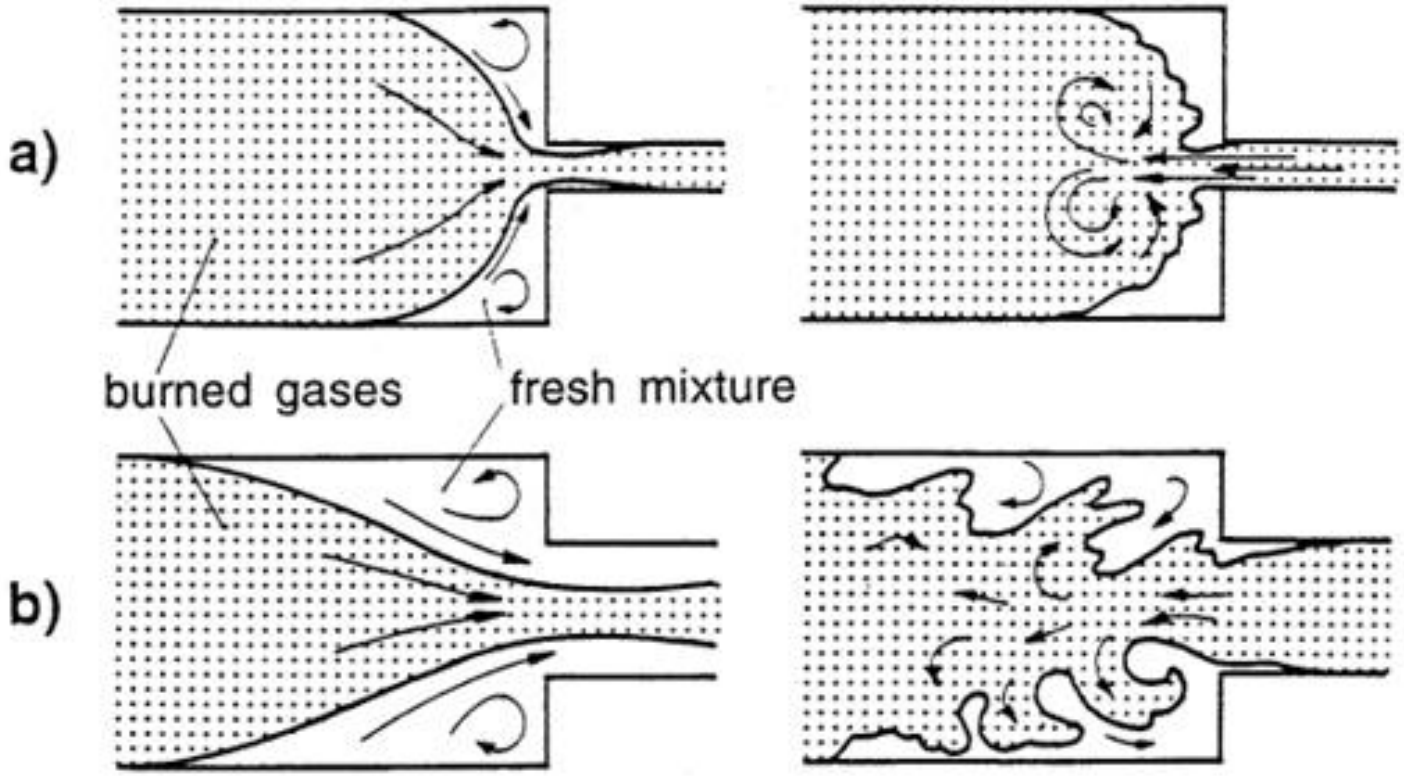
Experimental setup used by Ponizy & Leyer (1999). IGN, ignition (electrically heated wire); VP, vacuum pump; MI, mixture inlet; V, valves; PM, photomultipliers; PC, P1, P2, . . . Pn, pressure gauges; IIGN, I0, I1, . . . Im, ionization gauges. The tube diameter is 53 mm.

Peculiarities of vented deflagrations: flame distortion by vent ducts



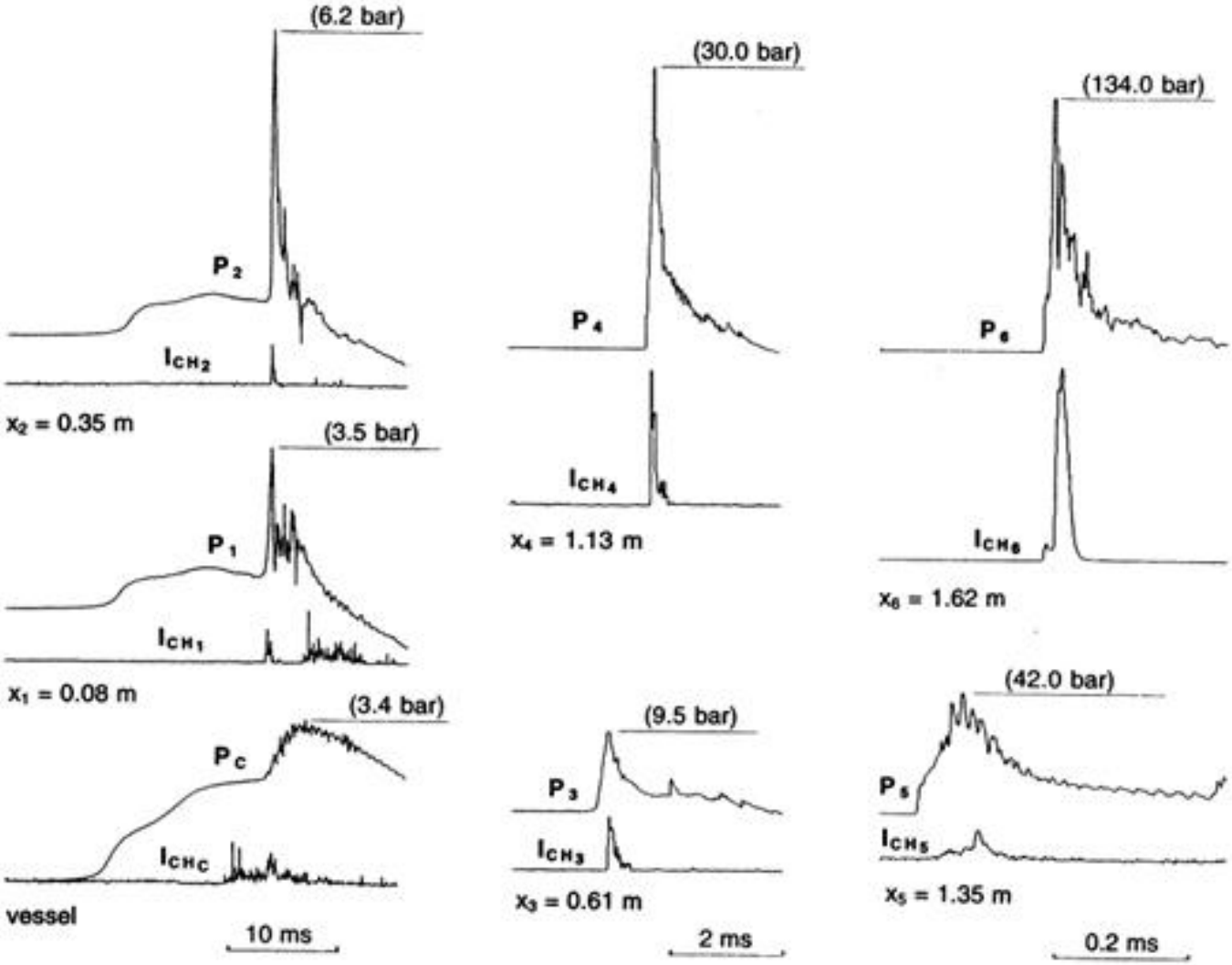
Flow pattern inside the duct. After Ponizy & Leyer (1999).

Peculiarities of vented deflagrations: flame distortion by vent ducts



Flow patterns in vessel before and after combustion in the duct, effect of flame front distortion; a) narrow ducts, b) wide ducts. After Ponizy & Leyer (1999).

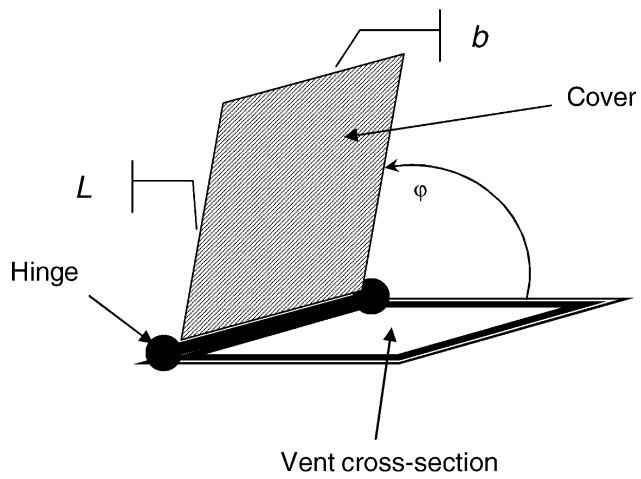
Peculiarities of vented deflagrations: flame distortion by vent ducts



Deflagration to detonation transition (detonation onset at 1.7 m from duct entrance). After Ponizy & Leyer (1999).

Vented deflagrations with hinged inertial vent covers

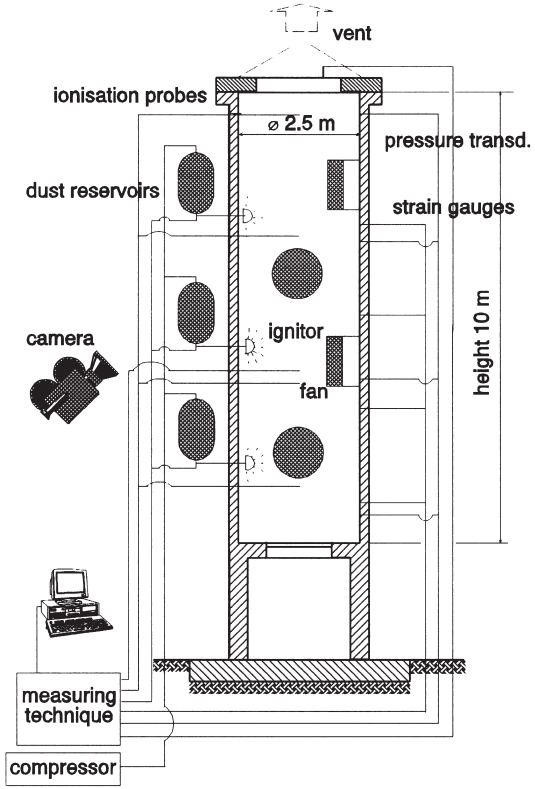
Molkov V.V., Grigorash A.V., Eber R.M., and Makarov D.V. Vented gaseous deflagrations: Modelling of hinged inertial vent covers. Journal of Hazardous Materials, A116:1-10, 2004.
Höchst S. and Leuckel W. On the effect of venting large vessels with mass inert panels. Journal of Loss Prevention in the Process Industries, 11:89-97, 1998.



Dynamic venting area:

$$F(\phi) = \min\left[F_N, 2L\sin\left(\frac{\phi}{2}\right)\left[b + L\cos\left(\frac{\phi}{2}\right)\right]\right] \qquad (15)$$

F_N = vent cross-sectional area. Dynamic vent area $F(\phi) \to F_N$ for $\phi = 0 \to \phi_N$ and $F(\phi) \equiv F_N$ for $\phi_N \leq \phi \leq \frac{1}{2}\pi$.



Experimental apparatus (H/D=4, 10.7 vol% methane).

Vented deflagrations with hinged inertial vent covers

Equations for prediction of dynamic deflagration pressure ($\tau = tS_{uL}^{\circ}/R_s$, $\Pi = P/P_0$, $n_u = m_u/m_{u0}$ and $n_b = m_b/m_{u0}$). S_{uL}° is the laminar burning velocity at reference conditions and R_s is the radius of a sphere with a volume equal to that of the enclosure.

$$\frac{d\Pi}{d\tau} = 3\Pi \frac{\chi(\tau) Z \Pi^{\epsilon+\frac{1}{\gamma_u}} \left(1 - n_u \Pi^{-\frac{1}{\gamma_u}}\right)^{\frac{2}{3}} - \gamma_b W_\Sigma(\tau) R_\Sigma}{\Pi^{\frac{1}{\gamma_u}} - \left(\gamma_u - \frac{\gamma_b}{\gamma_u}\right) n_u} \tag{16}$$

$$\frac{dn_b}{d\tau} = 3 \left\{ \chi(\tau) \Pi^{\epsilon+\frac{1}{\gamma_u}} \left(1 - n_u \Pi^{-\frac{1}{\gamma_u}}\right)^{\frac{2}{3}} - R_b^{\#} W_\Sigma(\tau) \frac{\sum_j A_j(\tau) \mu_j F_j(\tau)}{\sum_j \mu_j F_j(\tau)} \right\} \tag{17}$$

$$\frac{dn_u}{d\tau} = 3 \left\{ \chi(\tau) \Pi^{\epsilon+\frac{1}{\gamma_u}} \left(1 - n_u \Pi^{-\frac{1}{\gamma_u}}\right)^{\frac{2}{3}} + R_u^{\#} W_\Sigma(\tau) \frac{\sum_j \left[1 - A_j(\tau)\right] \mu_j F_j(\tau)}{\sum_j \mu_j F_j(\tau)} \right\} \tag{18}$$

$$R_\Sigma = R_u^{\#} W_\Sigma(\tau) \frac{\sum_j \left[1 - A_j(\tau)\right] \mu_j F_j(\tau)}{\sum_j \mu_j F_j(\tau)} + R_b^{\#} W_\Sigma(\tau) \frac{\sum_j A_j(\tau) \mu_j F_j(\tau)}{\sum_j \mu_j F_j(\tau)} \tag{19}$$

Vented deflagrations with hinged inertial vent covers

$$R^{\#}_{u\vee b} = \begin{cases} \left[\frac{2\gamma}{\gamma-1}\Pi\sigma_{u\vee b}\left[\left(\frac{P_a}{P_0\Pi}\right)^{\frac{2}{\gamma}} - \left(\frac{P_a}{P_0\Pi}\right)^{\frac{\gamma+1}{\gamma}}\right]\right]^{\frac{1}{2}} & \text{(sub-sonic outflow)} \\ \left[\gamma\Pi\sigma_{u\vee b}\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{\gamma-1}}\right]^{\frac{1}{2}} & \text{(sonic outflow)} \end{cases} \tag{20}$$

where $\sigma_u = \rho_u/\rho_{u0} = \Pi_u^{1/\gamma}$ and $\sigma_b = \rho_b/\rho_{u0} = \Pi_b^{1/\gamma}$.

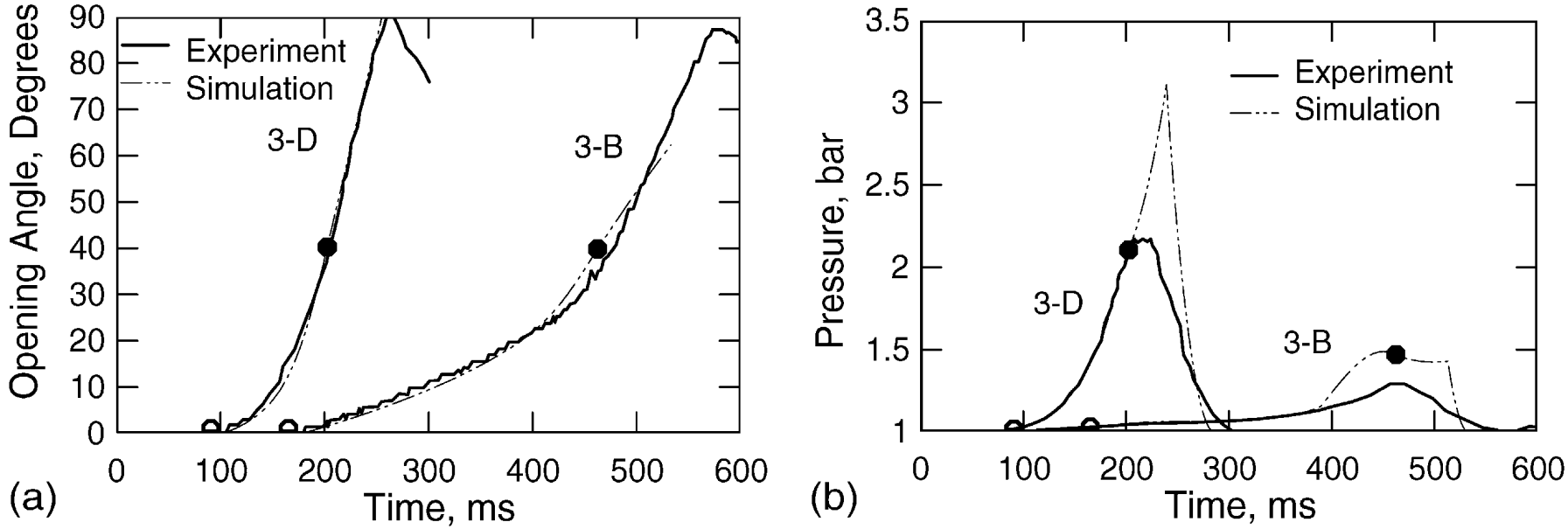
$$Z = \gamma_b\left[E - \frac{\gamma_u}{\gamma_b}\frac{\gamma_b-1}{\gamma_u-1}\right]\Pi^{1-\frac{\gamma_b}{u}} + \frac{\gamma_b-\gamma_u}{\gamma_u-1} \tag{21}$$

where E is an expansion coefficient of the combustion products. For the transient venting parameter W_Σ:

$$W_\Sigma = \frac{1}{\sqrt[3]{36\pi}}\frac{1}{\sqrt{\gamma}}\frac{c_0}{S^{\circ}_{uL}}\frac{\sum_j \mu_j F_j(\tau)}{V^{2/3}} \tag{22}$$

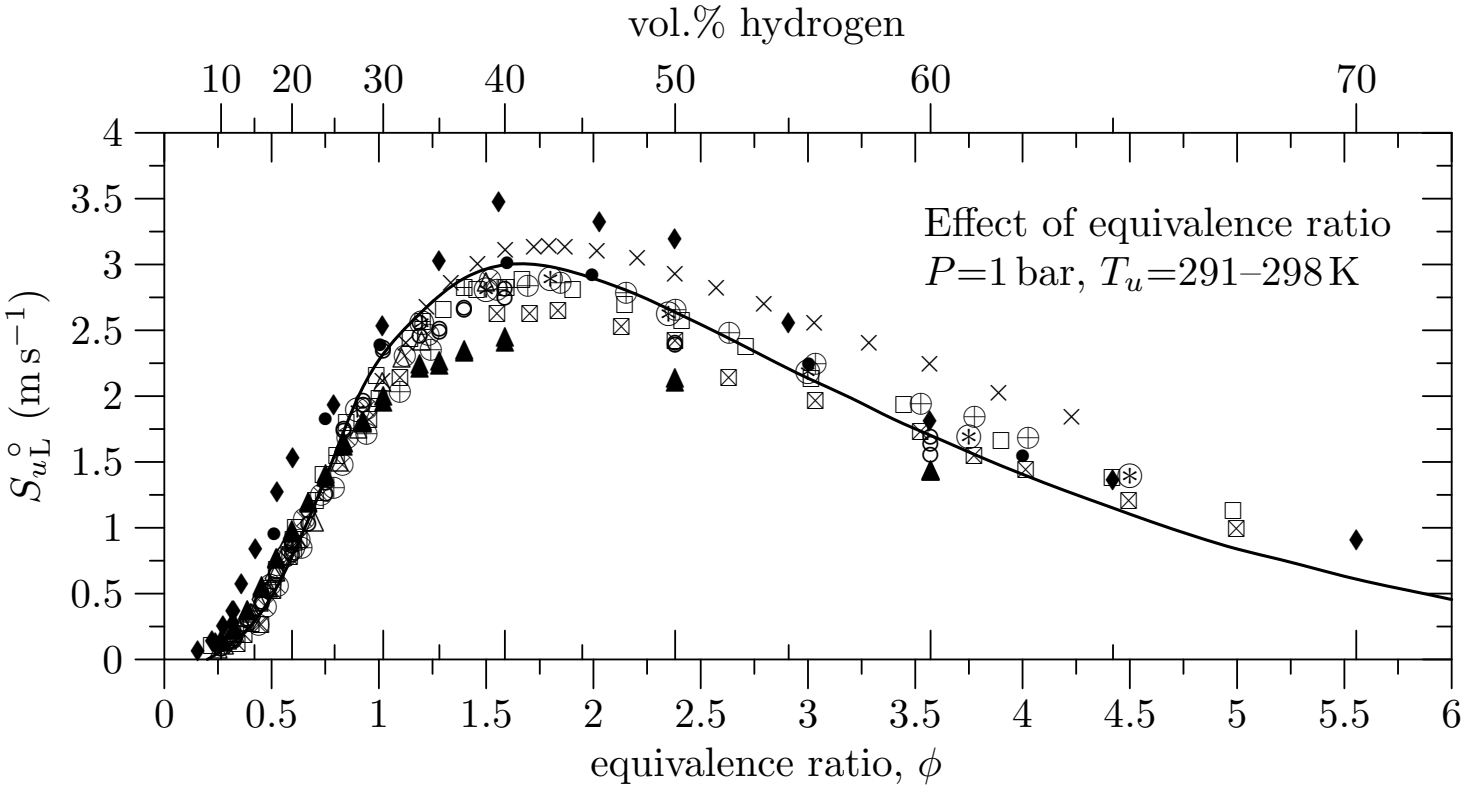
A detailed analysis for $F(\phi)$ to include torque and pressure forces is given in Molkov, Grigorash, Eber & Makarov (2004).

Vented deflagrations with hinged inertial vent covers



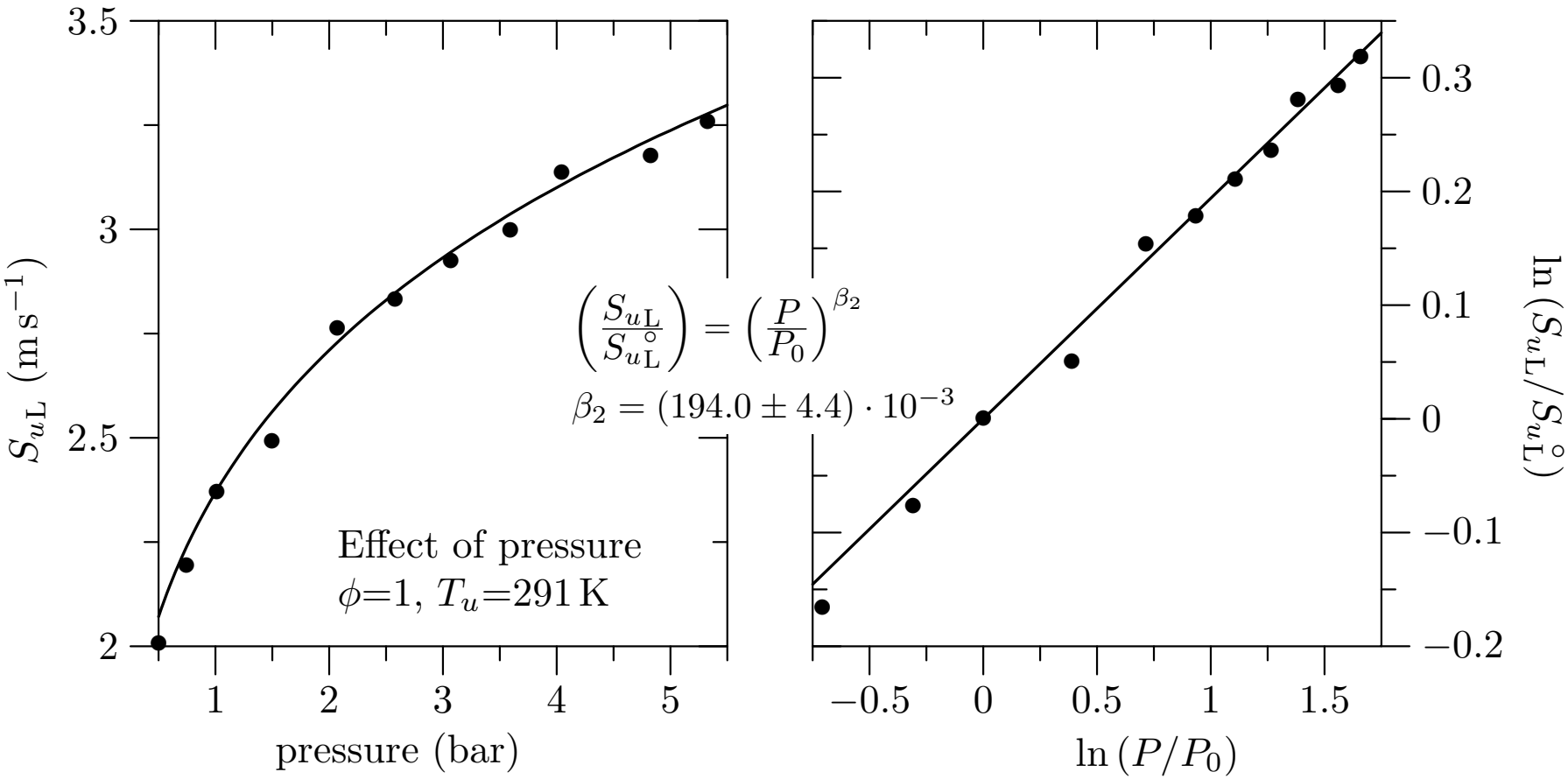
Comparison between equations (16)–(22) and experiments; ○ vent starts to open; ● vent 100% open.

Correlations for the laminar burning velocity



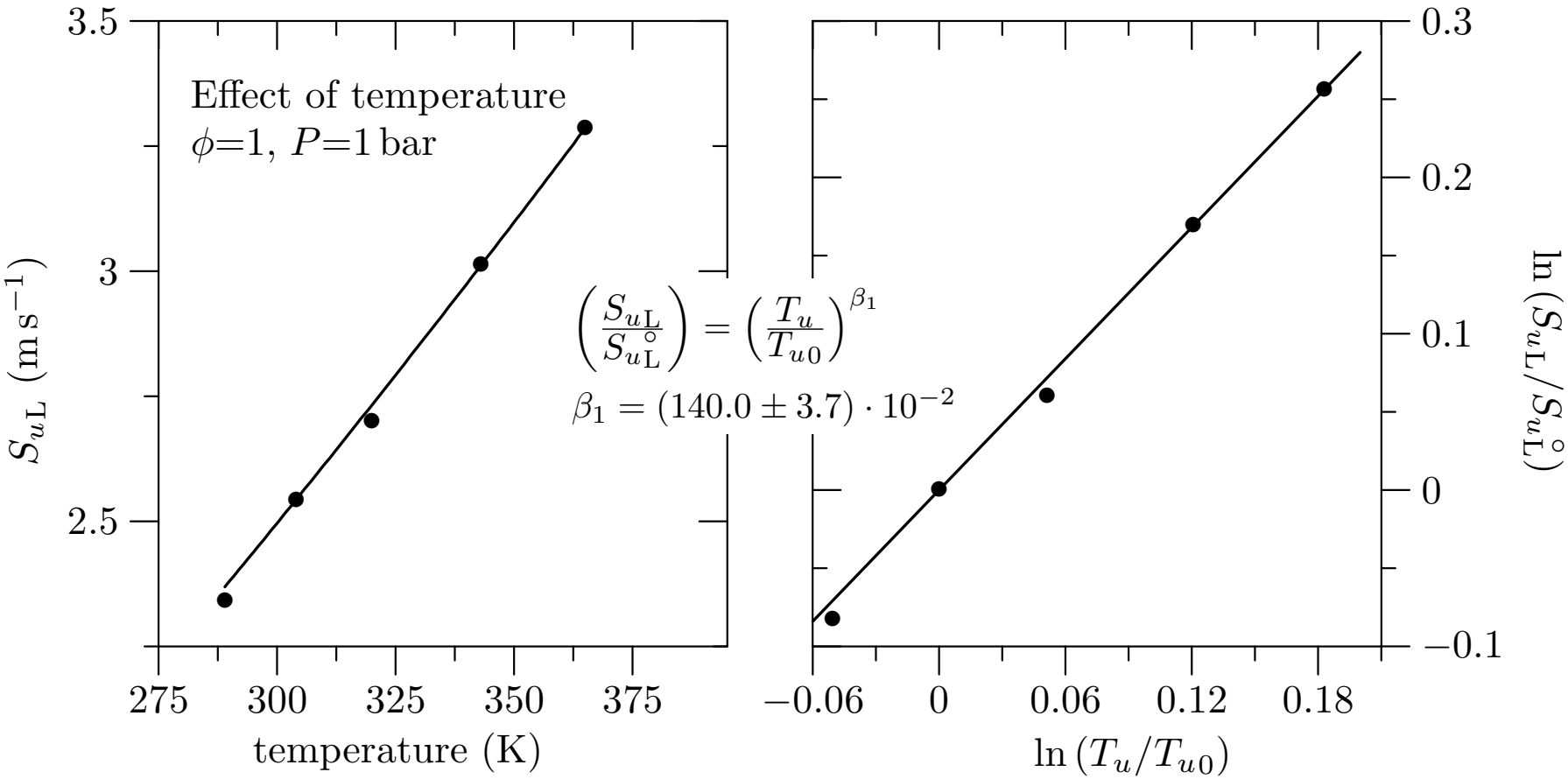
Laminar burning velocity of hydrogen-air mixtures as a function of equivalence ratio at T_0=293.15–298.15 K and P_0=1 bar.

Correlations for the laminar burning velocity



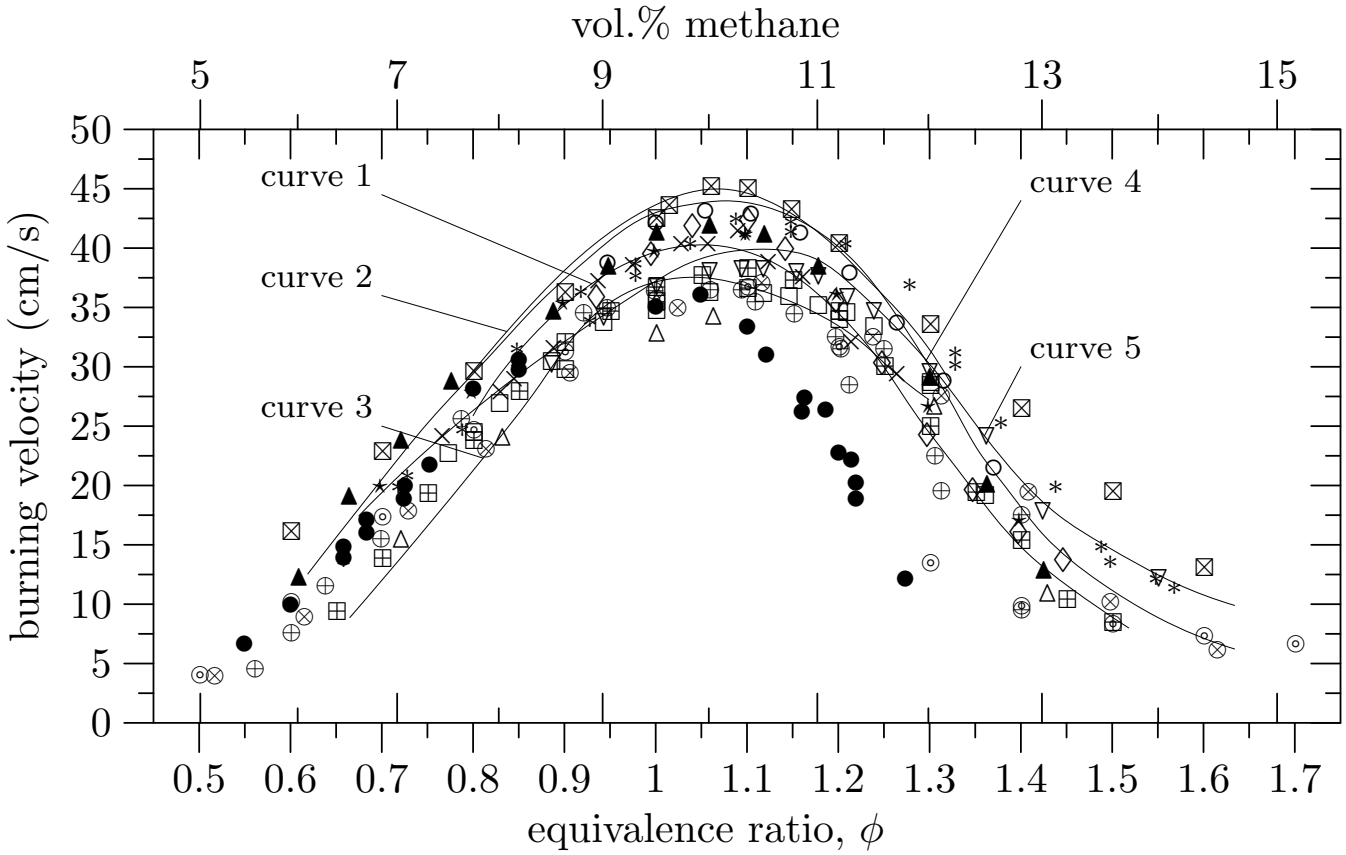
Laminar burning velocity of stoichiometric hydrogen-air as a function of pressure.

Correlations for the laminar burning velocity



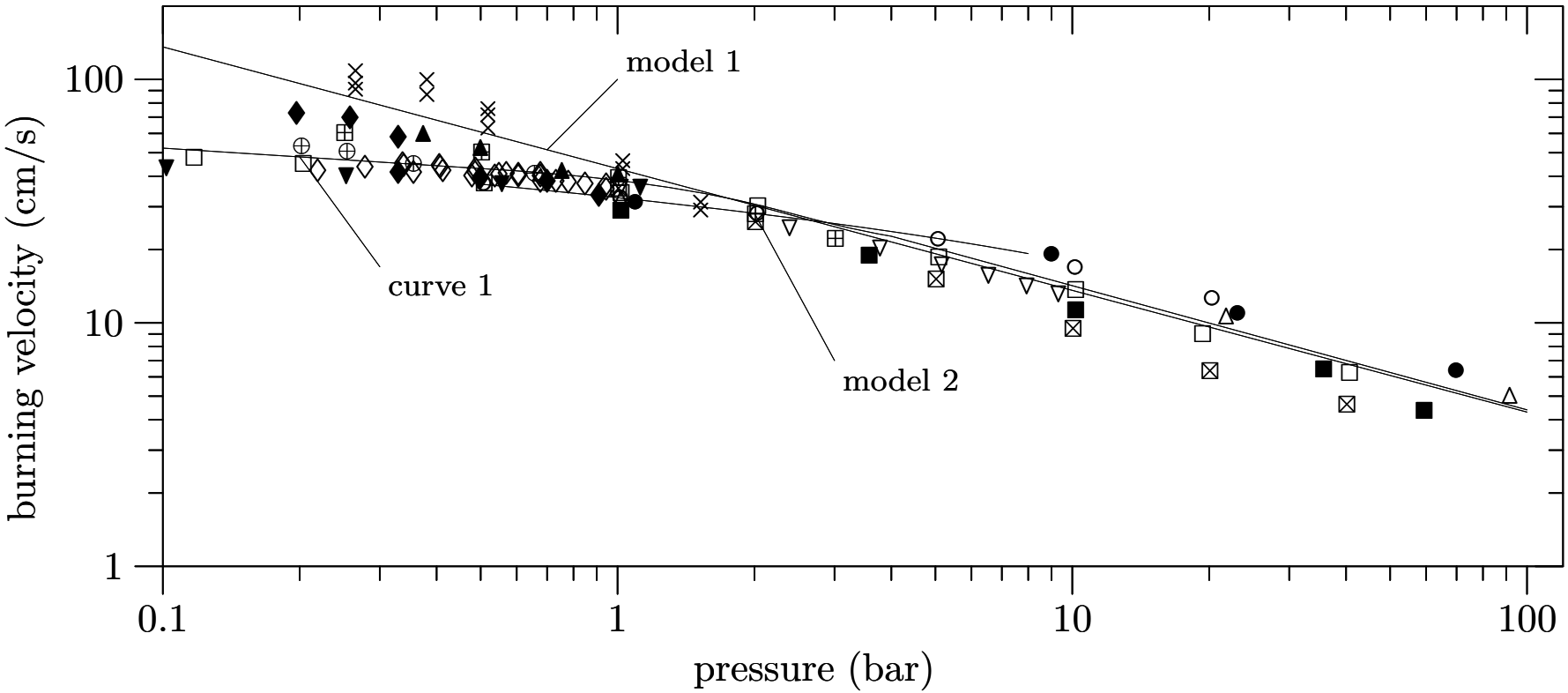
Laminar burning velocity of stoichiometric hydrogen-air as a function of temperature.

Correlations for the laminar burning velocity



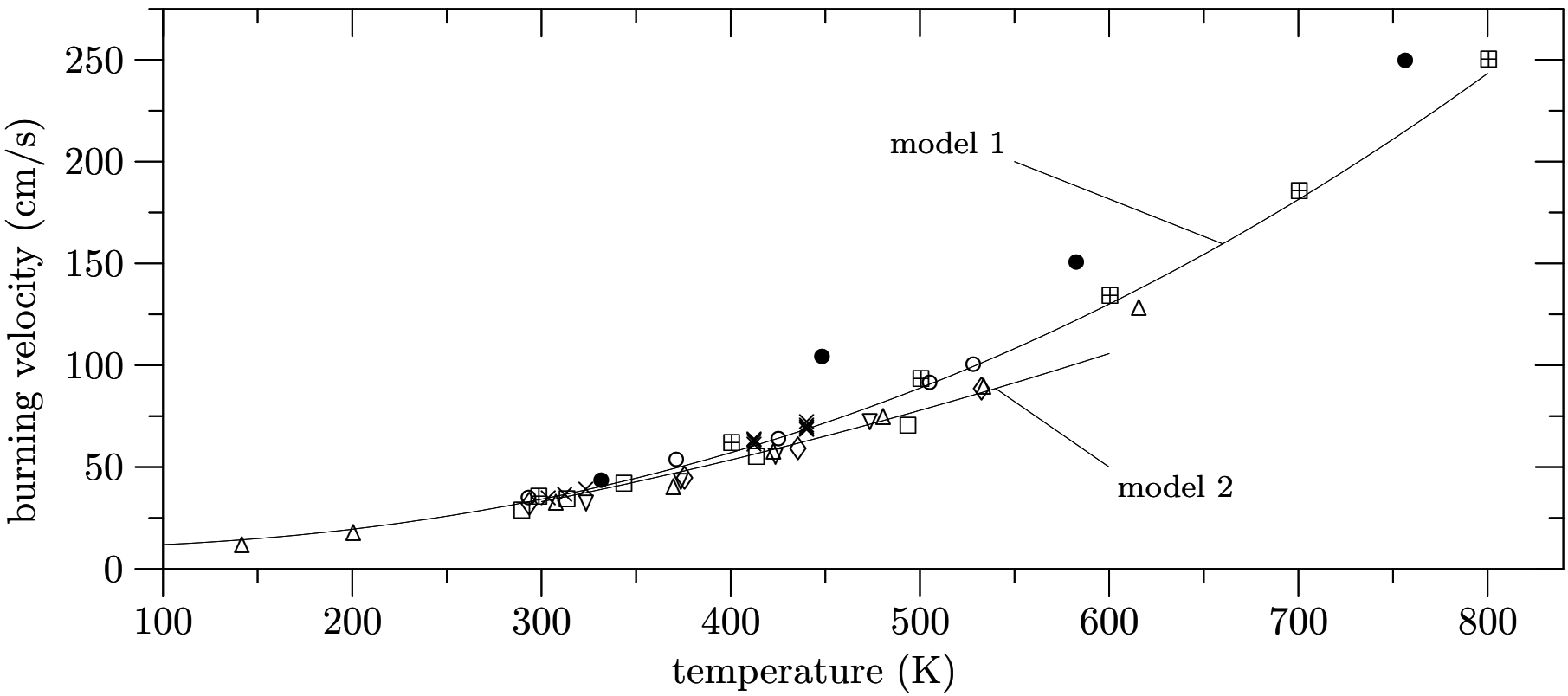
Laminar burning velocity of methane-air mixtures as a function of equivalence ratio at T_0=293.15–298.15 K and P_0=1 bar.

Correlations for the laminar burning velocity



Laminar burning velocity of stoichiometric methane-air as a function of pressure.

Correlations for the laminar burning velocity



Laminar burning velocity of stoichiometric methane-air as a function of temperature.

Correlations for the laminar burning velocity

Objective:
Find an expression for the pressure and temperature dependence of the laminar burning velocity and the laminar flame thickness

Governing equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = 0 \tag{23}$$

$$\frac{\partial (\rho \boldsymbol{v})}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}\boldsymbol{v}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \sum_{i=1}^{N} \rho Y_i \boldsymbol{f}_i \tag{24}$$

$$\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho \boldsymbol{v} Y_i) = -\nabla \cdot [\rho Y_i \boldsymbol{V}_i] + \dot{w}_i \tag{25}$$

$$\begin{aligned} \frac{\partial (\rho h)}{\partial t} + \nabla \cdot (\rho \boldsymbol{v} h) &= \frac{\partial p}{\partial t} + \boldsymbol{v} \cdot \nabla p + \boldsymbol{\tau} : \nabla \boldsymbol{v} - \nabla \cdot [\lambda \nabla T] + \nabla \cdot \boldsymbol{q} \\ &+ \nabla \cdot \left[\sum_{i=1}^{N} \rho Y_i h_i \boldsymbol{V}_i + \mathrm{R}T \sum_{i=1}^{N} \sum_{j=1}^{N} \left(\frac{X_j \alpha_i}{\mathcal{M}_i \mathcal{D}_{ij}} \right) (\boldsymbol{V}_i - \boldsymbol{V}_j) \right] + \sum_{i=1}^{N} \rho Y_i \boldsymbol{f}_i \cdot \boldsymbol{V}_i \end{aligned} \tag{26}$$

$$\frac{p}{\rho} = \frac{\gamma - 1}{\gamma} \sum_{i=1}^{N} Y_i \left[h_{f_i}^{\circ} + \int_{T^{\circ}}^{T} \mathrm{C}_{\mathrm{P}i}(T)\, dT \right] \tag{27}$$

$$\text{where} \quad \boldsymbol{\tau} = \mu \left[\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^{\dagger} \right] + \left(\kappa - \tfrac{2}{3}\mu \right) [\nabla \cdot \boldsymbol{v}]\, \boldsymbol{I} \tag{28}$$

$$\text{and} \quad \boldsymbol{q} = \epsilon \sigma T^4 \tag{29}$$

Assumptions:

- **Steady state**
- **Uniform pressure field**
- **Neglect viscous dissipation in energy equation**
- **Neglect effect of body forces in momentum and energy equation**
- **Neglect Dufour effect in energy equation**
- **Keep Soret effect in species and energy equation**

Correlations for the laminar burning velocity

Step 1: **Make use of the fact that $h = \sum Y_i h_i$ to restate equations (25) and (26) as:**

$$\nabla \cdot \left[\rho Y_i \left(\boldsymbol{v} + \boldsymbol{V}_i\right)\right] = \dot{w}_i \tag{30}$$

$$\nabla \cdot \left[\sum_{i=1}^{N} \rho Y_i h_i \left(\boldsymbol{v} + \boldsymbol{V}_i\right) - \lambda \nabla T\right] = 0 \tag{31}$$

Step 2: Use

$$h_i = h_{f_i}^{\circ} + \int_{T^{\circ}}^{T} \mathrm{C}_{\mathrm{P}i}\, dT \tag{32}$$

to rewrite equation (31) as

$$\nabla \cdot \left[\sum_{i=1}^{N} \rho Y_i \left(\boldsymbol{v} + \boldsymbol{V}_i\right) h_{f_i}^{\circ} + \sum_{i=9}^{N} \rho Y_i \left(\boldsymbol{v} + \boldsymbol{V}_i\right) \int_{T^{\circ}}^{T} \mathrm{C}_{\mathrm{P}i}\, dT - \lambda \nabla T\right] = 0 \tag{33}$$

and apply equation (30) to the first term of the left hand side to obtain

$$\nabla \cdot \left[\rho \boldsymbol{v} \sum_{i=6}^{N} \int_{T^{\circ}}^{T} Y_i \mathrm{C}_{\mathrm{P}i}\, dT + \rho \sum_{i=1}^{N} \boldsymbol{V}_i \int_{T^{\circ}}^{T} Y_i \mathrm{C}_{\mathrm{P}i}\, dT - \lambda \nabla T\right] = -\sum_{i=1}^{N} h_{f_i}^{\circ} \dot{w}_i \tag{34}$$

Correlations for the laminar burning velocity

Step 3: Assume a background fluid so that

$$\rho Y_i \boldsymbol{V}_i = -\rho \mathbb{D} \nabla Y_i \tag{35}$$

Since

$$\mathrm{C_P} = \sum Y_i \mathrm{C_P} \tag{36}$$

it is possible to rewrite equation (34) as

$$\nabla \cdot \left[\rho \boldsymbol{v} \int_{T^\circ}^{T} \mathrm{C_P}\, dT + \rho \mathbb{D} \sum_{i=1}^{N} (\nabla Y_i) \int_{T^\circ}^{T} Y_i \mathrm{C_P}_i\, dT - \rho \mathbb{D} \frac{\lambda}{\rho \mathrm{C_P} \mathbb{D}} \mathrm{C_P} \nabla T \right] = -\sum_{i=1}^{N} h_{f_i}^{\circ} \dot{w}_i \tag{37}$$

and because of the equality,

$$\nabla \int_{T^\circ}^{T} \mathrm{C_P}\, dT = \nabla \sum_{i=1}^{N} Y_i \int_{T^\circ}^{T} \mathrm{C_P}_i\, dT = \sum_{i=1}^{N} (\nabla Y_i) \int_{T^\circ}^{T} \mathrm{C_P}_i\, dT + \sum_{i=1}^{N} Y_i \nabla \int_{T^\circ}^{T} \mathrm{C_P}_i\, dT \tag{38}$$

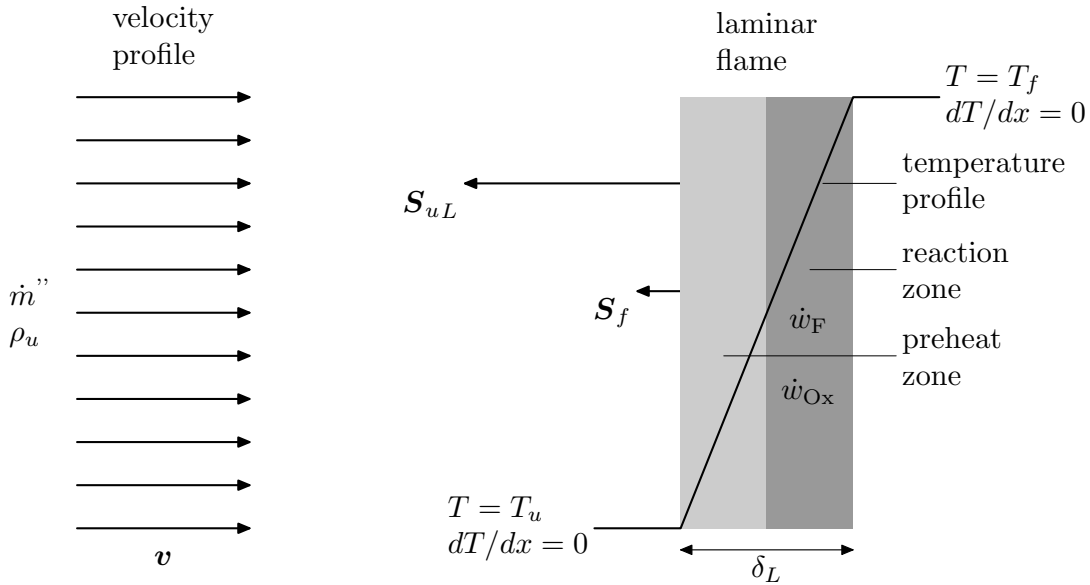
$$= \sum_{i=1}^{N} (\nabla Y_i) \int_{T^\circ}^{T} \mathrm{C_P}_i\, dT + \sum_{i=1}^{N} Y_i \mathrm{C_P}_i \nabla T = \sum_{i=6}^{N} (\nabla Y_i) \int_{T^\circ}^{T} \mathrm{C_P}_i\, dT + \mathrm{C_P} \nabla T \tag{39}$$

equation (37) may be rewritten as

$$\boxed{\nabla \cdot \left[\rho \boldsymbol{v} \int_{T^\circ}^{T} \mathrm{C_P}\, dT + \rho \mathbb{D} \nabla \int_{T^\circ}^{T} \mathrm{C_P}\, dT - \rho \mathbb{D} \left[\mathrm{Le} - 1 \right] \mathrm{C_P} \nabla T \right] = -\sum_{i=1}^{N} h_{f_i}^{\circ} \dot{w}_i} \tag{40}$$

Correlations for the laminar burning velocity

Step 4:



Assume unity Lewis number in equation (40):

$$\nabla \cdot \left[\rho \boldsymbol{v} \int_{T^\circ}^{T} \mathrm{C_P}\, dT + \rho \mathbb{D} \nabla \int_{T^\circ}^{T} \mathrm{C_P}\, dT \right] = -\sum_{i=1}^{N} h_{f_i}^\circ \dot{w}_i \tag{41}$$

If Le = 1 then $\rho\mathbb{D}$ may be replaced by $\lambda/\mathrm{C_P}$! From figure with simplified flame structure: $\rho_u \boldsymbol{v} = \rho_u \boldsymbol{S}_{uL} = \dot{m}''$ = constant.

Finally

$$\boxed{\dot{m}'' \mathrm{C_P} \nabla T + \nabla \cdot [\lambda \nabla T] = -\sum_{i=1}^{N} h_{f_i}^\circ \dot{w}_i} \tag{42}$$

Correlations for the laminar burning velocity

Step 5:

Express the combustion reaction in terms of a mass balance:

$$1\,\text{kg Fuel} + \nu\,\text{kg Oxidizer} \longrightarrow (\nu+1)\,\text{kg Products} \tag{43}$$

Then

$$-\dot{w}_{\mathrm{F}} = -\frac{1}{\nu}\dot{w}_{\mathrm{Ox}} = \frac{1}{\nu+1}\dot{w}_{\mathrm{Pr}} \tag{44}$$

and hence,

$$\begin{aligned}\sum_{i=1}^{N} h^{\circ}_{f_i}\dot{w}_i &= h^{\circ}_{f_{\mathrm{F}}}\dot{w}_{\mathrm{F}} + h^{\circ}_{f_{\mathrm{Ox}}}\dot{w}_{\mathrm{Ox}} + h^{\circ}_{f_{\mathrm{Pr}}}\dot{w}_{\mathrm{Pr}} \\ &= \left(h^{\circ}_{f_{\mathrm{F}}} + \nu\, h^{\circ}_{f_{\mathrm{Ox}}} - (\nu+1)\, h^{\circ}_{f_{\mathrm{Pr}}}\right)\dot{w}_{\mathrm{F}} \\ &= \Delta_c H\, \dot{w}_{\mathrm{F}}\end{aligned} \tag{45}$$

where $\Delta_c H$ denotes the fuel's heat of combustion. Equation (40) may then be restated as:

$$\boxed{\dot{m}''\mathrm{C_P}\nabla T + \nabla\cdot[\lambda\nabla T] = -\Delta_c H\dot{w}_i} \tag{46}$$

Step 6:

Integrate the one-dimensional form of equation (46) from $x \to -\infty$ to $x \to \infty$ for the simplified flame structure,

$$\dot{m}''\mathrm{C_P}\frac{dT}{dx} + \frac{d}{dx}\left(\lambda\frac{dT}{dx}\right) = -\Delta_c H\,\dot{w}_{\mathrm{F}} \tag{47}$$

subjected to the boundary conditions,

$$x \to -\infty: \quad T = T_u \qquad x \to \infty: \quad T = T_f \tag{48}$$

and the subsidiary conditions,

$$x \to -\infty: \quad \frac{dT}{dx} = 0 \qquad x \to \infty: \quad \frac{dT}{dx} = 0 \tag{49}$$

Inside the flame zone,

$$x \in \delta_L: \quad \frac{dT}{dx} = \frac{T_f - T_u}{\delta_L} \tag{50}$$

Integration of equation (47) gives:

$$\dot{m}''\mathrm{C_P}\,T\Big|_{T_u}^{T_f} + \lambda\,\frac{\partial T}{\partial x}\Bigg|_{dT/dx=0}^{dT/dx=0} = -\Delta_c H\int_{-\infty}^{\infty}\dot{w}_{\mathrm{F}}\,dx \tag{51}$$

Correlations for the laminar burning velocity

Step 7:

Apply a change of variables to the right hand side of equation (51) on the basis of the assumed temperature profile (50):

$$\frac{dT}{dx} = \frac{T_f - T_u}{\delta_L} \qquad \Longleftrightarrow \qquad dx = \frac{\delta_L}{T_f - T_u} dT \tag{52}$$

Hence,

$$\dot{m}^{"} \mathrm{C_P} \left(T_f - T_u\right) = -\frac{\delta_L \Delta_c H}{T_f - T_u} \int_{T_u}^{T_f} \dot{w}_\mathrm{F} dT = -\delta_L \Delta_c H \overline{\dot{w}}_\mathrm{F} \tag{53}$$

or, equivalently,

$$\boxed{\dot{m}^{"} \mathrm{C_P} \left(T_f - T_u\right) + \delta_L \, \Delta_c H \, \overline{\dot{w}}_\mathrm{F} = 0} \tag{54}$$

$\Longrightarrow$ A single *algebraic* equation with two unknowns:

- the mass flux $\dot{m}^{"} \left(\equiv \rho_u S_{uL}\right)$,
- and the laminar flame thickness δ_L.

Step 8:

Find a second algebraic equation by integrating equation (47) from $x \to -\infty$ to $x \to \delta_L/2$, subjected to the boundary conditions,

$$x \to -\infty : \quad T = T_u \qquad x = \frac{\delta_L}{2} : \quad T = \frac{T_u + T_f}{2} \tag{55}$$

and the subsidiary conditions,

$$x \to -\infty : \quad \frac{dT}{dx} = 0 \qquad x \to \frac{\delta_L}{2} : \quad \frac{dT}{dx} = \frac{T_f - T_u}{\delta_L} \tag{56}$$

Integration of equation (42) results in

$$\dot{m}^{"} \mathrm{C_P} \, T \Big|_{T_u}^{(T_u + T_f)/2} + \lambda \, \frac{\partial T}{\partial x} \Bigg|_{dT/dx = 0}^{(T_f - T_u)/\delta_L} = -\Delta_c H \int_{-\infty}^{\delta_L/2} \dot{w}_\mathrm{F} \, dx \tag{57}$$

and hence,

$$\boxed{\tfrac{1}{2} \mathrm{C_P} \dot{m}^{"} \left(T_f - T_u\right) - \lambda \frac{T_f - T_u}{\delta_L} = 0} \tag{58}$$

since $\dot{w}_\mathrm{F}$ is practically zero in the preheat zone.

Correlations for the laminar burning velocity

Step 9:

Solve equations (54) and (58) for S_{uL} and δ_L:

$$S_{uL} = \left[-2\frac{\lambda}{\rho_u \mathrm{C_P}}\frac{\Delta_c H}{\mathrm{C_P}\left(T_f - T_u\right)}\frac{\overline{\dot{w}}_\mathrm{F}}{\rho_u}\right]^{\frac{1}{2}} \tag{59}$$

$$\delta_L = \left[-2\frac{\lambda}{\rho_u \mathrm{C_P}}\frac{\mathrm{C_P}\left(T_f - T_u\right)}{\Delta_c H}\frac{\rho_u}{\overline{\dot{w}}_\mathrm{F}}\right]^{\frac{1}{2}} \tag{60}$$

Express the heat of combustion of the fuel as

$$\Delta_c H = (\nu + 1)\mathrm{C_P}(T_f - T_u) \tag{61}$$

and substitute this into equations (59) and (60):

$$S_{uL} = \left[-2\frac{\lambda}{\rho_u \mathrm{C_P}}(\nu + 1)\frac{\overline{\dot{w}}_\mathrm{F}}{\rho_u}\right]^{\frac{1}{2}} \tag{62}$$

$$\delta_L = \left[-2\frac{\lambda}{\rho_u \mathrm{C_P}}\frac{1}{\nu + 1}\frac{\rho_u}{\overline{\dot{w}}_\mathrm{F}}\right]^{\frac{1}{2}} \tag{63}$$

Step 10:

Assume a generalized overall reaction,

$$\sum_{i=1}^{N}\nu_i^{'}\mathrm{M}_i \longrightarrow \sum_{i=1}^{N}\nu_i^{''}\mathrm{M}_i \tag{64}$$

with a an overall reaction order $n = \sum_{i=1}^{N}\nu_i^{'}$

Mass consumption rate of each individual species:

$$\frac{d\left(\rho Y_i/\mathcal{M}_i\right)}{dt} = \left(\nu_i^{''} - \nu_i^{'}\right) BT^m \exp\left(-\frac{\mathrm{E_a}}{\mathrm{R}T}\right)\prod_{j=1}^{N}\left(\frac{\rho Y_j}{\mathcal{M}_j}\right)^{\nu_j^{'}} \tag{65}$$

$$\Longrightarrow \qquad \overline{\dot{w}}_\mathrm{F} \propto \rho^n BT^m \exp\left(-\frac{\mathrm{E_a}}{\mathrm{R}T}\right)\prod_{j=1}^{N}\left(Y_j/\mathcal{M}_j\right)^{\nu_j^{'}} \tag{66}$$

Since

$$\rho_u \propto T_u^{-1}P \tag{67}$$

and most of the combustion occurs in the reaction zone,

$$\overline{\dot{w}}_\mathrm{F} \propto T_f^{-n}P^n T_f^m \exp\left[-\frac{\mathrm{E_a}}{\mathrm{R}T_f}\right] \tag{68}$$

Correlations for the laminar burning velocity

Step 11:

Substitute equations (67) and (68) into equations (62) and (63) to obtain:

$$\frac{S_{uL}}{S_{uL}^{\circ}} \propto \sqrt{\frac{\lambda(T_u)}{\lambda(T_{u0})}} \frac{T_u}{T_{u0}} \left(\frac{P}{P_0}\right)^{\frac{n-2}{2}} \left(\frac{T_f}{T_f^{\circ}}\right)^{-\frac{n}{2}} \left(\frac{T_f}{T_f^{\circ}}\right)^{\frac{m}{2}} \exp\left[-\frac{\mathrm{E_a}}{2\mathrm{R}}\left(\frac{1}{T_f} - \frac{1}{T_f^{\circ}}\right)\right] \tag{69}$$

$$\frac{\delta_L}{\delta_L^{\circ}} \propto \sqrt{\frac{\lambda(T_u)}{\lambda(T_{u0})}} \left(\frac{P}{P_0}\right)^{-\frac{n}{2}} \left(\frac{T_f}{T_f^{\circ}}\right)^{\frac{n}{2}} \left(\frac{T_f}{T_f^{\circ}}\right)^{-\frac{m}{2}} \exp\left[+\frac{\mathrm{E_a}}{2\mathrm{R}}\left(\frac{1}{T_f} - \frac{1}{T_f^{\circ}}\right)\right] \tag{70}$$

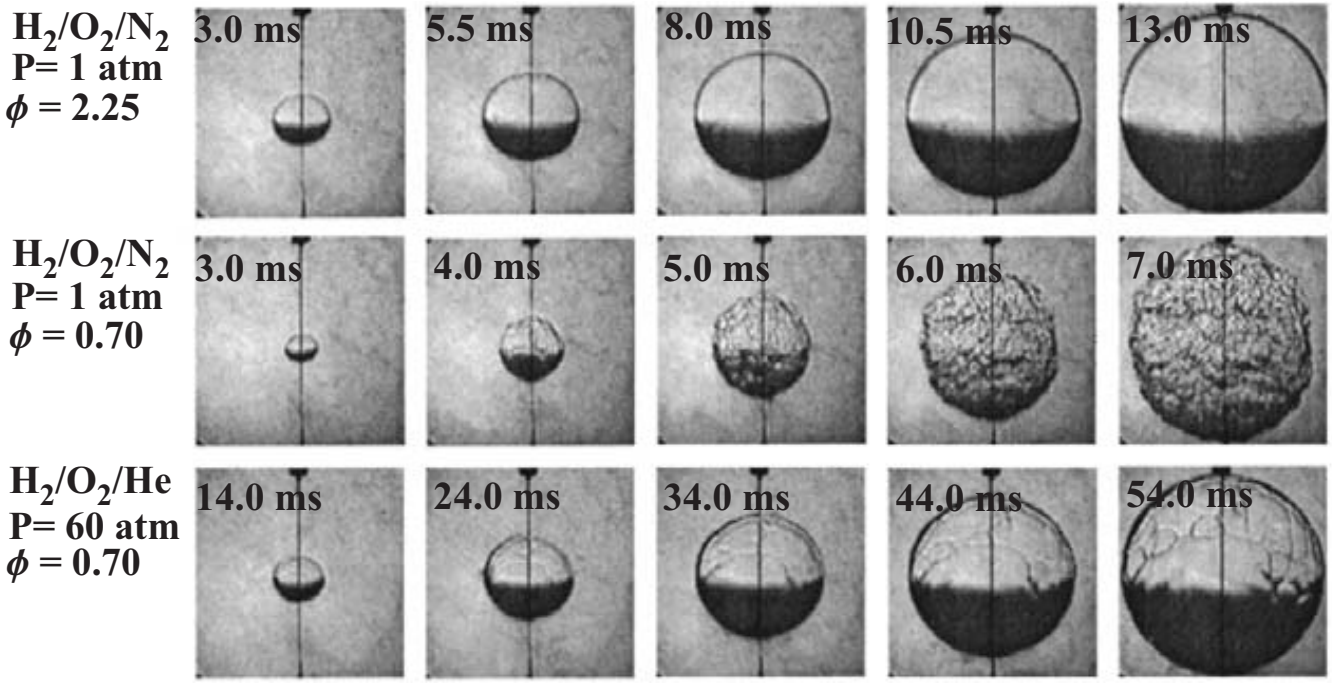
where S_{uL}°, δ_L° and T_f° are the laminar burning velocity, the laminar flame thickness and the flame temperature of the unburnt mixture at a reference state P_0 and T_{u0}.

When the variation in T_u is caused by adiabatic compression, equations (69) and (70) can be approximated by:

$$\frac{S_{uL}}{S_{uL}^{\circ}} = \left(\frac{P}{P_0}\right)^{c+\frac{\gamma-1}{\gamma}-1+\alpha} \tag{71}$$

$$\frac{\delta_L}{\delta_L^{\circ}} = \left(\frac{P}{P_0}\right)^{c-\alpha} \tag{72}$$

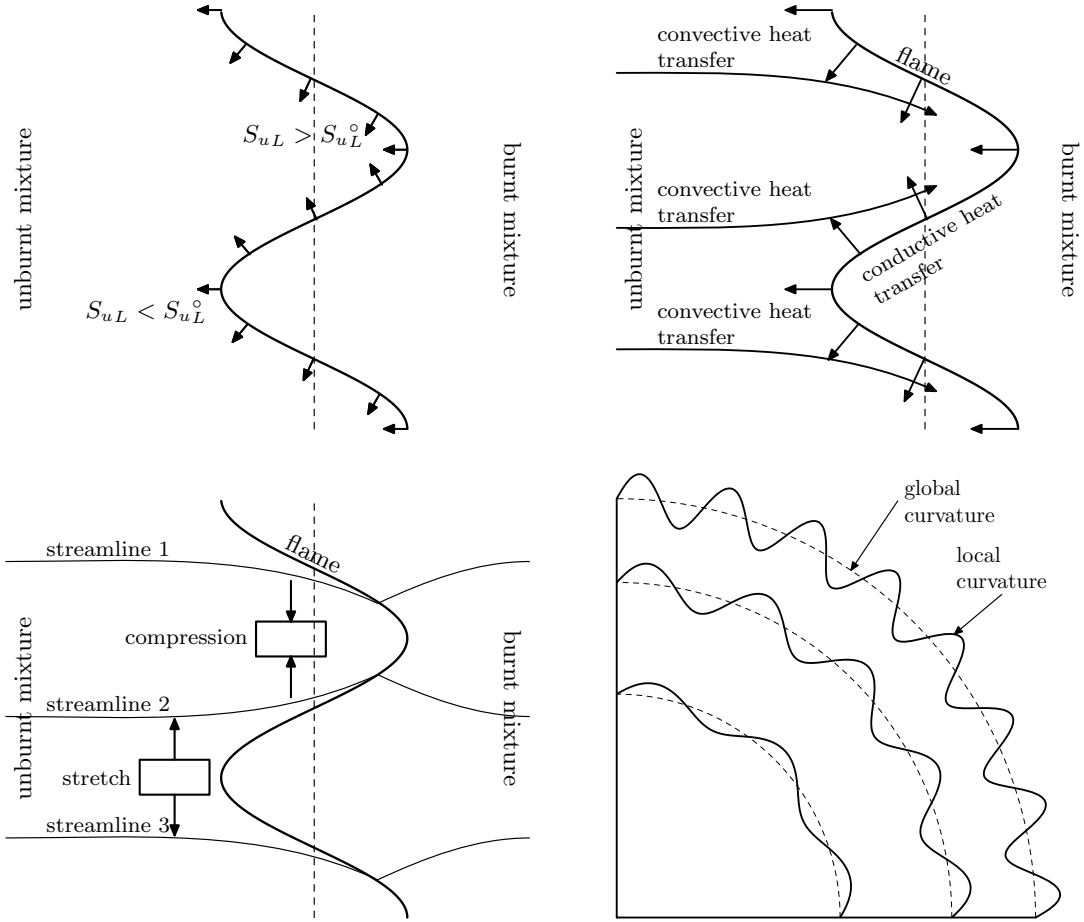
Effect of flame morphology on the laminar burning velocity



Flame morphology of propagating hydrogen-air flames.

From: Tse S.D., Zhu D.L., and Law C.K. Morphology and burning rates of expanding spherical flames in H2/O2/inert mixtures up to 60 atmospheres. In Proceedings of the Twenty-Eighth Symposium (International) on Combustion, pages 1793-1800, Pittsburgh, 2000. The Combustion Institute.

Effect of flame stretch and flame curvature on the laminar burning velocity



Effect of flame stretch and flame curvature on the laminar burning velocity.

Effect of flame stretch and flame curvature on the laminar burning velocity

Stretch rate of a surface element in a strained fluid:

$$\dot{s} = \frac{1}{A}\frac{dA}{dt} \tag{73}$$

Universal expression which relates the stretch rate of a flame surface element to the velocity field, $\boldsymbol{v}$, of a non-uniform flow-field:

$$\dot{s} = \underbrace{-\boldsymbol{nn}{:}\nabla\boldsymbol{v} + \nabla\cdot\boldsymbol{v}}_{\dot{s}_s} + \underbrace{S_{uL}^{\circ}\nabla\cdot\boldsymbol{n}}_{\dot{s}_c} \tag{74}$$

When a planar laminar flame with a thickness δ_L° is distorted into a bulge of size Λ, the local laminar burning velocity at each point can be related to the local stretch rate as

$$\frac{S_{uL}^{\circ} - S_{uL}}{S_{uL}^{\circ}} = \frac{\mathcal{L}}{S_{uL}^{\circ}}\left(\frac{1}{A}\frac{dA}{dt}\right) + \mathcal{O}\left(\epsilon^2\right) \tag{75}$$

where $\epsilon = \delta_L^{\circ}/\Lambda$. When $\Lambda \gg \delta_L^{\circ}$, ϵ is a small number so that:

$$S_{uL}^{\circ} - S_{uL} = \mathcal{L}\left(\frac{1}{A}\frac{dA}{dt}\right) + \mathcal{O}\left(\epsilon^2\right) \tag{76}$$

$$= \mathcal{L}\dot{s} + \mathcal{O}\left(\epsilon^2\right) \tag{77}$$

Effect of flame stretch and flame curvature on the laminar burning velocity

Express $\mathcal{L}\dot{s}$ as a linear combination of quantities that account for the separate effects of the strain rate, flame curvature, pressure, etc., each having its own Markstein length:

$$\mathcal{L}\dot{s} \equiv \mathcal{L}_s \dot{s}_s + \mathcal{L}_c \dot{s}_c + \ldots \tag{78}$$

$$\implies S_{uL}^{\circ} - S_{uL} = \left(\mathcal{L}_s \dot{s}_s + \mathcal{L}_c \dot{s}_c + \ldots\right) + \mathcal{O}\left(\epsilon^2\right) \tag{79}$$

Combine equations (74), (77) and (79):

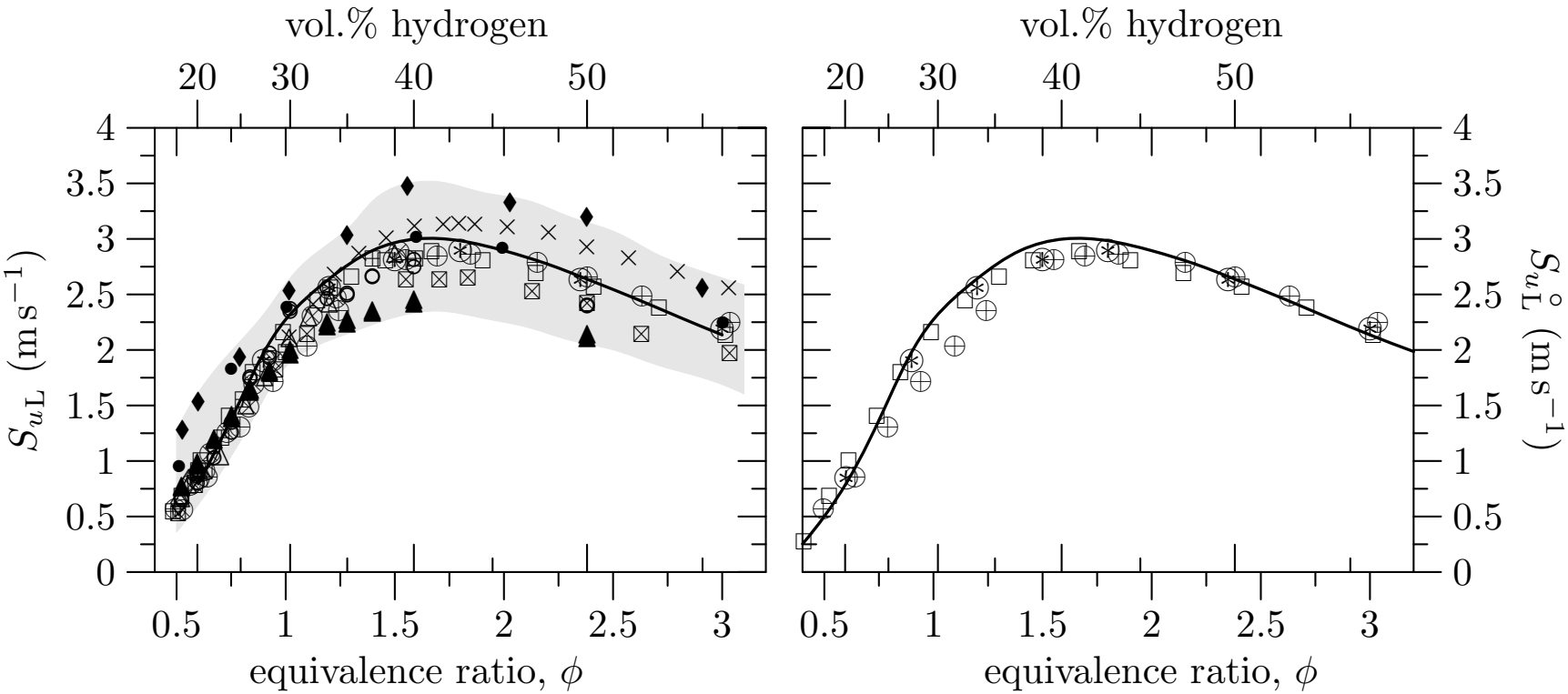
$$S_{uL} = \mathcal{L}_s \left[\boldsymbol{nn}{:}\nabla\boldsymbol{v} - \nabla\cdot\boldsymbol{v}\right] + \left[1 - \mathcal{L}_c \nabla\cdot\boldsymbol{n}\right] S_{uL}^{\circ} \tag{80}$$

$$= \mathcal{L}_s \left[\boldsymbol{nn}{:}\nabla\boldsymbol{v} - \nabla\cdot\boldsymbol{v}\right] + \left[1 + \frac{\mathcal{L}_c}{\kappa_1 + \kappa_2}\right] S_{uL}^{\circ} \tag{81}$$

$$= \mathcal{L}_s \left[\boldsymbol{nn}{:}\nabla\boldsymbol{v} - \nabla\cdot\boldsymbol{v}\right] + \left[1 + \frac{\mathcal{L}_c}{\mathcal{R}}\right] S_{uL}^{\circ} \tag{82}$$

The quantities denoted by $\mathcal{L}_s$ and $\mathcal{L}_c$ are called Markstein lengths.

Unstretched laminar burning velocity



Unstretched laminar burning velocity of hydrogen-air mixtures as a function of equivalence ratio at T_0=293.15–298.15 K and P_0=1 bar.

Correlations for the turbulent burning velocity

$$\text{Damköhler:} \quad \frac{S_{uT}}{S_{uL}} = 1 + \frac{v'_{\text{rms}}}{S_{uL}} \tag{83}$$

$$\text{Schelkin:} \quad \frac{S_{uT}}{S_{uL}} = \sqrt{1 + \left(\frac{v'_{\text{rms}}}{S_{uL}}\right)^2} \tag{84}$$

$$\text{Karloviz:} \quad \frac{S_{uT}}{S_{uL}} = 1 + \frac{v'_{\text{rms}}}{S_{uL}} \quad \text{(weak turbulence)} \tag{85}$$

$$\frac{S_{uT}}{S_{uL}} = 1 + \sqrt{\tfrac{5}{12}}\frac{v'_{\text{rms}}}{S_{uL}} \quad \text{(intermediate turbulence)} \tag{86}$$

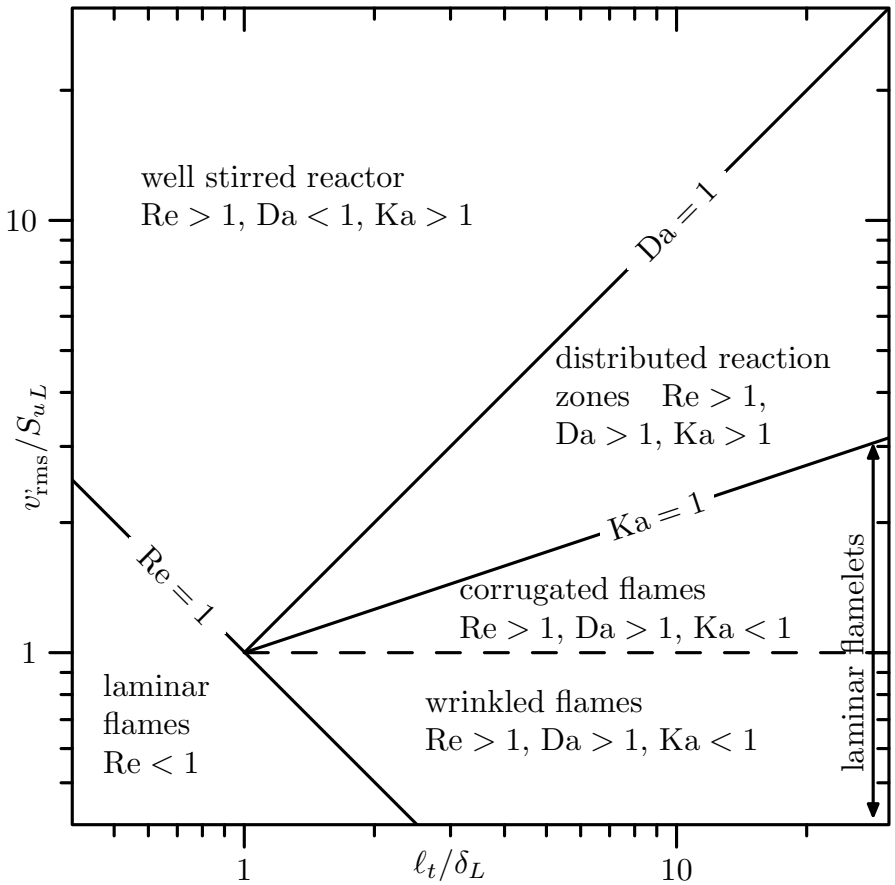
$$\frac{S_{uT}}{S_{uL}} = 1 + \sqrt{2}\left(\frac{v'_{\text{rms}}}{S_{uL}}\right)^{\frac{1}{2}} \quad \text{(strong turbulence)} \tag{87}$$

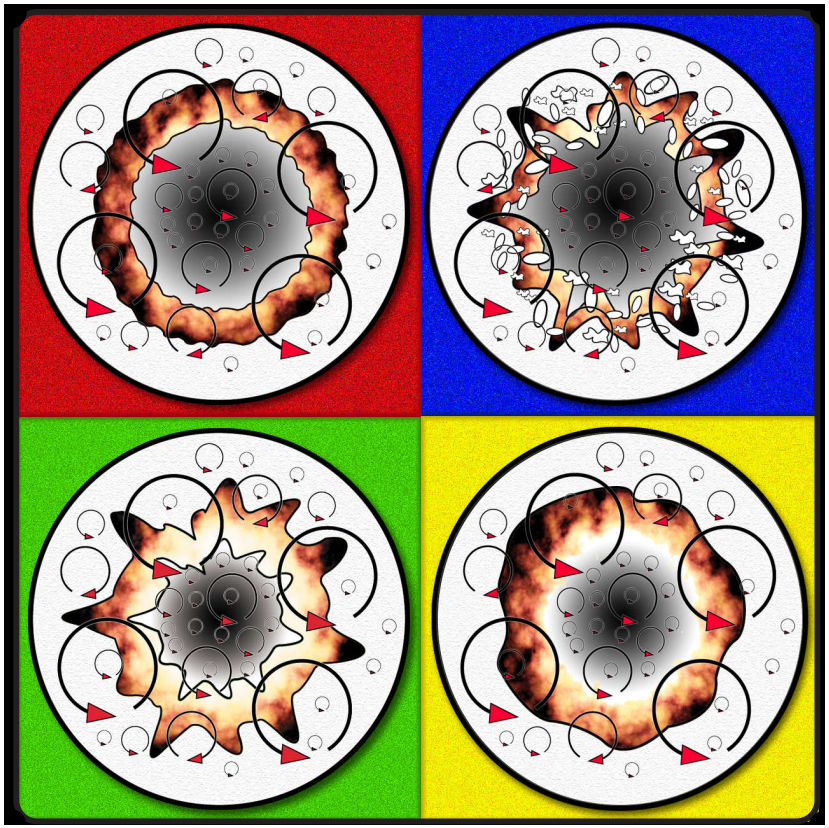
$$\text{Gülder:} \quad \frac{S_{uT}}{S_{uL}} = 1 + \sqrt[4]{\left(\tfrac{2}{15}\right)}\,\text{Re}_{\ell_t}^{\frac{1}{4}}\left(\frac{v'_{\text{rms}}}{S_{uL}}\right)^{\frac{1}{2}} \tag{88}$$

$$\text{Bradley:} \quad \frac{S_{uT}}{S_{uL}} = C\,(\text{Da}/\text{PrLe})^{0.3}\,\text{Re}_{\ell_t}^{-0.15}\left(\frac{v'_{\text{rms}}}{S_{uL}}\right) \tag{89}$$

$$\text{Yakhot:} \quad \frac{S_{uT}}{S_{uL}} = \exp\left[v'^2_{\text{rms}}/S_{uT}^2\right] \tag{90}$$

Correlations for the turbulent burning velocity





Damköhler's correlation for the turbulent burning velocity

Equate mass flux, $\dot{m}$, through cross sectional area of flame brush, A_T to mass flow of unburnt mixture through wrinkled laminar flame area, A_L:

$$\dot{m} = \rho_u A_T S_{uT} = \rho_u A_L S_{uL} \tag{91}$$

$$\Rightarrow \frac{S_{uT}}{S_{uL}} = \frac{A_L}{A_T} \tag{92}$$

Damköhler approximated the ratio of the area of wrinkled laminar flame and the cross section of the turbulent flame brush by

$$\frac{A_L}{A_T} = \frac{S_{uL} + v'_{\text{rms}}}{S_{uL}} = 1 + \frac{v'_{\text{rms}}}{S_{uL}} \tag{93}$$

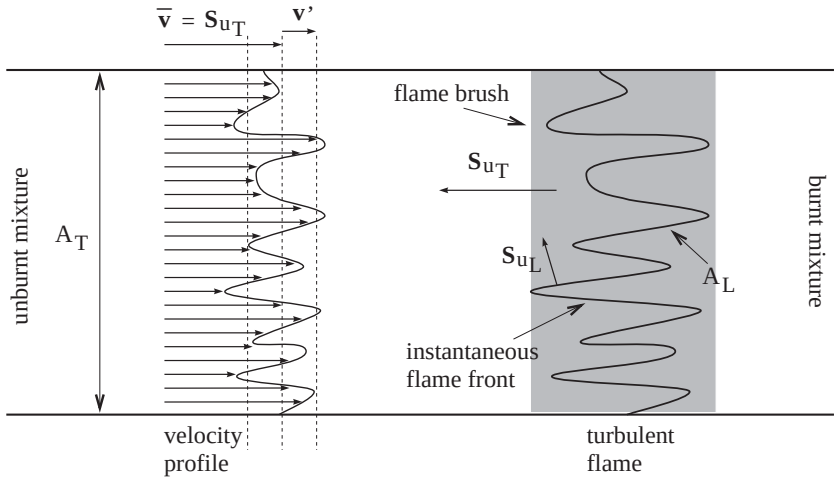
Substitution into equation (92) leads to

$$\boxed{\frac{S_{uT}}{S_{uL}} = 1 + \frac{v'_{\text{rms}}}{S_{uL}}} \tag{94}$$

In the limit $v'_{\text{rms}} \gg S_{uL}$, equation (94) implies that the turbulent burning velocity becomes independent of the laminar burning velocity

$$S_{uT} \sim v'_{\text{rms}} \tag{95}$$

This is known as Damköhler's hypothesis.



Schelkin's correlation for the turbulent burning velocity

Schelkin assumed:

• Turbulence creates conical bulges in a laminar flame.

• Increased flame surface is proportional to the average cone area divided by the average cone base.

• If the radius of the cone base and the apothem are denoted by R and h, then the surface area of the cone base and the cone mantle are equal to πR^2 and $\pi R\sqrt{R^2+h^2}$.

• When a circular element of a planar laminar flame is bulged into a cone, the surface area increases by a factor $\sqrt{R^2+h^2}/R$.

• Diameter of the cone base is proportional to the average length scale of the turbulence, $R \propto \frac{1}{2}\ell_t$.

• Diameter of the cone base is proportional to the average length scale of the turbulence, $R \propto \frac{1}{2}\ell_t$ and that the apothem scales as $h \propto v'_{\rm rms}\ell_t/S_{uL}$.

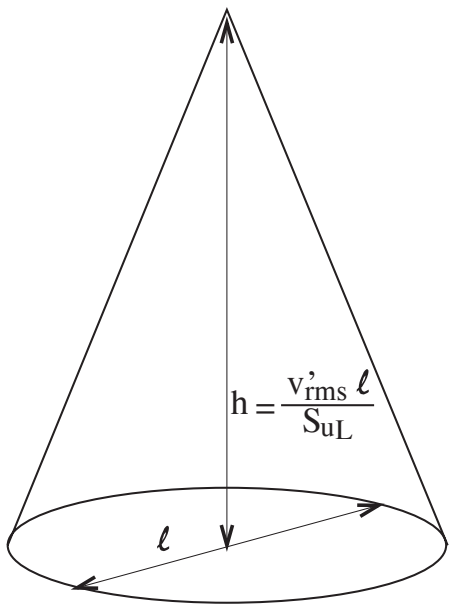
• Apothem to be proportional to the average fluctuating velocity $v'_{\rm rms}$ and the time during which an element of the flame interacts with an eddy, ℓ_t/S_{uL}.

These assumptions lead to

$$\frac{A_L}{A_T} = \frac{\sqrt{R^2+h^2}}{R} = \sqrt{1+\left(\frac{2v'_{\rm rms}}{S_{uL}}\right)^2} \qquad (96)$$

and substitution into equation (92) gives:

$$\boxed{\frac{S_{uT}}{S_{uL}} = \sqrt{1+\left(\frac{2v'_{\rm rms}}{S_{uL}}\right)^2}} \qquad (97)$$



Karloviz's correlations for the turbulent burning velocity

Define a turbulence macro velocity scale, a turbulence macro time scale and a turbulence macro length scale:

$$v_t = v'_{\mathrm{rms}} = (\overline{v'^2})^{\frac{1}{2}}$$

$$\tau_t = \int_0^\infty \rho(\tau) d\tau \qquad \text{where} \qquad \rho(\tau) = \frac{\overline{v'(t)v'(t+\tau)}}{\overline{v'^2(t)}}$$

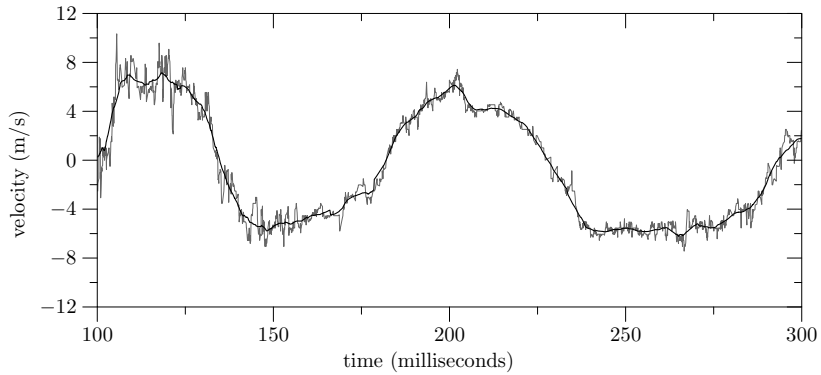
$$\ell_t = v_t \tau_t = v'_{\mathrm{rms}} \tau_t$$

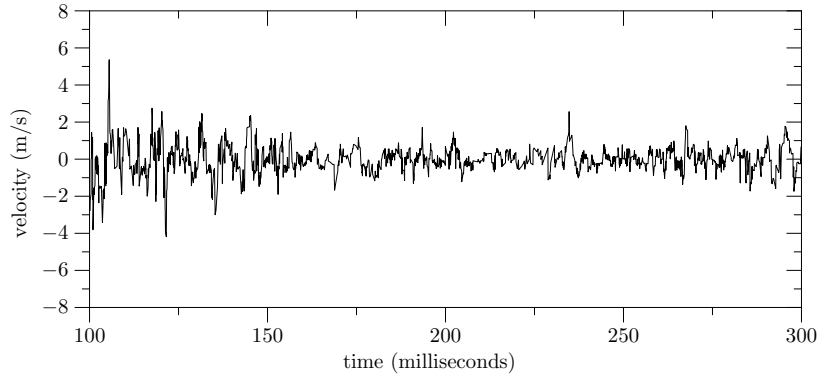
Karlovitz assumed that an additional velocity produced by the turbulent diffusion, ${S_u}^t$, has to be added to the laminar burning velocity:

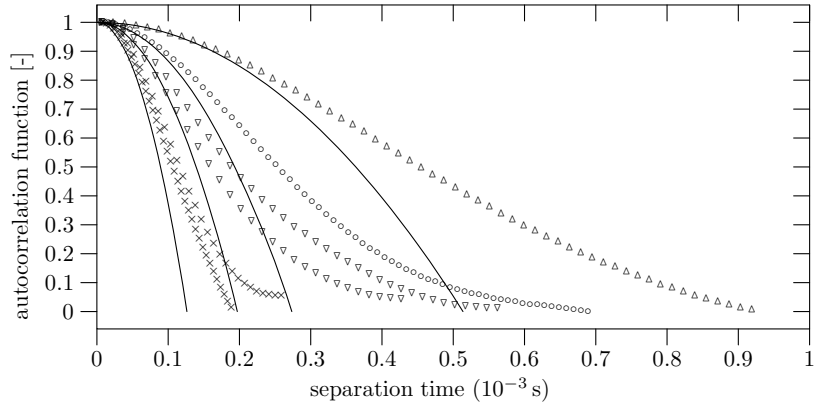
$$S_{uT} = S_{uL} + {S_u}^t \tag{98}$$

The additional velocity is taken into account by dividing the root-mean-square displacement due to the turbulence by the average time interval during which a flame element interacts with an eddy, $\mathcal{T} = \ell_t / S_{uL}$:

$${S_u}^t = \frac{(\overline{x'^2})^{\frac{1}{2}}}{\mathcal{T}} \tag{99}$$







Karloviz's correlations for the turbulent burning velocity

The root-mean-square displacement and root-mean-square velocity are interrelated through:

$$\frac{d\overline{x'^2}}{dt} = 2\,\overline{v'^2}\int_0^t \rho(\tau)\,d\tau = 2\,(v'_{\rm rms})^2\int_0^t \rho(\tau)\,d\tau \tag{100}$$

Weak turbulence: $v'_{\rm rms} \ll S_{uL}$. Hence $\mathcal{T}\,(\equiv \ell_t/S_{uL}) \ll \tau_t\,(\equiv \ell_t/v'_{\rm rms})$. Consequently, $\rho(\tau) \approx 1$ if $t \leq \mathcal{T}$ so that the root-mean-square displacement within the interaction time between a flame element and a turbulent eddy becomes (by integrating equation (100)): $(\overline{x'^2})^{\frac{1}{2}} = v'_{\rm rms}\mathcal{T}$

$$\Longrightarrow {S_u}^t = \frac{(\overline{x'^2})^{\frac{1}{2}}}{\mathcal{T}} = \frac{v'_{\rm rms}\mathcal{T}}{\mathcal{T}} = v'_{\rm rms} \tag{101}$$

Substitution into equation (98) and division by S_{uL} results in

$$\boxed{\frac{S_{uT}}{S_{uL}} = 1 + \frac{v'_{\rm rms}}{S_{uL}}} \tag{102}$$

Strong turbulence: $\mathcal{T}\,(\equiv \ell_t/S_{uL}) \gg \tau_t\,(\equiv \ell_t/v'_{\rm rms})$. The integral on the right hand side of equation (100) assumes a definite value which is equal to the time scale of the turbulence, τ_t. This leads to

$$(\overline{x'^2})^{\frac{1}{2}} = \sqrt{2\ell_t v'_{\rm rms}\mathcal{T}} \tag{103}$$

and

$${S_u}^t = \frac{(\overline{x'^2})^{\frac{1}{2}}}{\mathcal{T}} = \frac{\sqrt{2\ell_t v'_{\rm rms}\mathcal{T}}}{\ell_t/S_{uL}} = \sqrt{2S_{uL}v'_{\rm rms}} \tag{104}$$

Insertion into equation (98) and division by S_{uL} yields:

$$\boxed{\frac{S_{uT}}{S_{uL}} = 1 + \sqrt{2}\left(\frac{v'_{\rm rms}}{S_{uL}}\right)^{\frac{1}{2}}} \tag{105}$$

Intermediate turbulence: $\mathcal{T}\,(\equiv \ell_t/S_{uL}) \approx \tau_t\,(\equiv \ell_t/v'_{\rm rms})$, the root-mean-square displacement depends on the shape of the correlation function. If the shape of the correlation function is approximated by an osculation parabola, where τ_m denotes the Taylor microscale,

$$\rho(\tau) = 1 - \frac{1}{2}\frac{\tau^2}{{\tau_m}^2} \tag{106}$$

the integral in (100) may be solved for the variance of the displacement to give

$$\overline{x'^2} = \overline{v'^2}\left[\tfrac{1}{2}\mathcal{T}^2 - \tfrac{1}{12}(\mathcal{T}^4/\tau_m^2)\right] \approx \overline{v'^2}\left[\tfrac{1}{2}\mathcal{T}^2 - \tfrac{1}{12}\mathcal{T}^2\right] \approx \tfrac{5}{12}\overline{v'^2}\mathcal{T}^2 \tag{107}$$

Consequently,

$${S_u}^t = \frac{(\overline{x'^2})^{\frac{1}{2}}}{\mathcal{T}} = \frac{\sqrt{\frac{5}{12}}v'_{\rm rms}\mathcal{T}}{\mathcal{T}} = \sqrt{\tfrac{5}{12}}v'_{\rm rms} \tag{108}$$

and

$$\boxed{\frac{S_{uT}}{S_{uL}} = 1 + \sqrt{\tfrac{5}{12}}\frac{v'_{\rm rms}}{S_{uL}}} \tag{109}$$