JOINT EUROPEAN SUMMER SCHOOL ON FUEL CELL AND HYDROGEN TECHNOLOGIES

THE SAFETY OF HYDROGEN TECHNOLOGIES

MITIGATION OF HYDROGEN DEFLAGRATIONS

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MITIGATION STRATEGIES

- INERTISATION
- FLAME QUENCHING
  \[\Rightarrow\] PRESSURE RELIEF VENTING
The basic idea behind pressure relief venting
Deflagration parameters

\[ n_0 \text{Reactants} \rightarrow n_p \text{Products} \quad \implies \quad P_{\text{max}} = \frac{n_p T_f}{n_0 T_0} P_0 \]
Deflagration parameters

Experimental deflagration pressure curves of hydrogen-air mixtures at initial conditions $T_0=298.15\,\text{K}$ and $P_0=1\,\text{bar}$. 
Deflagration parameters

Experimental deflagration pressure curves of methane-air mixtures at initial conditions $T_0=298.15 \text{ K}$ and $P_0=1 \text{ bar}$.
Deflagration parameters

Determination of explosion parameters from experimental deflagration pressure curves.
Scaling an explosion: a matter of invariance across size?

\[ K_{St} = \left( \frac{dP}{dt} \right)_{max} V^{\frac{1}{3}} \]

\( P_{max} \quad \left( \frac{dP}{dt} \right)_{max} \)
Scaling an explosion: a matter of invariance across size?

Adiabatic flame temperature (K)

Equivalence ratio, $\phi$

vol.% hydrogen

$H_2-O_2$

$H_2$-air

isobaric

isochoric

$\square$ CHEMEQUIL
Scaling an explosion: a matter of invariance across size?

H₂-O₂; isochoric
△ expt. 6 dm³
● GASEQ
□ CHEMEQUIL

H₂-air; isochoric
○ expt. 169 mm³
△ expt. 6 dm³
× expt. 120 dm³
● GASEQ
□ CHEMEQUIL
Scaling an explosion: a matter of invariance across size?

Despite this similarity the inflection point occurs for a different reason in the 169 ml vessel used in the present work. As discussed previously by Dahoe and de Goey (2003), the duration of an explosion in a 20-l sphere is long enough to allow the flame ball to rise in the vessel due to buoyancy. As a result, there is still a layer of unburnt mixture present below the lower hemispherical part of the flame, after all reactants ahead of the upper hemispherical part of the flame have been consumed.

Because the surface area of the lower hemispherical part of the flame decreases progressively during the consumption of the remaining part of the reactants in the final stage of the explosion, the accompanying rate of pressure rise also decreases progressively. Although the role of buoyancy is negligible in the 169 ml vessel, there is still the effect of a progressively decreasing flame surface area in the final stage of the explosion. Initially, the flame ball grows with a progressively increasing flame surface area, until it reaches the wall of the vessel. From that moment onwards, the flame surface area, and hence the rate of pressure rise, decreases progressively as the reactants in the corners of the vessel are being consumed.

It may also be observed from Fig. 2 that, unlike with methane–air mixtures, the pressure–time curves of hydrogen–air mixtures exhibit oscillations whose magnitude may vary up to about 0.25 bar. These oscillations arise with both fuel-lean and fuel-rich mixtures, and tend to become zero when the mixture strength approaches the flammability limits. Their onset occurs before the maximum explosion pressure is reached, after an initial period of smooth pressure buildup, and their presence continues after the explosion has completed. The cause of this phenomenon is described by Garforth and Rallis (1976) and Lewis and von Elbe (1961), Chapter 15, and will be discussed in Section 3.

To enable a comparison with results presented by other researchers, the maximum explosion pressure, $P_{\text{max}}$, and the maximum rate of pressure rise, $(dP/dt)_{\text{max}}$, were determined as illustrated by the upper part of Fig. 3.
Application of deflagration parameters to vented explosions

\[
\Pi = \frac{P - P_0}{P_{\text{max}} - P_0} \quad \text{and} \quad \Gamma = C_d c_d \sqrt{\frac{\gamma + 1}{2}} \frac{A_v}{V^2/3} \frac{P_{\text{max}} - P_0}{K_G}
\]
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:

\[
\frac{m_u}{m_{u0}} = \frac{P_{max} - P}{P_{max} - P_0}
\]  

(1)

Differentiation with respect to time:

\[
\frac{dP}{dt} = -\frac{P_{max} - P_0}{m_{u0}} \frac{dm_u}{dt}
\]

(2)

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

\[
\frac{dm_u}{dt} = -4\pi r_f^2 \rho_u S_u
\]

(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

\[
\frac{dm_u}{dt} = -4\pi r_f^2 \rho_u S_u
\]

(4)

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

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

(5)
Derivation of a simple deflagration model

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

$$\frac{\rho_u}{\rho_u} = \left(\frac{P_0}{P}\right)^{\frac{1}{\gamma}}$$ \hspace{1cm} (6)

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

$$\frac{4}{3}\pi r_f^3 = V_{\text{vessel}} - \frac{m_uRT_u}{P}$$ \hspace{1cm} (7)

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

$$\frac{m_u\hat{R}T_u}{P} = V_{\text{vessel}}\rho_u P_{\text{max}} - P - \rho_u P_{\text{max}} - P_0 = V_{\text{vessel}} \left(\frac{\rho_u}{\rho_u}\right) \frac{P_{\text{max}} - P}{P_{\text{max}} - P_0} \hspace{1cm} (8)$$

$$= V_{\text{vessel}} \left(\frac{P_0}{P}\right)^{\frac{1}{\gamma}} \frac{P_{\text{max}} - P}{P_{\text{max}} - P_0}$$

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

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

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

(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 $P = P_{\text{max}}$. By substituting $P = P_{\text{max}}$ 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:

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

(11)

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


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:

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

(12)

where \( \rho \) 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

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

(13)
Derivation of a vented deflagration model

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

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

(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.

Peculiarities of vented deflagrations

Peculiarities of vented deflagrations: flame distortion by vent ducts


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

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


Dynamic venting area:

\[ F(\phi) = \min \left[ F_N, 2L \sin \left( \frac{\phi}{2} \right) \left( b + L \cos \left( \frac{\phi}{2} \right) \right) \right] \]  \hspace{1cm} (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 ($\tau = tS_{uL}/R_s$, $\Pi = P/P_0$, $n_u = m_u/m_{u0}$ 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.

\[
\frac{d\Pi}{d\tau} = 3\Pi \frac{\chi(\tau) \Pi^{\epsilon + \frac{1}{\gamma_u}} (1 - n_u \Pi^{-\frac{1}{\gamma_u}})^{\frac{2}{3}} - \gamma_b W_\Sigma(\tau) R_\Sigma}{\Pi^{\frac{1}{\gamma_u}} - (\frac{\gamma_u}{\gamma_b} n_u M_{\Sigma})} \tag{16}
\]

\[
\frac{dn_b}{d\tau} = 3 \left\{ \chi(\tau) \Pi^{\epsilon + \frac{1}{\gamma_u}} (1 - n_u \Pi^{-\frac{1}{\gamma_u}})^{\frac{2}{3}} - R^\#_b W_\Sigma(\tau) \frac{\sum A_j(\tau) \mu_j F_j(\tau)}{\sum \mu_j F_j(\tau)} \right\} \tag{17}
\]

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

\[
R_\Sigma = R^\#_u W_\Sigma(\tau) \frac{\sum A_j(\tau) \mu_j F_j(\tau)}{\sum \mu_j F_j(\tau)} + R^\#_b W_\Sigma(\tau) \frac{\sum A_j(\tau) \mu_j F_j(\tau)}{\sum \mu_j F_j(\tau)} \tag{19}
\]
Vented deflagrations with hinged inertial vent covers

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

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

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

where \( E \) is an expansion coefficient of the combustion products. For the transient venting parameter \( W_\Sigma \):

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

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.

\[
\frac{S_{uL}}{S_{uL_0}} = (\frac{T_u}{T_{u0}})^{\beta_1}
\]

\[
\beta_1 = (140.0 \pm 3.7) \cdot 10^{-2}
\]

Effect of temperature
\( \phi = 1, \ P = 1 \text{ bar} \)
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.
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:
\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (23)
\]
\[
\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p + \nabla \cdot \mathbf{\tau} + \sum_{i=1}^{N} \rho Y_i f_i \quad (24)
\]
\[
\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho \mathbf{v} Y_i) = -\nabla \cdot [\rho Y_i \mathbf{V}_i] + \dot{w}_i \quad (25)
\]
\[
\frac{\partial (\rho h)}{\partial t} + \nabla \cdot (\rho \mathbf{v} h) = \frac{\partial p}{\partial t} + \mathbf{v} \cdot \nabla p + \mathbf{\tau} : \nabla \mathbf{v} - \nabla \cdot [\lambda \nabla T] + \nabla \cdot \mathbf{q} + \sum_{i=1}^{N} \rho Y_i h_i \mathbf{V}_i \quad (26)
\]
\[
\rho = \frac{\gamma - 1}{\gamma} \sum_{i=1}^{N} Y_i \left[ h^0_{fi} + \int_{T_0}^{T} C_{Pi}(T) \, dT \right] \quad (27)
\]
where \( \mathbf{\tau} = \mu \left[ \nabla \mathbf{v} + \left( \nabla \mathbf{v} \right)^T \right] + \left( \kappa - \frac{2}{3} \mu \right) [\nabla \cdot \mathbf{v}] \mathbf{I} \quad (28) \]
and \( \mathbf{q} = \varepsilon \sigma T^4 \quad (29) \)

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:

\[
\nabla \cdot \left[ \rho Y_i (v + V_i) \right] = \dot{w}_i \tag{30}
\]
\[
\nabla \cdot \left[ \sum_{i=1}^{N} \rho Y_i h_i (v + V_i) - \lambda \nabla T \right] = 0 \tag{31}
\]

Step 2: Use

\[
h_i = h_{f_i}^\circ + \int_{T^\circ}^{T} C_{P_i} \, dT \tag{32}
\]

to rewrite equation (31) as

\[
\nabla \cdot \left[ \sum_{i=1}^{N} \rho Y_i (v + V_i) \, h_{f_i}^\circ \right. + \sum_{i=9}^{N} \rho Y_i (v + V_i) \int_{T^\circ}^{T} C_{P_i} \, dT - \lambda \nabla T \right] = 0 \tag{33}
\]

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

\[
\nabla \cdot \left[ \rho v \sum_{i=6}^{N} \int_{T^\circ}^{T} Y_i C_{P_i} \, dT + \rho \sum_{i=1}^{N} V_i \int_{T^\circ}^{T} Y_i C_{P_i} \, dT - \lambda \nabla T \right] = - \sum_{i=1}^{N} h_{f_i}^\circ \dot{w}_i \tag{34}
\]
Correlations for the laminar burning velocity

**Step 3:** Assume a background fluid so that
\[ \rho Y_i V_i = -\rho \mathbb{D} \nabla Y_i \]  
(35)

Since
\[ C_P = \sum Y_i C_P \]  
(36)

it is possible to rewrite equation (34) as
\[ \nabla \cdot \left[ \rho \mathbf{v} \int_{T^o}^T C_P \, dT + \rho \mathbb{D} \sum_{i=1}^N (\nabla Y_i) \int_{T^o}^T Y_i C_{P_i} \, dT - \rho \mathbb{D} \frac{\lambda}{\rho C_P \mathbb{D}} C_P \nabla T \right] = -\sum_{i=1}^N h_i^\circ \dot{w}_i \]  
(37)

and because of the equality,
\[ \nabla \int_{T^o}^T C_P \, dT = \nabla \sum_{i=1}^N Y_i \int_{T^o}^T C_{P_i} \, dT = \sum_{i=1}^N (\nabla Y_i) \int_{T^o}^T C_{P_i} \, dT + \sum_{i=1}^N Y_i \nabla \int_{T^o}^T C_{P_i} \, dT \]
(38)

\[ = \sum_{i=1}^N (\nabla Y_i) \int_{T^o}^T C_{P_i} \, dT + \sum_{i=1}^N Y_i C_{P_i} \nabla T = \sum_{i=6}^N (\nabla Y_i) \int_{T^o}^T C_{P_i} \, dT + C_P \nabla T \]  
(39)

equation (37) may be rewritten as
\[ \nabla \cdot \left[ \rho \mathbf{v} \int_{T^o}^T C_P \, dT + \rho \mathbb{D} \nabla \int_{T^o}^T C_P \, dT - \rho \mathbb{D} \left[ \text{Le} - 1 \right] C_P \nabla T \right] = -\sum_{i=1}^N h_i^\circ \dot{w}_i \]  
(40)
Correlations for the laminar burning velocity

Step 4:

Assume unity Lewis number in equation (40):

\[ \nabla \cdot \left[ \rho \mathbf{v} \int_{T_0}^{T} C_p \, dT + \rho D \nabla \int_{T_0}^{T} C_p \, dT \right] = - \sum_{i=1}^{N} h_{f,i}^o \dot{w}_i \]  

(41)

If \( Le = 1 \) then \( \rho D \) may be replaced by \( \lambda / C_p \) ! From figure with simplified flame structure: \( \rho_u \mathbf{v} = \rho_u S_{uL} = \dot{m}^\prime = \) constant.

Finally

\[ \dot{m}^\prime C_p \nabla T + \nabla \cdot [\lambda \nabla T] = - \sum_{i=1}^{N} h_{f,i}^o \dot{w}_i \]  

(42)
Correlations for the laminar burning velocity

Step 5:
Express the combustion reaction in terms of a mass balance:

\[ 1 \text{ kg Fuel} + \nu \text{ kg Oxidizer} \rightarrow (\nu + 1) \text{ kg Products} \quad (43) \]

Then

\[ -\dot{w}_F = -\frac{1}{\nu} \dot{w}_{Ox} = \frac{1}{\nu + 1} \dot{w}_{Pr} \quad (44) \]

and hence,

\[
\sum_{i=1}^{N} h_i^o \dot{w}_i = h_F^o \dot{w}_F + h_{Ox}^o \dot{w}_{Ox} + h_{Pr}^o \dot{w}_{Pr}
\]

\[ = \left( h_F^o + \nu h_{Ox}^o - (\nu + 1) h_{Pr}^o \right) \dot{w}_F
\]

\[ = \Delta_c H \dot{w}_F \quad (45) \]

where \( \Delta_c H \) denotes the fuel’s heat of combustion.

Equation (40) may then be restated as:

\[ \dot{m}^* C_P \nabla T + \nabla \cdot [\lambda \nabla T] = -\Delta_c H \dot{w}_F \quad (46) \]

Step 6:
Integrate the one-dimensional form of equation (46) from \( x \rightarrow -\infty \) to \( x \rightarrow \infty \) for the simplified flame structure,

\[ \dot{m}^* C_P \frac{dT}{dx} + \frac{d}{dx} \left( \lambda \frac{dT}{dx} \right) = -\Delta_c H \dot{w}_F \quad (47) \]

subjected to the boundary conditions,

\[ x \rightarrow -\infty : \quad T = T_u \quad x \rightarrow \infty : \quad T = T_f \quad (48) \]

and the subsidiary conditions,

\[ x \rightarrow -\infty : \quad \frac{dT}{dx} = 0 \quad x \rightarrow \infty : \quad \frac{dT}{dx} = 0 \quad (49) \]

Inside the flame zone,

\[ x \in \delta_L : \quad \frac{dT}{dx} = \frac{T_f - T_u}{\delta_L} \quad (50) \]

Integration of equation (47) gives:

\[ \dot{m}^* C_P T \bigg|_{T_u}^{T_f} + \lambda \frac{\partial T}{\partial x} \bigg|_{dT/dx=0} = -\Delta_c H \int_{-\infty}^{\infty} \dot{w}_F \, dx \quad (51) \]
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):

\[
\frac{dT}{dx} = \frac{T_f - T_u}{\delta_L} \quad \iff \quad dx = \frac{\delta_L}{T_f - T_u}dT
\]

(52)

Hence,

\[
m^*C_P \left( T_f - T_u \right) = -\frac{\delta_L \Delta H}{T_f - T_u} \int \dot{w}_F dT = -\delta_L \Delta H \bar{w}_F
\]

(53)

or, equivalently,

\[
\boxed{m^*C_P \left( T_f - T_u \right) + \delta_L \Delta H \bar{w}_F = 0}
\]

(54)

⇒ A single algebraic equation with two unknowns:
- the mass flux \( m^* \) (\( \equiv \rho u S_uL \)),
- and the laminar flame thickness \( \delta_L \).

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,

\[
x \to -\infty : \quad T = T_u \quad x = \delta_L/2 : \quad T = \frac{T_u + T_f}{2}
\]

(55)

and the subsidiary conditions,

\[
x \to -\infty : \quad \frac{dT}{dx} = 0 \quad x \to \delta_L/2 : \quad \frac{dT}{dx} = \frac{T_f - T_u}{\delta_L}
\]

(56)

Integration of equation (42) results in

\[
\boxed{m^*C_P T \frac{(T_u + T_f)}{T_u} + \lambda \frac{\partial T}{\partial x} \frac{(T_f - T_u)}{\delta_L} \left. \right|_{dt/dx=0} = -\Delta H \int_{-\infty}^{\delta_L/2} \dot{w}_F dx}
\]

(57)

and hence,

\[
\boxed{\frac{1}{2}C_P \dot{m}^* \left( T_f - T_u \right) - \lambda \frac{T_f - T_u}{\delta_L} = 0}
\]

(58)

since \( \dot{w}_F \) is practically zero in the preheat zone.
Correlations for the laminar burning velocity

**Step 9:**

Solve equations (54) and (58) for $S_uL$ and $\delta_L$:

\[
S_uL = \left[ -2 \frac{\lambda}{\rho_u C_P} \frac{\Delta_c H}{C_P (T_f - T_u)} \frac{\bar{w}_F}{\rho_u} \right]^{\frac{1}{2}}
\] (59)

\[
\delta_L = \left[ -2 \frac{\lambda}{\rho_u C_P} \frac{C_P (T_f - T_u) \rho_u}{\Delta_c H} \frac{\bar{w}_F}{\rho_u} \right]^{\frac{1}{2}}
\] (60)

Express the heat of combustion of the fuel as

\[
\Delta_c H = (\nu + 1) C_P (T_f - T_u)
\] (61)

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

\[
S_uL = \left[ -2 \frac{\lambda}{\rho_u C_P} (\nu + 1) \frac{\bar{w}_F}{\rho_u} \right]^{\frac{1}{2}}
\] (62)

\[
\delta_L = \left[ -2 \frac{\lambda}{\rho_u C_P} \frac{1}{\nu + 1} \frac{\rho_u}{\bar{w}_F} \right]^{\frac{1}{2}}
\] (63)

**Step 10:**

Assume a generalized overall reaction,

\[
\sum_{i=1}^{N} \nu_i^{\star} M_i \rightarrow \sum_{i=1}^{N} \nu_i M_i
\] (64)

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

Mass consumption rate of each individual species:

\[
\frac{d (\rho Y_i / M_i)}{dt} = (\nu_i^{\star} - \nu_i) BT^m \exp \left( -\frac{E_a}{R T} \right) \prod_{j=1}^{N} \left( \frac{\rho Y_j}{M_j} \right)^{\nu_j}
\] (65)

\[
\Rightarrow \bar{\dot{w}}_F \propto \rho^n BT^m \exp \left( -\frac{E_a}{R T_f} \right) \prod_{j=1}^{N} \left( Y_j / M_j \right)^{\nu_j}
\] (66)

Since

\[
\rho_u \propto T_u^{-1} P
\] (67)

and most of the combustion occurs in the reaction zone,

\[
\bar{\dot{w}}_F \propto T_f^{-n} P^n T_f^m \exp \left[ -\frac{E_a}{R T_f} \right]
\] (68)
Correlations for the laminar burning velocity

Step 11:

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

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

(69)

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

(70)

where \( S_{uL}^\circ, \delta_L^\circ \) and \( T_f^\circ \) 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:

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

(71)

\[
\frac{\delta_L}{\delta_L^\circ} = \left( \frac{P}{P_0} \right)^{c-\alpha}
\]

(72)
Effect of flame morphology on the laminar burning velocity

Flame morphology of propagating hydrogen-air flames.

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:

\[ \dot{s} = \frac{1}{A} \frac{dA}{dt} \quad (73) \]

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

\[ \dot{s} = -n_n : \nabla \mathbf{v} + \nabla \cdot \mathbf{v} + S_u^0 \nabla \cdot n \quad (74) \]

\( \dot{s}_s \) stretch rate due to stretching, \( \dot{s}_c \) stretch rate due to curvature.

When a planar laminar flame with a thickness \( \delta^0_L \) is distorted into a bulge of size \( \Lambda \), the local laminar burning velocity at each point can be related to the local stretch rate as

\[ \frac{S_{uL} - S_u^0}{S_u^0} = \frac{\mathcal{L}}{S_u^0} \left( \frac{1}{A} \frac{dA}{dt} \right) + \mathcal{O}(\epsilon^2) \quad (75) \]

where \( \epsilon = \delta^0_L / \Lambda \). When \( \Lambda \gg \delta^0_L \), \( \epsilon \) is a small number so that:

\[ S_{uL} - S_u^0 = \mathcal{L} \left( \frac{1}{A} \frac{dA}{dt} \right) + \mathcal{O}(\epsilon^2) \quad (76) \]

\[ = \mathcal{L} \dot{s} + \mathcal{O}(\epsilon^2) \quad (77) \]
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:

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

$$\implies S_{u_L} - S_{uL} = (\mathcal{L}_s\dot{s}_s + \mathcal{L}_c\dot{s}_c + \ldots) + \mathcal{O}(\epsilon^2)$$

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

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

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

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

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

Damköhler: \[ \frac{S_{uT}}{S_{uL}} = 1 + \frac{v'_{\text{rms}}}{S_{uL}} \] (83)

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

Karloviz: \[ \frac{S_{uT}}{S_{uL}} = 1 + \frac{v'_{\text{rms}}}{S_{uL}} \] (weak turbulence) (85)
\[ \frac{S_{uT}}{S_{uL}} = 1 + \sqrt{\frac{5}{12}} \frac{v'_{\text{rms}}}{S_{uL}} \] (intermediate turbulence) (86)
\[ \frac{S_{uT}}{S_{uL}} = 1 + \sqrt{2} \left( \frac{v'_{\text{rms}}}{S_{uL}} \right)^{\frac{1}{2}} \] (strong turbulence) (87)

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

Bradley: \[ \frac{S_{uT}}{S_{uL}} = C \left( \frac{\text{Da}}{\text{PrLe}} \right)^{0.3} \text{Re}_{\ell}^{-0.15} \left( \frac{v'_{\text{rms}}}{S_{uL}} \right) \] (89)

Yakhot: \[ \frac{S_{uT}}{S_{uL}} = \exp \left[ \frac{v'_{\text{rms}}^2}{S_{uT}^2} \right] \] (90)
Correlations for the turbulent burning velocity

\[
\text{well stirred reactor} \quad \text{Re} > 1, \text{Da} < 1, \text{Ka} > 1
\]

\[
\text{distributed reaction zones} \quad \text{Re} > 1, \text{Da} > 1, \text{Ka} > 1
\]

\[
\text{corrugated flames} \quad \text{Re} > 1, \text{Da} > 1, \text{Ka} < 1
\]

\[
\text{well stirred reactor} \quad \text{Re} = 1, \text{Da} = 1, \text{Ka} = 1
\]

\[
\text{laminar flames} \quad \text{Re} < 1
\]

\[
\text{wrinkled flames} \quad \text{Re} > 1, \text{Da} > 1, \text{Ka} < 1
\]
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

\[
\frac{S_{uT}}{S_{uL}} = 1 + \frac{v_{\text{rms}}}{S_{uL}} \tag{94}
\]

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 $\pi R^2$ 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 $h \propto \frac{v_{\text{rms}} \ell_t}{S_{uL}}$.
- Apothem to be proportional to the average fluctuating velocity $v_{\text{rms}}$ and the time during which an element of the flame interacts with an eddy, $\ell_t/S_{uL}$.

These assumptions lead to

$$\frac{A_L}{A_T} = \frac{\sqrt{R^2 + h^2}}{R} = \sqrt{1 + \left(\frac{2v_{\text{rms}}}{S_{uL}}\right)^2} \quad (96)$$

and substitution into equation (92) gives:

$$\frac{S_{uT}}{S_{uL}} = \sqrt{1 + \left(\frac{2v_{\text{rms}}}{S_{uL}}\right)^2} \quad (97)$$
Define a turbulence macro velocity scale, a turbulence macro time scale and a turbulence macro length scale:

\[ v_t = v_{\text{rms}} = \left( \frac{v^2}{2} \right)^{\frac{1}{2}} \]

\[ \tau_t = \int_{0}^{\infty} \rho(\tau)d\tau \quad \text{where} \quad \rho(\tau) = \frac{v(t)v(t+\tau)}{v^2(t)} \]

\[ \ell_t = v_t \tau_t = v_{\text{rms}} \tau_t \]

Karlovitz assumed that an additional velocity produced by the turbulent diffusion, \( S_{uT} \), has to be added to the laminar burning velocity:

\[ S_{uT} = S_{uL} + S_{uT} \]  \hspace{1cm} (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, \( \tau = \ell_t/S_{uL} \):

\[ S_{uT} = \frac{(x^2)^{\frac{1}{2}}}{\tau} \]  \hspace{1cm} (99)
Karloviz’s correlations for the turbulent burning velocity

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

\[
\frac{d\bar{x}^2}{dt} = 2 \bar{v}^2 \int_0^t \rho(\tau) d\tau = 2 (v_{\text{rms}})^2 \int_0^t \rho(\tau) d\tau \quad (100)
\]

**Weak turbulence:** \( v_{\text{rms}} \ll S_{uL} \). Hence \( T (\equiv \ell_t/S_{uL}) \ll \tau_t (\equiv \ell_t/v_{\text{rms}}) \). Consequently, \( \rho(\tau) \approx 1 \) if \( t \leq T \) so that the root-mean-square displacement within the interaction time between a flame element and a turbulent eddy becomes (by integrating equation (100)):

\[
(x^2)^{\frac{1}{2}} = v_{\text{rms}} T
\]

\[
\Rightarrow S_u^t = \frac{(x^2)^{\frac{1}{2}}}{T} = v_{\text{rms}} T = v_{\text{rms}} \quad (101)
\]

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

\[
\frac{S_u T}{S_{uL}} = 1 + \frac{v_{\text{rms}}}{S_{uL}} \quad (102)
\]

**Intermediate turbulence:** \( T (\equiv \ell_t/S_{uL}) \approx \tau_t (\equiv \ell_t/v_{\text{rms}}) \). The integral on the right hand side of equation (100) assumes a definite value which is equal to the time scale of the turbulence, \( \tau_t \). This leads to

\[
(x^2)^{\frac{1}{2}} = \sqrt{2} \ell_t v_{\text{rms}} T
\]

and

\[
S_u^t = \frac{(x^2)^{\frac{1}{2}}}{T} = \frac{\sqrt{2} \ell_t v_{\text{rms}} T}{\ell_t / S_{uL}} = \sqrt{2 S_{uL} v_{\text{rms}}} \quad (104)
\]

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

\[
\frac{S_u T}{S_{uL}} = 1 + \sqrt{2 \left( \frac{v_{\text{rms}}}{S_{uL}} \right)^2} \quad (105)
\]

**Intermediate turbulence:** \( T (\equiv \ell_t/S_{uL}) \approx \tau_t (\equiv \ell_t/v_{\text{rms}}) \), 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 \( \tau_m \) denotes the Taylor microscale,

\[
\rho(\tau) = 1 - \frac{1}{2} \frac{\tau^2}{\tau_m^2} \quad (106)
\]

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

\[
\bar{x}^2 = \bar{v}^2 \left[ \frac{1}{2} T^2 \frac{\tau^2}{\tau_m^2} - \frac{1}{12} (T^4 / \tau_m^2) \right] \approx \bar{v}^2 \left[ \frac{1}{2} T^2 - \frac{1}{12} T^2 \right] \approx \frac{5}{12} \bar{v}^2 T^2 \quad (107)
\]

Consequently,

\[
S_u^t = \frac{(x^2)^{\frac{1}{2}}}{T} = \frac{\sqrt{\frac{5}{12} v_{\text{rms}} T}}{T} = \sqrt{\frac{5}{12} v_{\text{rms}}} \quad (108)
\]

and

\[
\frac{S_u T}{S_{uL}} = 1 + \sqrt{\frac{5}{12} \frac{v_{\text{rms}}}{S_{uL}}} \quad (109)
\]