Fundamentals of Explosions Definitions of Basic Combustion Parameters

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- Consequences of an explosion:
  - Blast
  - Fire
  - Toxicity

- Given an accidental scenario, what is the volume of explosive mixture?
  - A fluid mechanics problem of dispersion and turbulent mixing

- Given a volume of explosive gas mixture (within the flammability limits), what is the blast pressure?
    - Depends on the burning rate (flame speed)

- What is the turbulent flame speed for initial and boundary conditions?
    - Central problem in explosion risk assessment

Explosion Dynamics

- Chemical thermodynamics (stoichiometry, energetics)
- Chemical kinetics (reaction mechanisms, rates of reactions)
- Combustion (ignition, flame propagation and flammability limits, quenching, MESG)
- Gas dynamics (detonation waves, initiation, limits, DDT)

Chemical Thermodynamics

- Equilibrium species and concentrations in products

- Energetics of a reaction (for a given path, i.e., constant volume, pressure across a combustion wave)

Stoichiometry

- Relationship between the composition of the reactants and products.
  - Atoms are conserved in a chemical reaction
  - Stoichiometric mixture – just the right amount of oxidizer for the given fuel
  - Assume complete combustion
    - $C \rightarrow CO_2$, $H \rightarrow H_2O$, $S \rightarrow SO_2$, $N_2 \rightarrow N_2$

- e.g. $H_2 + ½\ O_2 \rightarrow H_2O$
  $H_2 + ½\ (O_2 + 3.76N_2) \rightarrow H_2O + 1.88N_2$
  $H_2 + 2.38\ \text{air} \rightarrow H_2O + 1.88\ N_2$
- Percentage by mole 66.6% H_2, 33.4% O_2
- Percentage by weight 11.1 % H_2 ,88.9% O_2
- Percentage by mole 29.6% H_2, 70.4% air

Fuel-air ratio

$$FA = \frac{\text{moles of fuel}}{\text{moles of air}}$$

e.g. $H_2 + ½ (O_2 + 3.76N_2) \rightarrow H_2O + 1.88N_2$

$$FA = \frac{1}{2.38} = 0.42$$

- by mass $2\ H_2 + 68.64$ air

$$FA_{mass} = \frac{2}{68.64} = 0.029$$

Equivalence Ratio

$$\phi = \frac{(\mathrm{FA})_{\mathrm{mixture}}}{(\mathrm{FA})_{\mathrm{stoichiometric}}}$$

$\phi = 1$ stoichiometric composition

$H_2 + 2.38\ \mathrm{air} \rightarrow H_2O + 1.88\ N_2$

$\phi < 1$ fuel lean

$\phi > 1$ fuel rich

Enthalpy of a Compound

$$\begin{aligned}\tilde{h}(T) &= \tilde{h}_{\mathrm{f}}^{\mathrm{o}} + \int_{298}^{T} \mathrm{c_p}\, dT \\ &= \tilde{h}_{\mathrm{f}}^{\mathrm{o}} + \Delta\tilde{h}(T)\end{aligned}$$

- $\tilde{h}_{\mathrm{f}}^{\mathrm{o}}$ enthalpy of formation
  - enthalpy change when a compound is formed from its stable elements at standard reference state, i.e. 298K, 1 atm.
- $\tilde{h}_{\mathrm{f}}^{\mathrm{o}} = 0$ for stable elements at reference state

Enthalpy (heat) of Reaction

- heat exchange when reactants go to products at constant pressure and temperature

$$\Delta\tilde{h}_R = \frac{\sum\limits_{\text{products}} n_i\tilde{h}_i(T) - \sum\limits_{\text{reactants}} n_i\tilde{h}_i(T)}{\text{moles of fuel}}$$

Adiabatic Flame Temperature T_a

- temperature of products in an adiabatic constant pressure process

$$\Delta \mathrm{H} = \sum_{\text{products}} n_i\tilde{h}_i(T_{\mathrm{a}}) - \sum_{\text{reactants}} n_i\tilde{h}_i(298) = 0$$

Constant Volume Explosion Pressure

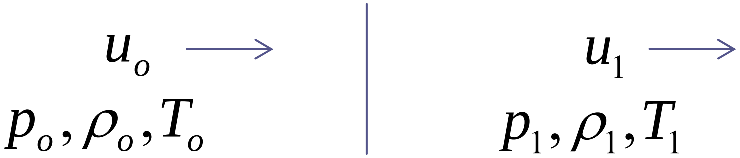
- pressure rise in a constant volume adiabatic process

$$\Delta U = \sum_{\text{products}} n_i \widetilde{U}_i - \sum_{\text{reactants}} n_i \widetilde{U}_i = 0$$

$$\widetilde{U}_i = \widetilde{h}_i(T) - P_i \widetilde{V}$$

$$\frac{P_{\text{product}}}{P_{\text{reactant}}} = \frac{n_{\text{product}} T_{\text{a}}}{n_{\text{reactant}} T_{\text{o}}}$$

Combustion Wave



$$u_o \longrightarrow \qquad\qquad u_1 \longrightarrow$$

$$p_o, \rho_o, T_o \qquad\qquad p_1, \rho_1, T_1$$

- Conservation law

$$\rho_o u_o = \rho_1 u_1$$

$$p_o + \rho_o u_o^2 = p_1 + \rho_1 u_1^2$$

$$h_o + \frac{u_o^2}{2} = h_1 + \frac{u_1^2}{2}$$

$$h_o = \sum_{\text{reactants}} x_i h_i \qquad h_1 = \sum_{\text{products}} x_i h_i$$

$$h_i = h_{f_i}^o + \int_{298K}^{T} c_{p_i} T$$

$$Pv = \rho R T$$

Chemical Kinetics

- Deals with reaction mechanisms (details steps) and the rates of chemical reactions

Reaction Mechanisms

- Global
  - Fuel + Oxidizer → Products

- Elementary

e.g. $H_2 + \frac{1}{2} O_2 \rightarrow H_2O$ (global)

$H_2 + M \rightarrow H + H + M$

$O_2 + M \rightarrow O + O + M$

$O + H_2 \rightarrow OH + H$

$H + O_2 \rightarrow OH + O$

$H_2 + OH \rightarrow H_2O + H$

etc.

Reduced mechanisms

- A few important intermediate steps to represent the overall reaction
  - e.g. $H_2 - O_2$
    - Chain initiation: $H_2 + O_2 \rightarrow H + HO_2$
    - Main branching: $H + O_2 \rightarrow O + OH$
    - Main heat release: $H_2 + OH \rightarrow H_2O + H$
    - Chain termination: $H + O_2 \rightarrow HO_2$
    - Secondary chain termination: $HO_2 + HO_2 \rightarrow H_2O_2$ +O2
    - Secondary chain branching: $H_2O_2 \rightarrow OH + OH$

Reaction Rate

- Unimolecular $\mathrm{A} \xrightarrow{\mathrm{k}} \mathrm{B}$

$$-\frac{d[\mathrm{A}]}{dt} = k[\mathrm{A}]$$

- Bimolecular $\mathrm{A} + \mathrm{B} \xrightarrow{\mathrm{k}} \mathrm{C}$

$$-\frac{d[\mathrm{A}]}{dt} = -\frac{d[\mathrm{B}]}{dt} = k[\mathrm{A}][\mathrm{B}]$$

- Termolecular $\mathrm{A} + \mathrm{B} + \mathrm{C} \xrightarrow{\mathrm{k}} \mathrm{D}$

$$-\frac{d[\mathrm{A}]}{dt} = -\frac{d[\mathrm{B}]}{dt} = -\frac{d[\mathrm{C}]}{dt} = k[\mathrm{A}][\mathrm{B}][\mathrm{C}]$$

- k → rate constant fit to a law of the form

$$k(T) = AT^{b}\exp\left(\frac{E_a}{RT}\right)$$

  - Can also fit global reaction to a global rate constant.
    - e.g. Hydrocarbon fuel CnHm

$$C_nH_m + \left(n + \frac{m}{4}\right)O_2 \xrightarrow{k_g} nCO_2 + \frac{m}{2}H_2O$$

$$k_g = AT^{n}[C_nH_m]^{a}[O_2]^{b}\exp\left(-\frac{E_a}{RT}\right)$$

- Since for high activation energy the temperature dependence is controlled by the exponential term, the power law dependence is dropped, i.e.

$$k = \mathrm{A}[\mathrm{fuel}]^{\mathrm{a}}[\mathrm{O}_2]^{\mathrm{b}} \exp\left(-\frac{E_{\mathrm{a}}}{RT}\right)$$

- The exponential form of the rate law is referred to as the Arrhenius rate law.

Explosion (Rapid Runaway Reactions)

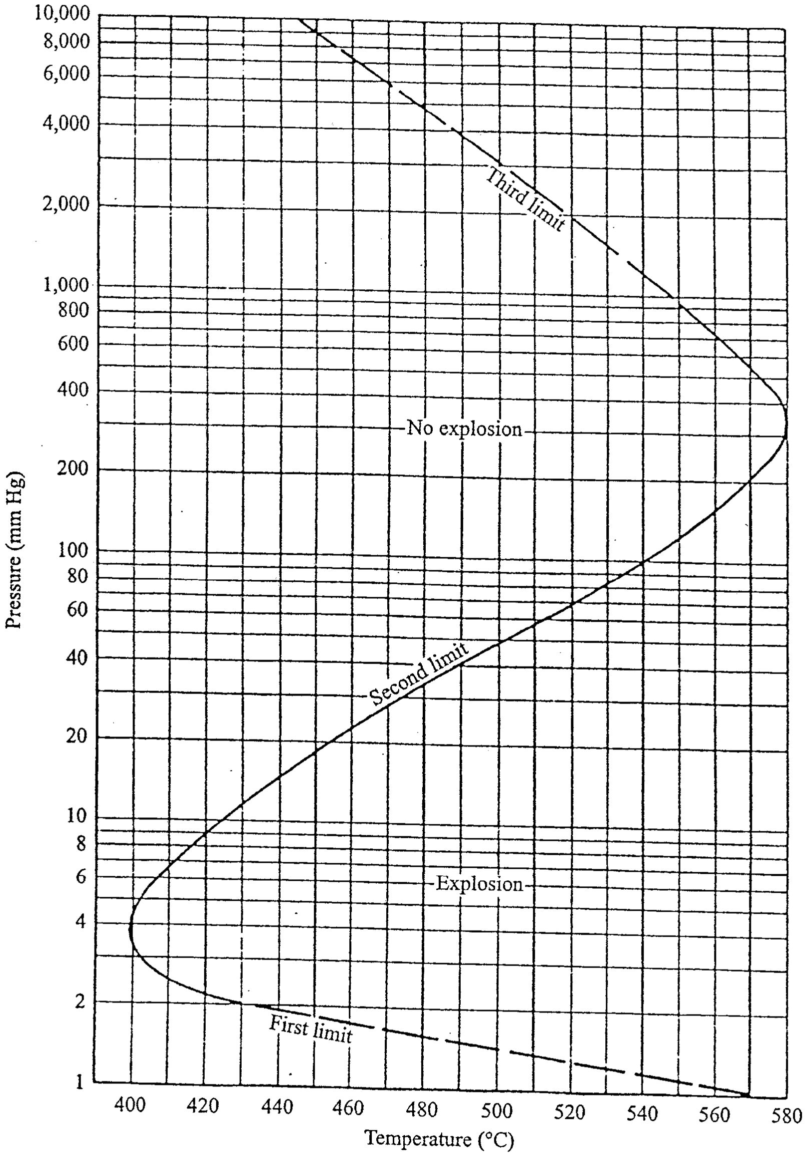
- Can be a consequence of rapid chain branching reaction

- Thermal runaway is a result of strong temperature dependence of reaction rate.

Explosion Limit

- Reaction rates are temperature and pressure dependent. There exist a critical state that defines if runaway reactions will occur or not
- Represented by a curve in the thermodynamic state (p,T) plane bounding regions of “explosion” and “no explosions”.

- Classical example is the Z-shaped curve for the explosion limit of H_2 – O_2 reaction
- For a fixed temperature, “explosion” or “no explosion” depends on pressure



Explosion limits for hydrogen-oxygen mixture.

- Consider a fixed temperature of 500°C
  - For $p \leq 1.5$ torr, no explosion
    - diffusion losses to wall (1st limit)
  - For 1.5 torr $\leq p \leq$ 50 torr, explosion occurs
    - chain branching dominates
  - For 50 torr $\leq p \leq$ 3000 torr, no explosion
    - Three body recombination chain terminating reactions dominate over chain branching

- For $p \geq 3000$ torr, explosion occurs
  - Formation of $HO_2 + H_2 \rightarrow H_2O_2 + H$ dominates over diffusion losses of HO_2
- For $T \geq 580$ °C, explosion occurs for all pressures
  - Dissociation of H_2O_2 is important

Homogeneous Adiabatic Constant Volume Thermal Explosion

- First law

$$\frac{dU}{dt} = \dot{q}_{\mathrm{R}} Q$$

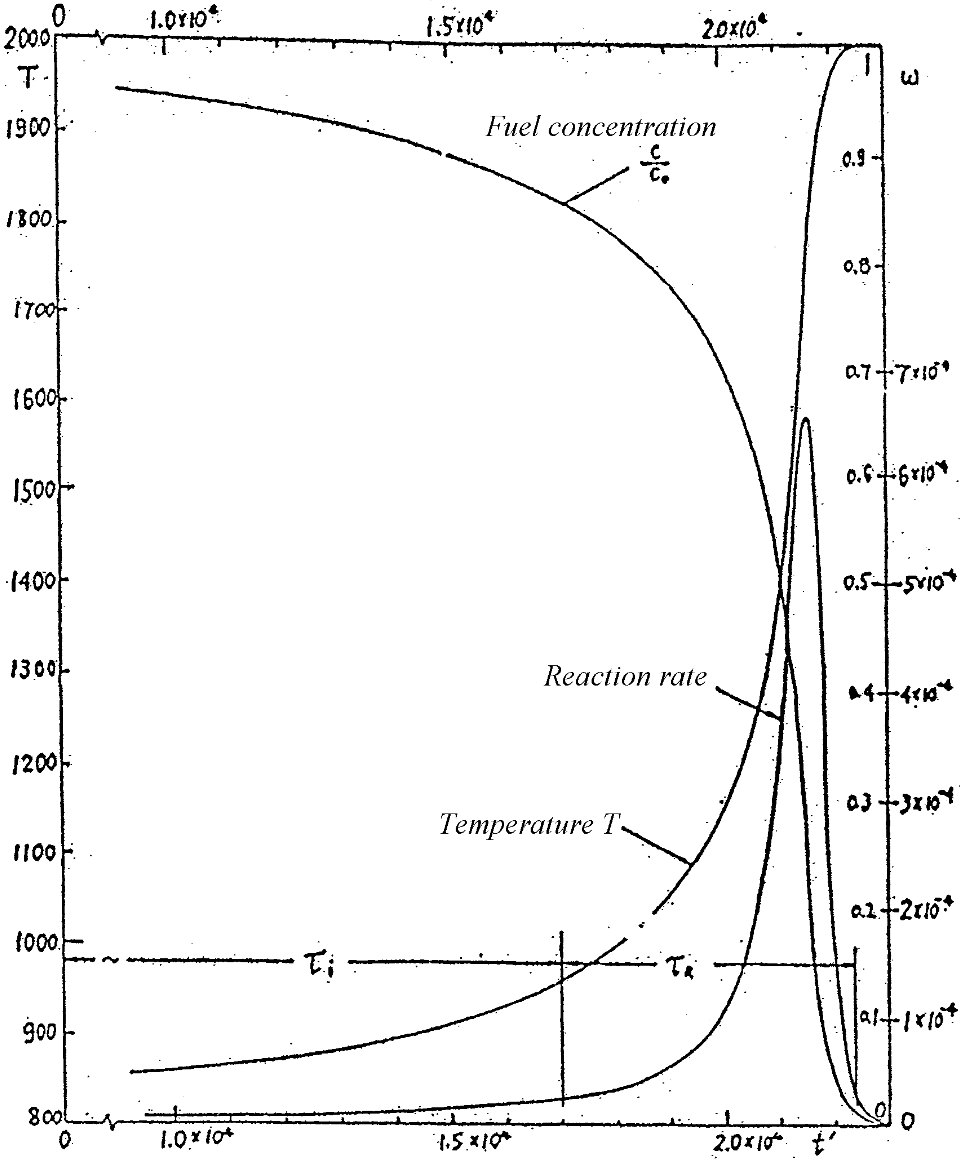
$$\dot{Q}_R = \mathrm{k_o} c^n \exp\left(-\frac{E_{\mathrm{a}}}{RT}\right) Q$$

$$\Delta T \sim -\Delta c$$

$$\frac{dT}{dt^*} = (T_{\max} - T)^{\mathrm{n}} \exp\left(-\frac{E_{\mathrm{a}}}{RT}\right)$$

$t^* = k_{\mathrm{o}} t$, consider n=1

- Integrating numerically from T_o to T_{max}
  - e.g.: T_o = 800 K, T_{max} = 2000 K, E_a = 20 kcal/mol, R = 1.98 cal/(mol K)
  - Results：
    - Very slow initial temperature rise
    - Very rapid rise in T where $T \approx 1100$ K
    - Very rapid decrease in fuel when $T \geq 1100$K



Temperature, concentration and reaction rate profile.

- Induction period $\tau_i \rightarrow$ negligible duration of temperature rise
- Reaction time $\tau_R \rightarrow$ period of rapid temperature rise to T_{max}
- Strong dependence of $\frac{\tau_R}{\tau_i}$ on E_a

e.g. $\frac{\tau_R}{\tau_i} \approx 0.3$ for $E_a = 20$kcal

$\frac{\tau_R}{\tau_i} \approx 0.00035$ for $E_a \approx 40$kcal

Thermal Runaway (Ignition)

- Reaction rates are finite at finite temperatures, without losses all explosive mixtures will eventually undergo runaway reaction

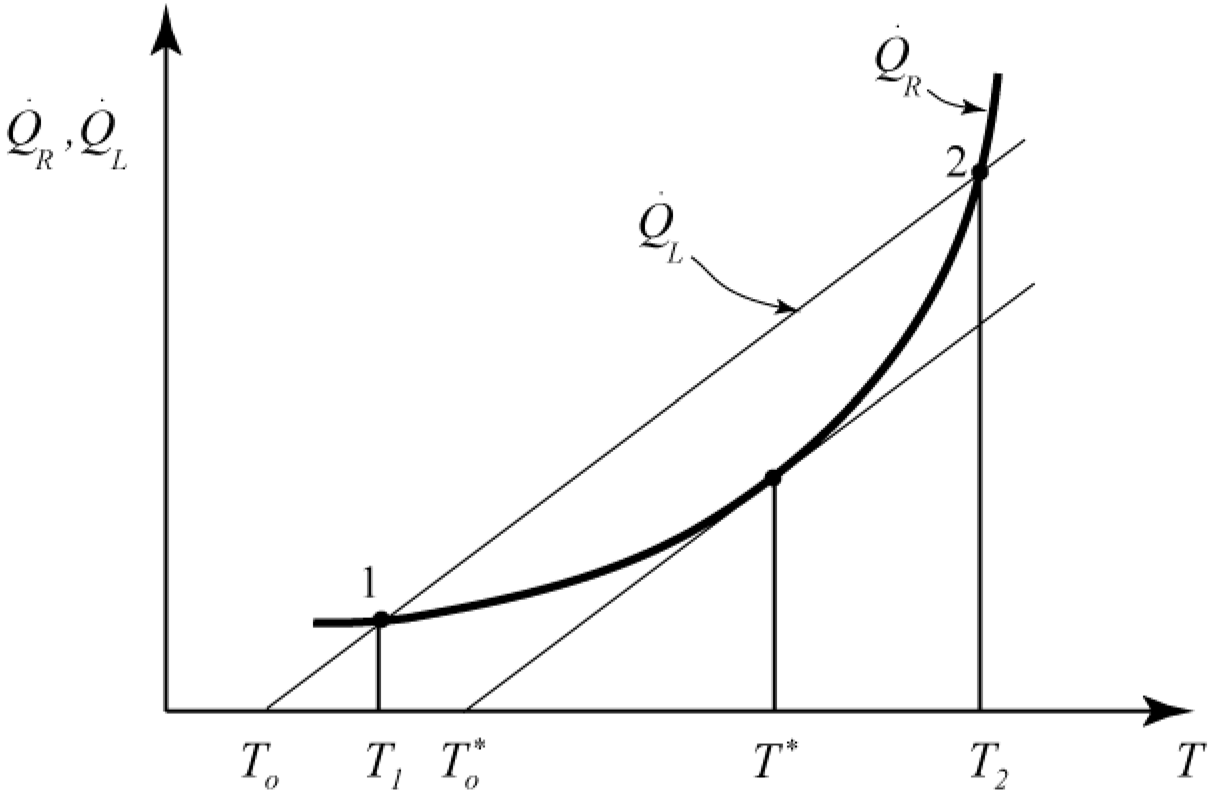
- Runaway reaction occurs when rate of heat production due to reaction exceed rate of heat loss

- First law $$\frac{n\tilde{c}_{\mathrm{v}}}{V}\frac{dT}{dt} = \dot{q}_R - \dot{q}_L$$
  - L.H.S. Rate of change of internal energy per unit volume
  - Rate of energy release per unit volume

$$\dot{q}_R = A[\mathrm{F}]^{\mathrm{a}}[\mathrm{O}]^{\mathrm{b}}\exp\left(-\frac{E_{\mathrm{a}}}{RT}\right)Q$$

  - Rate of heat loss per volume

$$\dot{q}_L = \frac{hS}{V}(T - T_{\mathrm{o}})$$



- At 1, stable if $T<T_1$ $\quad \dot{q}_R > \dot{q}_L$

  $T>T_1$ $\quad \dot{q}_L > \dot{q}_R$

- At 2, unstable T<T_2 , $\dot{q}_L > \dot{q}_R$

  system $\rightarrow$ 1

  T>T_2 , $\dot{q}_R > \dot{q}_L$ runaway

  T>T*, $\dot{q}_R > \dot{q}_L$ ignition

T* - ignition temperature

- At critical ignition point * ($T = T^*$)

$$\dot{q}_R = \dot{q}_L \qquad \left(\frac{d\dot{q}_\mathrm{R}}{dT}\right)^* = \left(\frac{d\dot{q}_\mathrm{L}}{dT}\right)^*$$

$$AQ[F]^\mathrm{a}[O]^\mathrm{b}\exp\left(-\frac{E_\mathrm{a}}{RT_\mathrm{i}}\right) = \frac{hS}{V}(T - T_\mathrm{o})$$

$$AQ[F]^\mathrm{a}[O]^\mathrm{b}\,\frac{E_\mathrm{a}}{RT_\mathrm{i}^{\,2}}\exp\left(-\frac{E_\mathrm{a}}{RT_\mathrm{i}}\right) = \frac{hS}{V}$$

- Dividing the two equations yield

$$\frac{RT^{*2}}{E_{\mathrm{a}}} = T^{*} - T_{o}$$

- Solving for T^{*}

$$T^{*} = \frac{E_{\mathrm{a}}}{2R}\left\{1 \pm \sqrt{1 - \frac{4RT_{\mathrm{o}}}{E_{\mathrm{a}}}}\right\}$$

- Take the negative root

$$0 \le T_{\mathrm{o}} \le \frac{E_{\mathrm{a}}}{4\mathrm{R}} \qquad 0 \le T^{*} \le \frac{E_{\mathrm{a}}}{2\mathrm{R}}$$

- In general $T_o << \dfrac{E_a}{4R}$

$$T^* \simeq \frac{E_a}{2R}\left\{1-\left(1-2\frac{RT_o}{E_a}-2\frac{R^2T_o^2}{E_a^2}....\right)\right\}$$

- First approximation

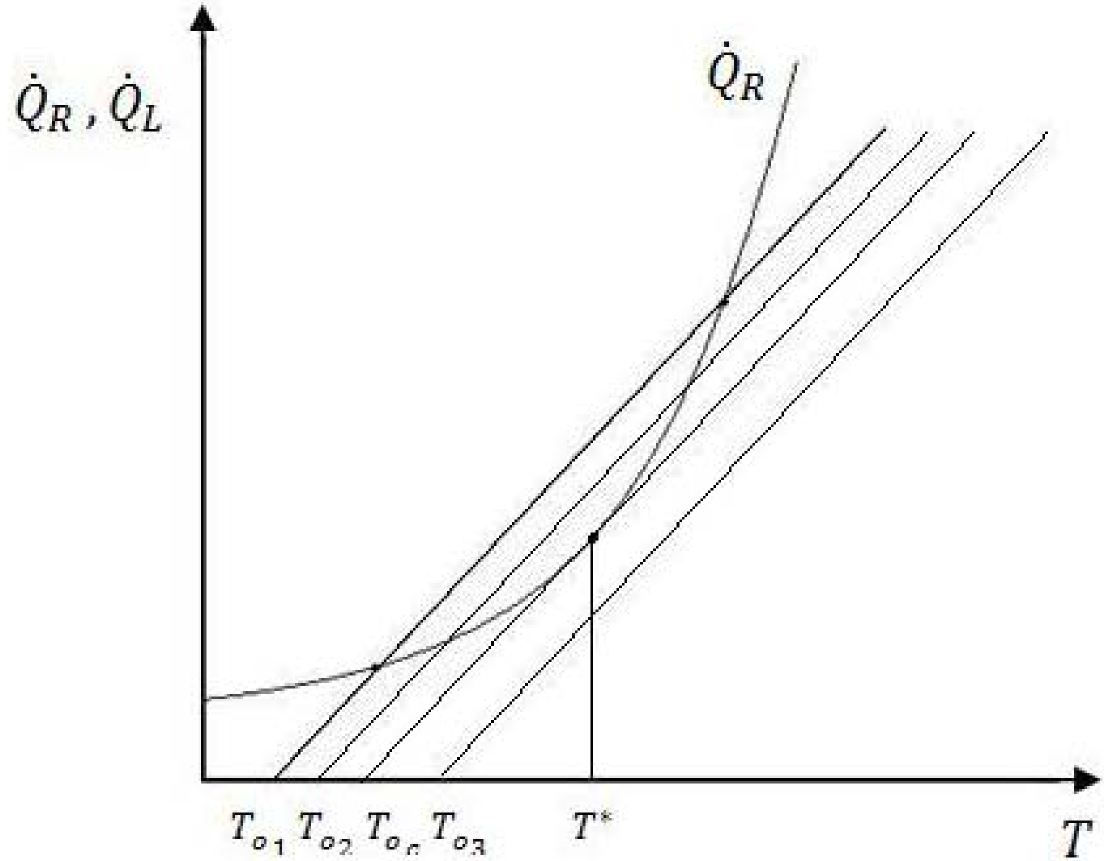
$$T^* \simeq T_o$$

- Second approximation

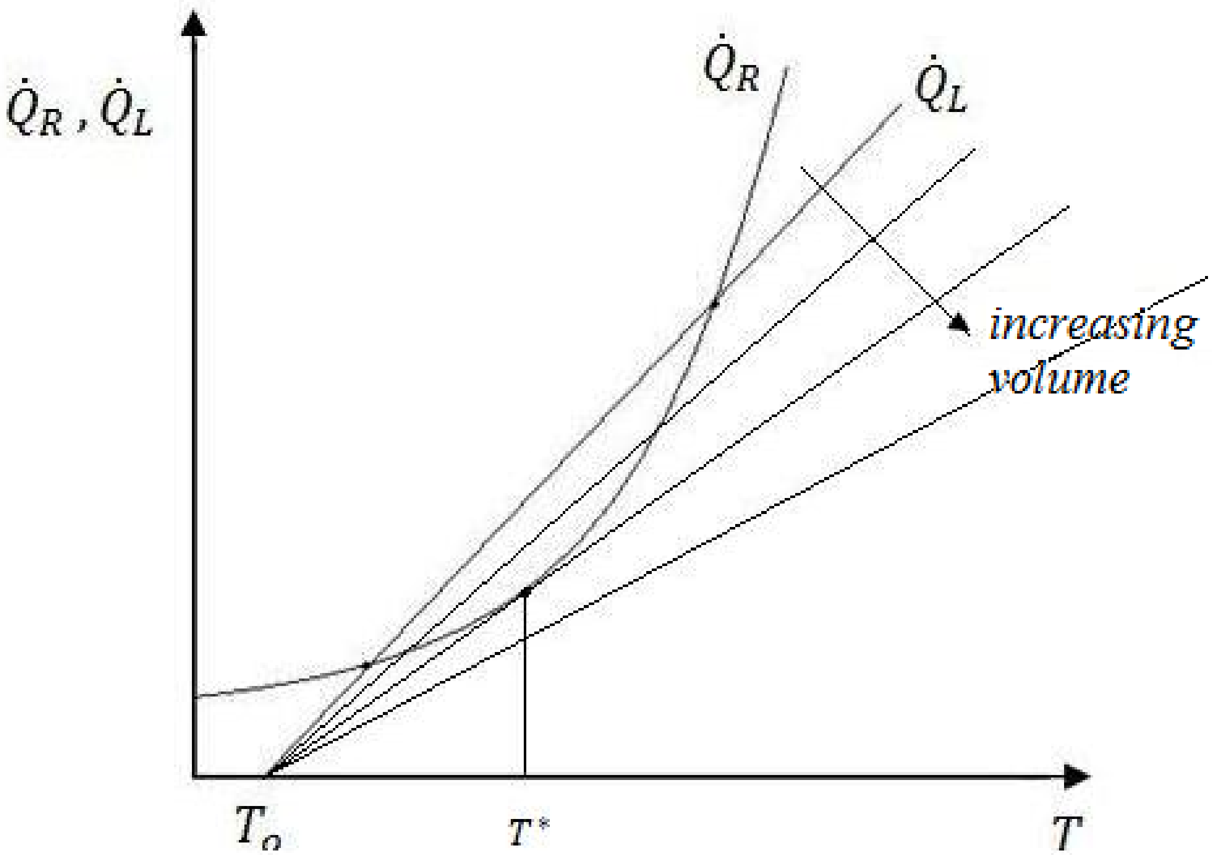
$$T^* \simeq T_o + \frac{RT_o^2}{E_a}$$

$$\frac{T^* - T_o}{T_o} = \frac{T^*}{T_o} - 1 \simeq \frac{RT_o}{E_a}$$

- Given a heat release curve and the size of the volume there exist a critical value of T_o when runaway occurs



- Given a T_o and heat release curve $\dot{Q}_R$ there exist a critical volume above which runaway occurs



$$\frac{d\dot{Q}_L}{dT} = \frac{A}{V}$$

Minimum ignition energy

- Assume spherical volume $V = \frac{4\pi}{3} r^3$
- From $\dot{q}_R = \dot{q}_L$

$$AQ[F]^{\mathrm{a}}[O]^{\mathrm{b}} \exp\left(-\frac{E_{\mathrm{a}}}{RT}\right) = \frac{hS}{V}(T - T_{\mathrm{o}})$$

$$\frac{S}{V} = \frac{4\pi r^{*2}}{\frac{4\pi}{3} r^{*3}} = \frac{3}{r^*}$$

$$r^* = \frac{3h(T_{\mathrm{a}} - T_{\mathrm{o}})}{AQ[F]^{\mathrm{a}}[O]^{\mathrm{b}} \exp\left(-\frac{E_{\mathrm{a}}}{RT}\right)}$$

- Adiabatic flame temperature $T^* \simeq T_{\mathrm{a}}$

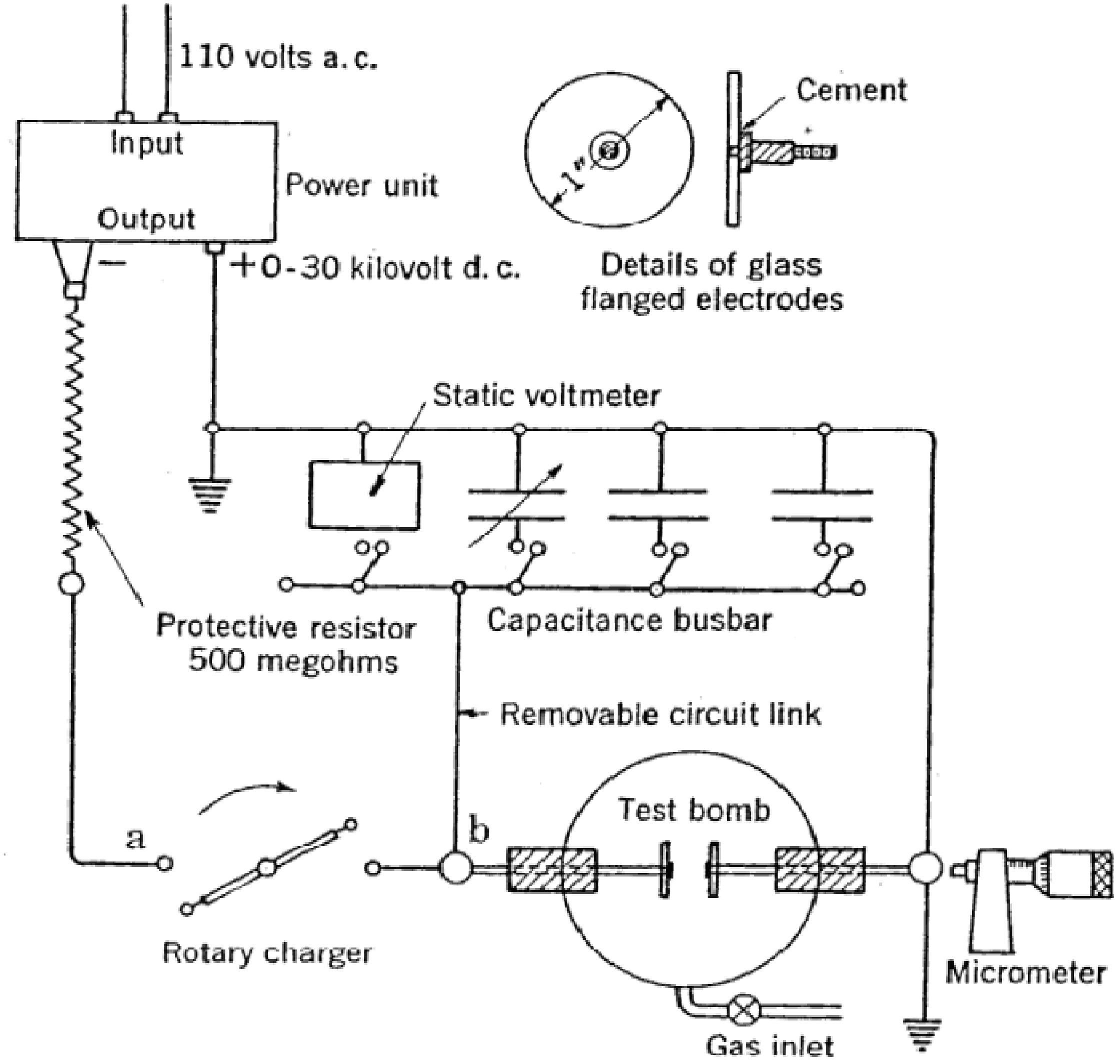
Minimum ignition energy

- External energy to heat flame kernel to ignition temperature $T^* \approx T_a$

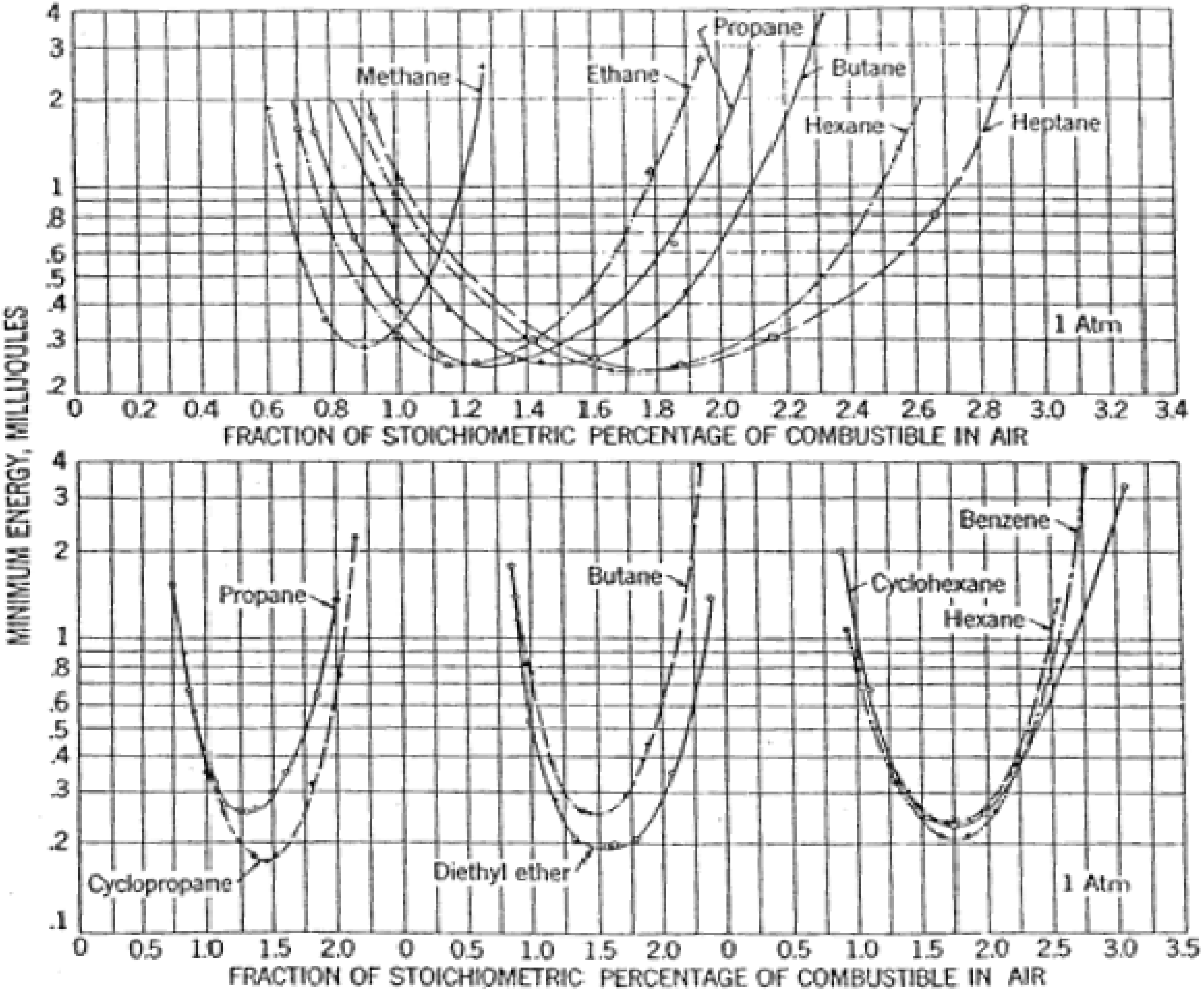
$$E_{\min} = \rho \frac{4\pi r^{*3}}{3} c_p (T_a - T_o)$$

$$r^* = \frac{3h(T_a - T_o)}{AQ[F]^a[O]^b \exp\left(-\frac{E_a}{RT}\right)}$$

- Minimum ignition spark energy determined experimentally
  - Circuit parameter, electrode configuration, etc.
  - Standardized ASTM E582-07



Scheme of apparatus for determining minimum ignition energies for electric-spark ignition



Minimum ignition energies of combustible-air mixtures in relation to the stoichiometric percentage in air.

Quenching distance d_q

- Minimum tube diameter (or gap) in which self-sustained flame propagation is possible

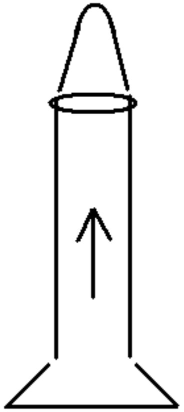
- Balance between heat production by chemical reactions in flame zone and losses from boundaries of reaction zone, i.e. $\dot{q}_R = \dot{q}_L$

$$\mathrm{d}_\mathrm{q} \simeq r^* \simeq \delta$$

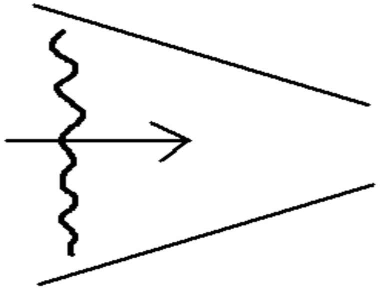
- δ →Laminar flame thickness

- Different methods used to determine quenching distance

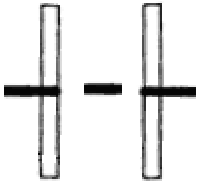
- Flash back method

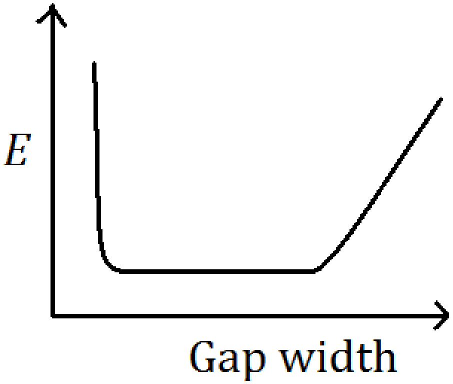


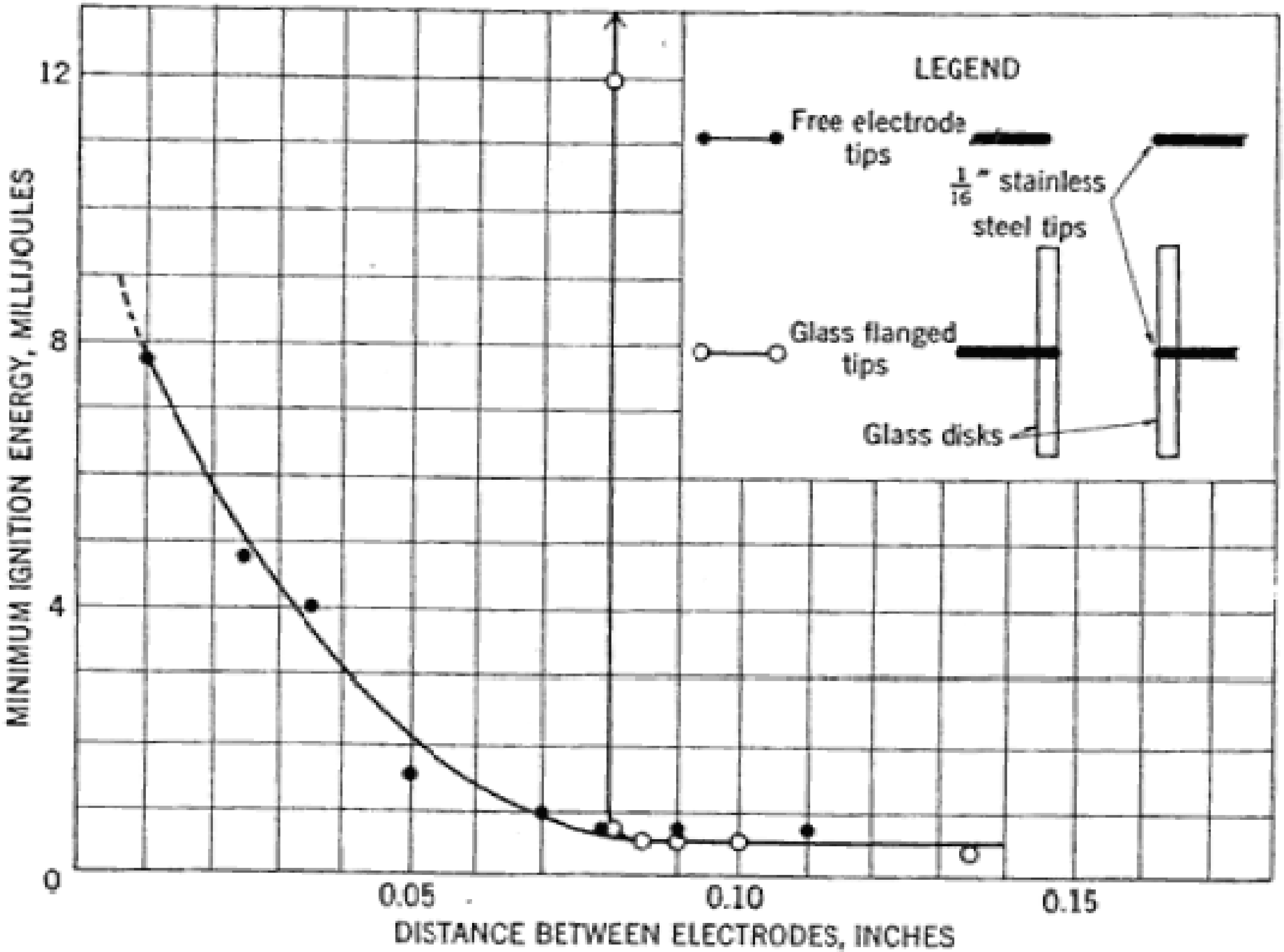
- Tapered tube



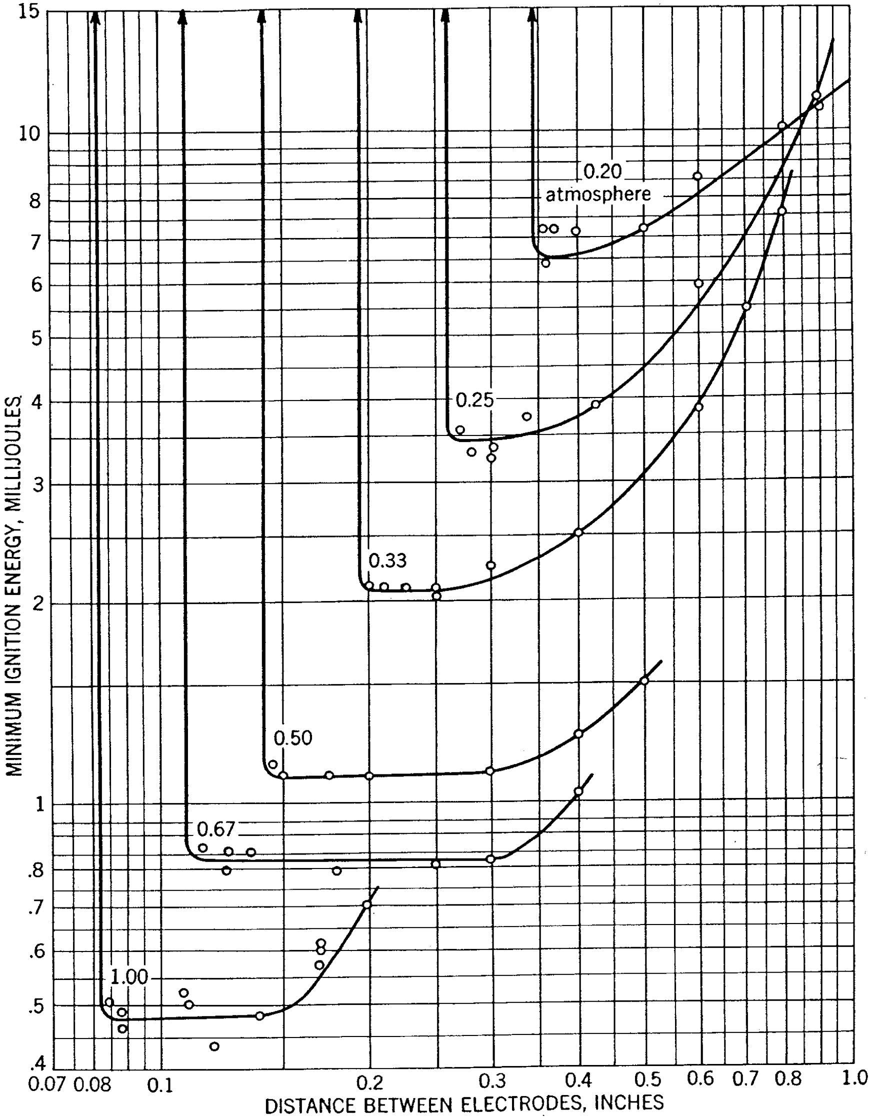
- Flanged electrode



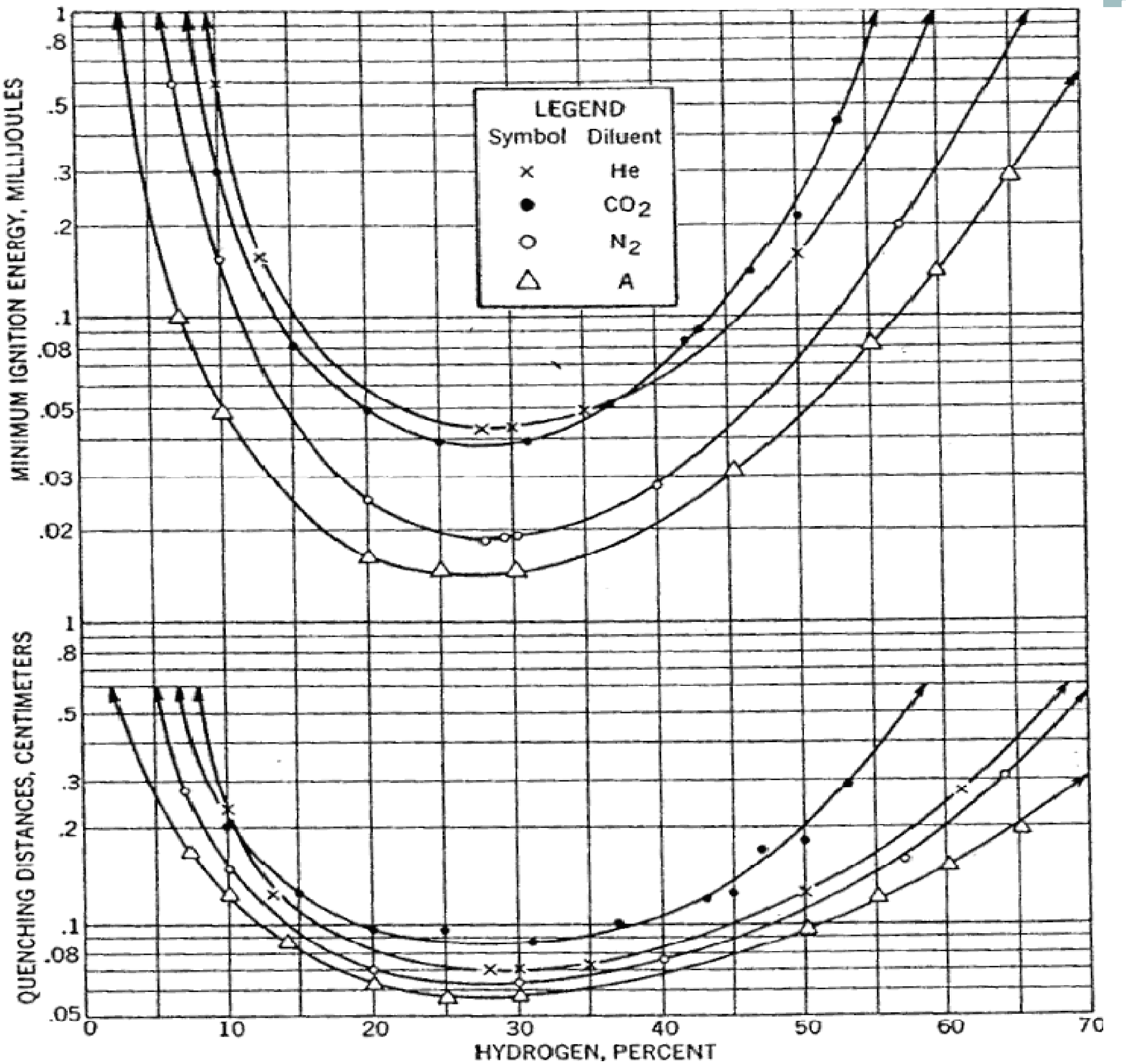




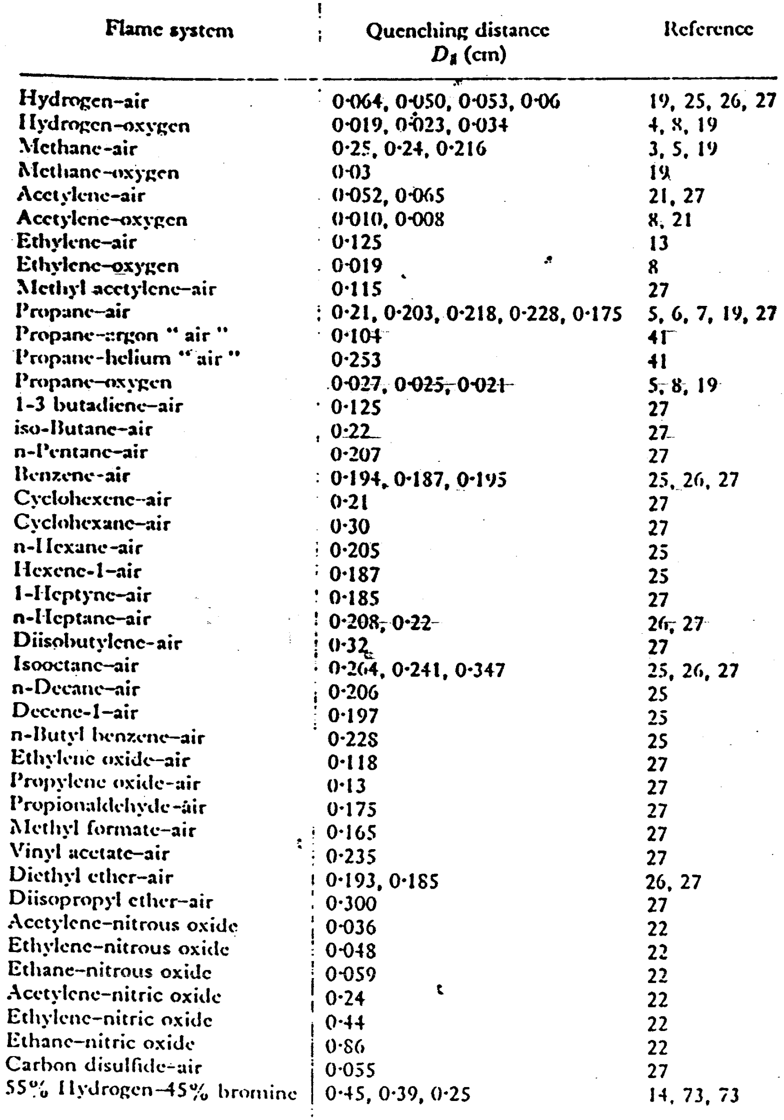
Minimum ignition energies for free and glass-flanged electrode tips as function of electrode distance.



Minimum ignition energies for glass-flanged electrode tips as function of electrode distance and pressure

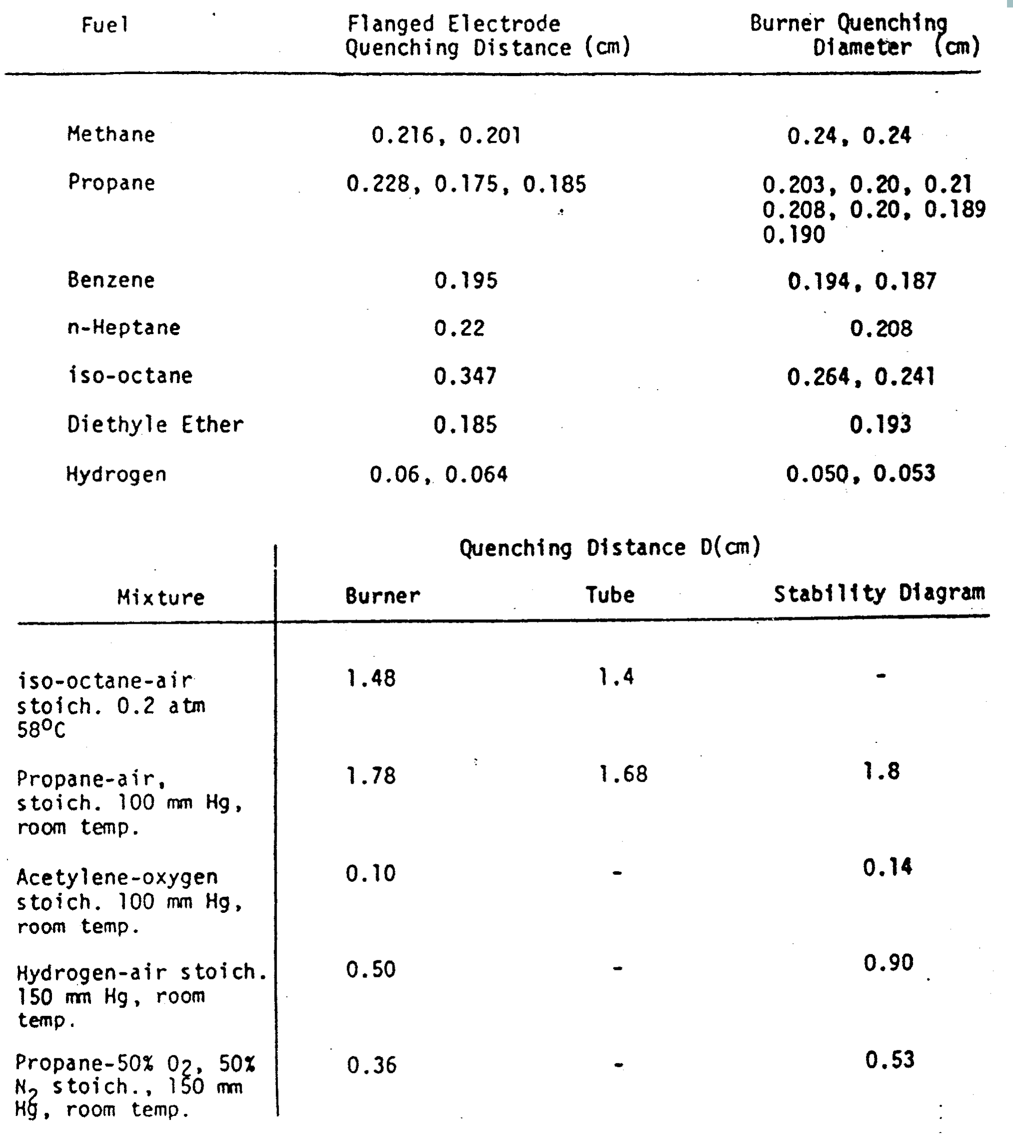


Minimum ignition energies and quenching distances for hydrogen-oxygen-inert gas mixtures at atmospheric pressure. $O_2/(O_2 + \text{inert gas}) = 0.21$



Flame system	Quenching distance $D_\parallel$ (cm)	Reference
Hydrogen–air	0·064, 0·050, 0·053, 0·06	19, 25, 26, 27
Hydrogen–oxygen	0·019, 0·023, 0·034	4, 8, 19
Methane–air	0·25, 0·24, 0·216	3, 5, 19
Methane–oxygen	0·03	19
Acetylene–air	0·052, 0·065	21, 27
Acetylene–oxygen	0·010, 0·008	8, 21
Ethylene–air	0·125	13
Ethylene–oxygen	0·019	8
Methyl acetylene–air	0·115	27
Propane–air	0·21, 0·203, 0·218, 0·228, 0·175	5, 6, 7, 19, 27
Propane–argon " air "	0·104	41
Propane–helium " air "	0·253	41
Propane–oxygen	0·027, 0·025, 0·021	5, 8, 19
1-3 butadiene–air	0·125	27
iso-Butane–air	0·22	27
n-Pentane–air	0·207	27
Benzene–air	0·194, 0·187, 0·195	25, 26, 27
Cyclohexene–air	0·21	27
Cyclohexane–air	0·30	27
n-Hexane–air	0·205	25
Hexene-1–air	0·187	25
1-Heptyne–air	0·185	27
n-Heptane–air	0·208, 0·22	26, 27
Diisobutylene–air	0·32	27
Isooctane–air	0·264, 0·241, 0·347	25, 26, 27
n-Decane–air	0·206	25
Decene-1–air	0·197	25
n-Butyl benzene–air	0·228	25
Ethylene oxide–air	0·118	27
Propylene oxide–air	0·13	27
Propionaldehyde–air	0·175	27
Methyl formate–air	0·165	27
Vinyl acetate–air	0·235	27
Diethyl ether–air	0·193, 0·185	26, 27
Diisopropyl ether–air	0·300	27
Acetylene–nitrous oxide	0·036	22
Ethylene–nitrous oxide	0·048	22
Ethane–nitrous oxide	0·059	22
Acetylene–nitric oxide	0·24	22
Ethylene–nitric oxide	0·44	22
Ethane–nitric oxide	0·86	22
Carbon disulfide–air	0·055	27
55% Hydrogen–45% bromine	0·45, 0·39, 0·25	14, 73, 73

Quenching distance for various flames at 1 atmosphere for stoichiometric mixtures at room temperature.



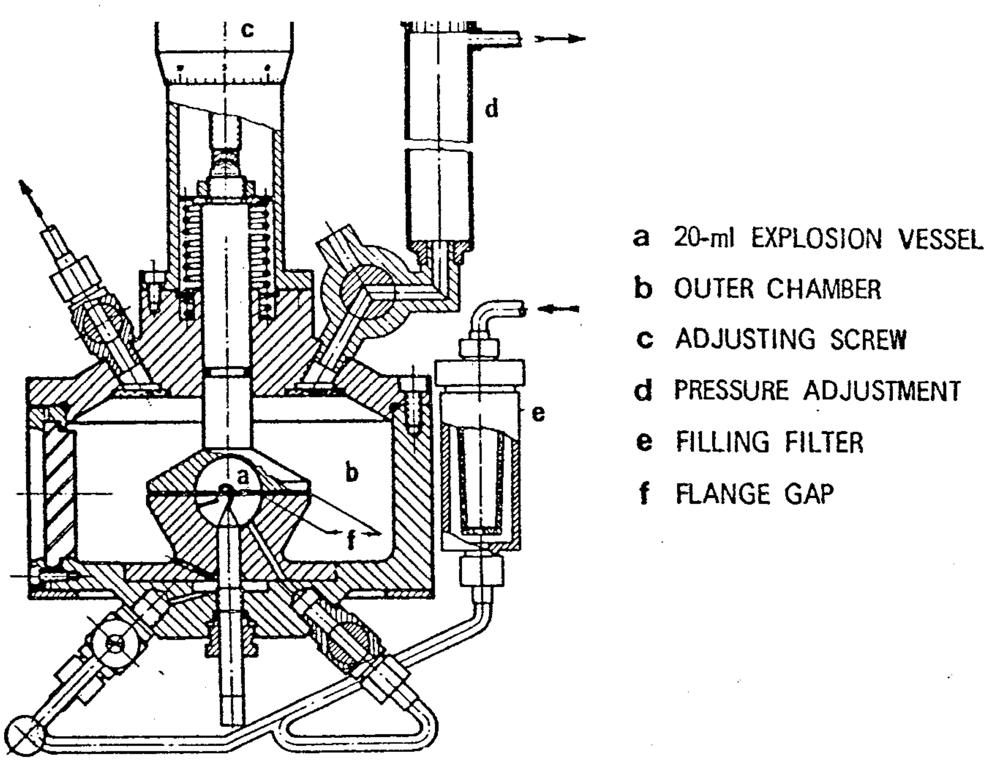
Fuel	Flanged Electrode Quenching Distance (cm)	Burner Quenching Diameter (cm)
Methane	0.216, 0.201	0.24, 0.24
Propane	0.228, 0.175, 0.185	0.203, 0.20, 0.21 0.208, 0.20, 0.189 0.190
Benzene	0.195	0.194, 0.187
n-Heptane	0.22	0.208
iso-octane	0.347	0.264, 0.241
Diethyle Ether	0.185	0.193
Hydrogen	0.06, 0.064	0.050, 0.053

Mixture	Quenching Distance D(cm)		
	Burner	Tube	Stability Diagram
iso-octane-air stoich. 0.2 atm 58^oC	1.48	1.4	-
Propane-air, stoich. 100 mm Hg, room temp.	1.78	1.68	1.8
Acetylene-oxygen stoich. 100 mm Hg, room temp.	0.10	-	0.14
Hydrogen-air stoich. 150 mm Hg, room temp.	0.50	-	0.90
Propane-50% O_2, 50% N_2 stoich., 150 mm Hg, room temp.	0.36	-	0.53

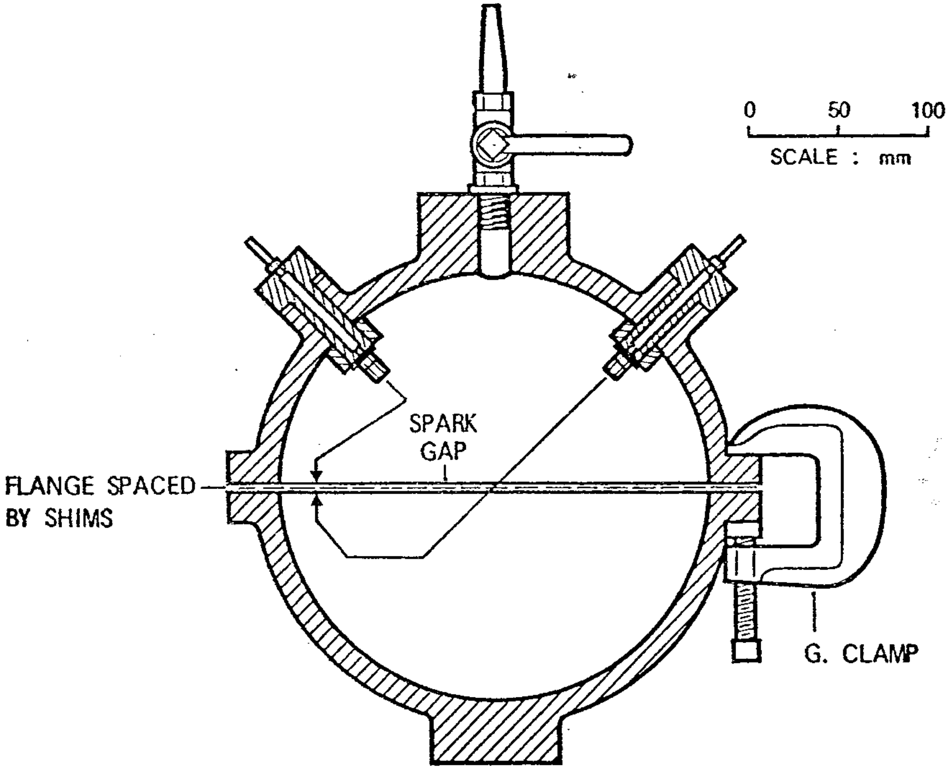
Comparison of quenching distances from different methods

MESG (maximum experimental safe gap)

- Maximum gad in which explosion can be transmitted from one chamber to another standard apparatus used 20 ml vessel European standard 8 L sphere
- Westerburg apparatus
  - (Underwriter's lab)



20 ml explosion vessel.



8 L explosion vessel. (SMRE 25.4 mm (1 inch) Flanges, Assembly: 4 or 6 G Clamps

Flammability Limits

- Conditions that define whether self-sustained flame propagation is possible or not
    - Conditions :
        - Thermodynamic state (p,T)
        - Boundary condition (tube diameter)
        - Composition (equivalence ratio)
        - Percentage of inert diluent

- Physics involved in flammability limits – very diverse (heat losses, flame stretch, buoyancy, stability)

- In general, flammability limits are defined for fuel composition, lean and rich limit

- Effect of buoyancy give rise to upward, downward, horizontal limits

- Effect of tube diameter resolved by choosing a sufficiently large diameter where dependence is weak $d \geq 5$ cm

- Standard apparatus → Flammability tube used by Coward and Jones 1.5m long, 5cm diameter

- Closed explosion vessel also used criterion based on achieving some arbitrary pressure rise
- Flame stretch and thermo-diffusive instability play important role near limits

- For mixture of different fuels Le Chatelier rule is used, i.e.

$$\frac{c_A}{c_A^*} + \frac{c_B}{c_B^*} = 1$$

  - c_A, c_B - concentration of fuel A and B of mixture
  - c_A^*, c_B^* - limiting concentration of fuel A and B respectively

- Le Chatelier rule is essentially based on energetics of fuels.
  - Works for fuels having same physical properties, i.e.
    - molecular weights
    - diffusivity
    - reaction rates, etc.

Combustion in a closed vessel

- Can be used to determine flammability limits
- Constant volume explosion pressure → energetics of mixture
- Burning velocity
- k_g factor for explosion venting design

- Can derive relationship between p, $\Delta P_{\max}$, $\frac{d\Delta p}{dt}$ and S

$$\frac{d\Delta p}{dt} = \frac{3\Delta p_{\max} S}{R}\left(\frac{p}{p_o}\right)^{\frac{1}{\gamma}}\left\{1-\left(\frac{p_o}{p}\right)^{\frac{1}{\gamma}}\left(1-\frac{\Delta p}{\Delta p_{\max}}\right)\right\}^{\frac{2}{3}}$$

  - *P(t)* , $\Delta P_{\max}$ measured
  - *S* is the burning velocity and can be determined

- k_g factor is defined as

$$k_g = V^{\frac{1}{3}}\left(\frac{d\Delta p}{dt}\right)_{\max} = V^{\frac{1}{3}}\left(\Delta p_{\max}, S\right)$$

- A measure of the rate of pressure rise in the vessel

- $V^{\frac{1}{3}}$ ~ Length scale of the vessel to normalize the rate of pressure rise for different size vessel

Explosion Venting

- Reactants (or products) are discharged from vessel to limit maximum over pressure developed
- Rate of enthalpy vented equal rate of chemical energy release
- NFPA Guideline 68 for vent area-volume ratio, k_g factor

- Given explosive mixture at given initial conditions (p, T, chemical composition, etc.), there are two mode of combustion:
  - deflagration
  - detonation

- Product temperature more or less the same but combustion rate differs by 10^4 times

Deflagration Wave (Propagating Flame)

- Subsonic relative to unburned mixture ahead of it

- Expansion wave, pressure drops across flame

- Unburned mixture ahead is set into motion due to increase in specific volume across flame

- Burning velocity *S* relative to mixture ahead
- Flame speed $\dot{R}_{\mathrm{f}}$ relative to fixed coordinate system
- If the deflagration is fast, there is a precursor shock ahead of flame front

- Deflagration propagates as a diffusion wave
  - Heat and radical species diffuses from reaction zone ahead to effect ignition
  - Burning velocity $S \sim \sqrt{\frac{\alpha}{t_c}}$ α-diffusivity $t_c \sim \frac{1}{\omega_c}$ reaction time, *S*~cm/s
  - Laminar flame thickness δ~1mm
  - Effect of curvature and stretch on burning velocity
  - Laminar flame unstable-cellular

- Propagating flame – deflagration
  - Self accelerate due to positive feed back mechanism

- Max deflagration speed ~ ½ CJ detonation speed

- DDT transition to detonation

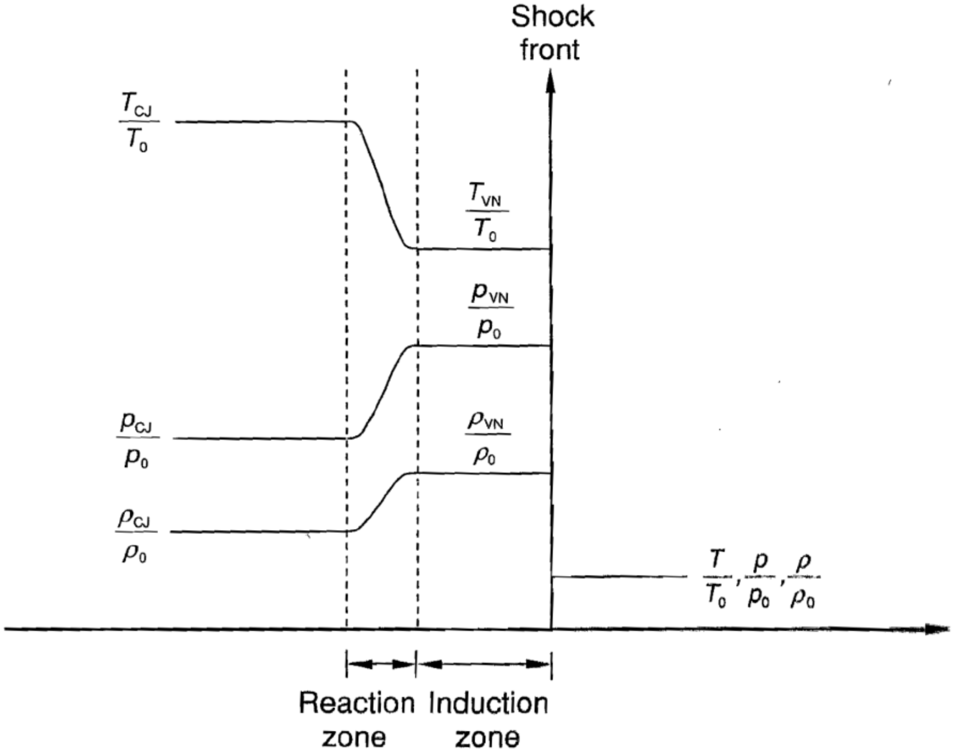
Detonation Wave

- Propagate at supersonic speed relative to reactants in front of it

- Compression shock wave that initiate chemical reaction via adiabatic compression to auto-ignition temperature

- Expansion in reaction zone and products (Taylor wave) produce forward thrust to derive leading shock front

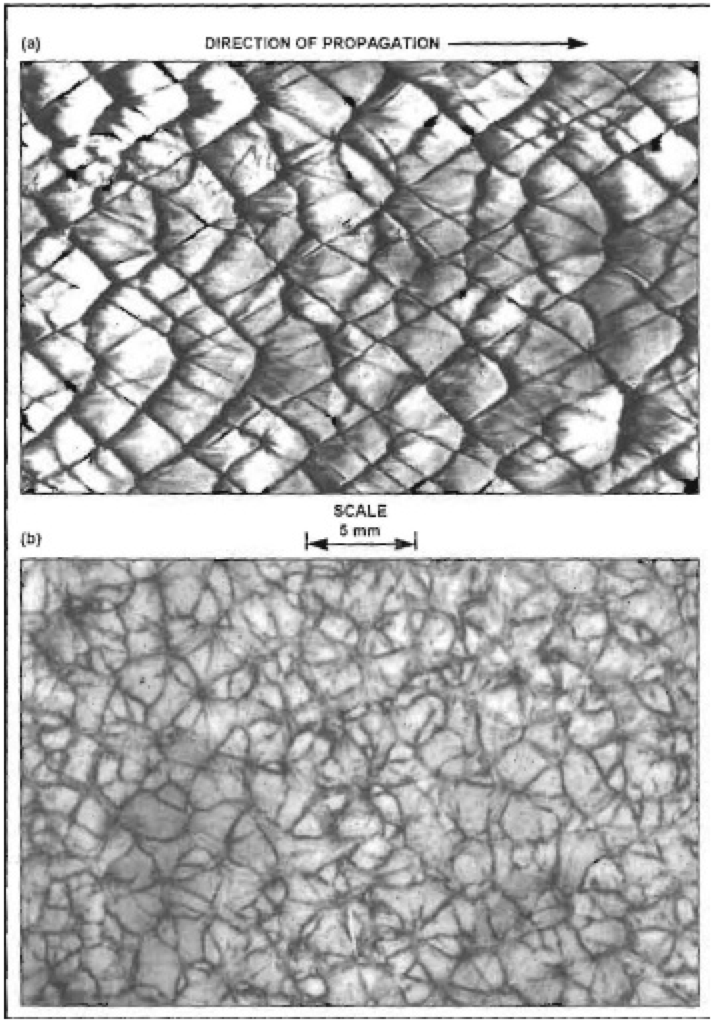
- ZND structure (Zeldovich- von Neumann – Döring) model of detonation zone – leading shock followed by induction zone and reaction zone



- Chapman-Jouguet detonation → sonic velocity of product (relative to the detonation)
    - Minimum velocity solution of steady conservation laws (tangent of Rayleigh line to Hugoniot)

- Typical stoichiometric mixtures at 1atm, 298K, D_{CJ}~1800ms
- Detonation pressure $\Delta p_{\mathrm{CJ}} \simeq 15$
- A detonation is generally unstable
- Longitudinal instability → Pulsating detonation

- Transverse instability → cellular structure
- Detonation cell size measure by smoked foil technique
- Useful length scale to characterize detonation zone thickness
- Cell size ~ ZND reaction zone length
- Spinning detonation – lowest transverse unstable mode in a circular tube. Stationary structure with respect to rotating frame fixed to spinning head



(a) Side wall and (b) end-on soot records of a multiheaded detonation

Courtesy of S.B. Murray

Detonability Limits

- Critical conditions that define if self-sustained detonation can propagate

- Critical conditions :
  - initial state (p,T), composition, amount of inert diluent, tube diameter, nature of tube wall

- Composition limit → given a tube diameter, lean and rich limits

- Given a mixture composition there is a limiting:
  - tube diameter
  - pressure limit (e.g. too low, too high)
- No theory for detonation limit prediction
- Experiment determination lacks an operational definition of a limit criterion
- Complex near limit phenomena:
  - Single headed spin, pulsating, galloping detonation, etc.

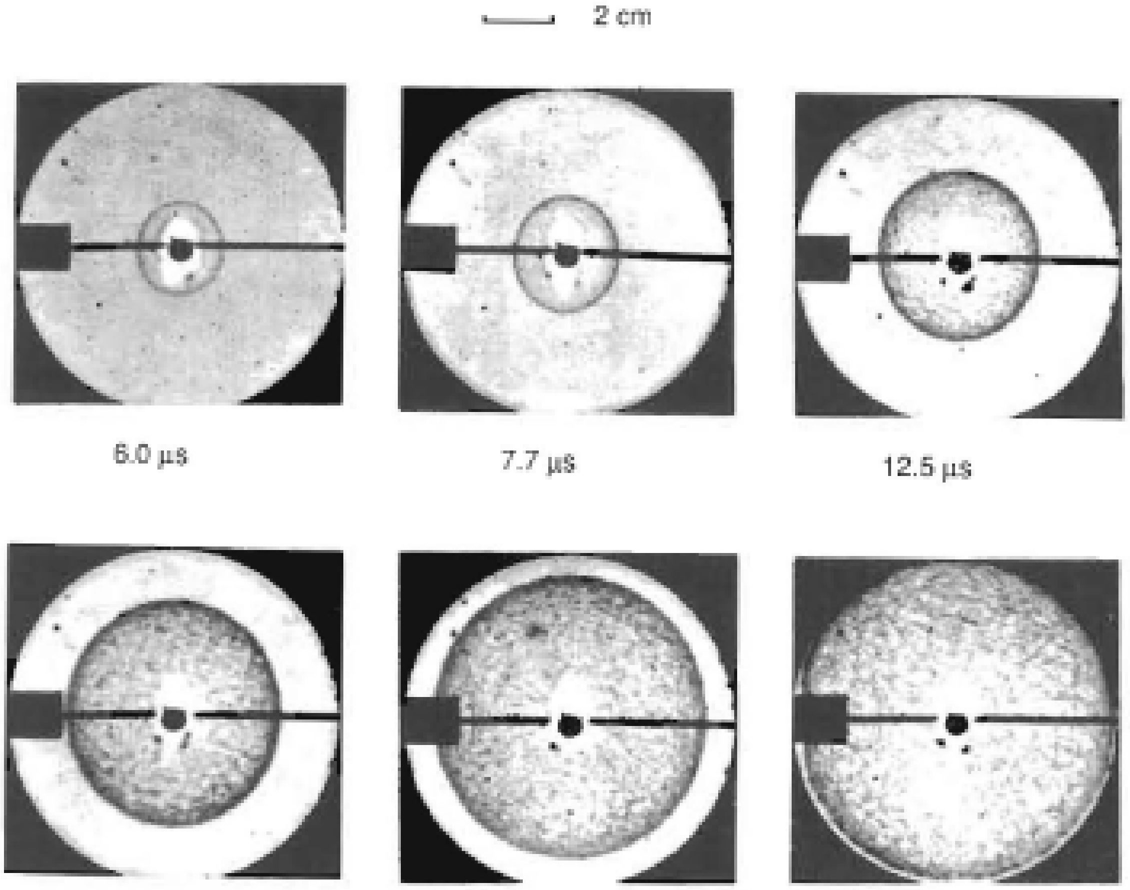
- Failure mechanism
  - Stable detonation → curvature
  - Unstable detonation → suppressing instability
- Sensitivity of mixture measured by detonation cell size λ.
- λ depends on mixture composition, inert diluent, initial pressure, etc.

- Boundary conditions characterized by tube diameter

- $\lambda = \pi d$ may serve as limit criterion for spinning detonation

Direct Initiation

- Formation of detonation from the conditions generated by the ignition source directly
- By pass the flame acceleration and pre-detonation deflagration stage
- Blast initiation → strong decaying blast wave generated by powerful ignition source
  - high energy spark, exploding wire, condensed explosive charge



6.0 µs

7.7 µs

12.5 µs

17.9 µs

23.0 µs

27.8 µs

Sequence of schlieren photographs of supercritical regime

Lee, J.H. et al. Comb. Flame, 18,1972

- Direct initiation possible if decaying blast is of sufficient duration
- Zeldovich criterion :
  - blast strength > Chapman-Jouguet detonation for a duration > induction time
- Propagation distance of black wave (above Chapman-Jouguet detonation strength) > detonation zone thickness

- Blast decay characterized by explosion length

$$R_o = \left(\frac{E_c}{p_o} \right)^{\frac{1}{3}}$$

- Detonation sensitivity characterized by reaction zone thickness (or cell size λ)

- Zeldovich criterion $\rightarrow \quad E_c \sim \lambda^3$

- Explosion length scaling for different geometry

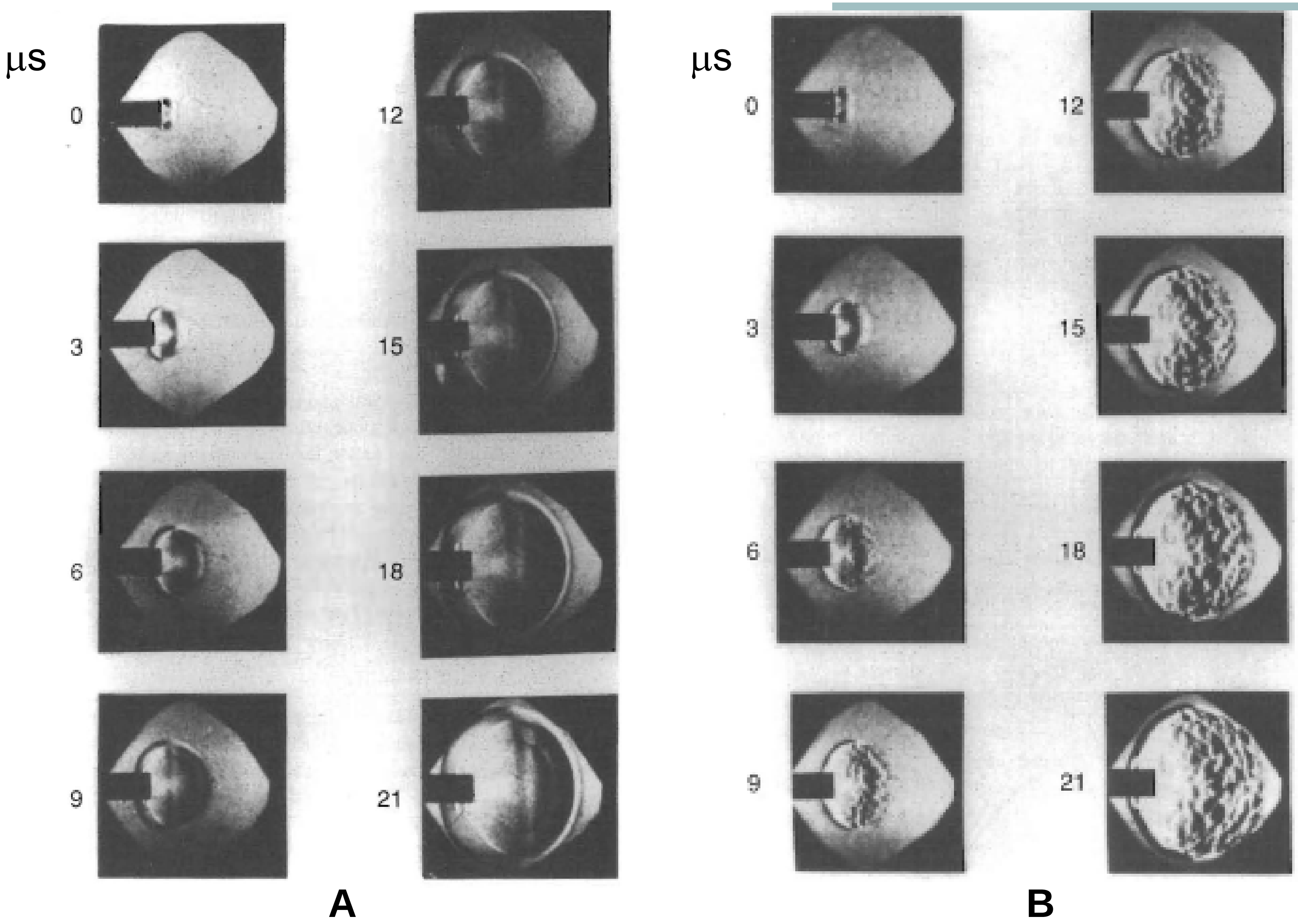
$$\left(\frac{E_c}{p_o}\right)_{\text{planar}} = \left(\frac{E_c}{p_o}\right)_{\text{cylindrical}}^{1/2} = \left(\frac{E_c}{p_o}\right)_{\text{spherical}}^{1/3}$$

- Direct initiation also possible by flash photolysis, turbulent jet mixing

- SWACER mechanism → induction time gradient to permit energy release in phase with shock wave

Critical Tube Diameter

- Minimum diameter of tube that permits planar detonation to diffract to a spherical detonation
  - Failure mechanisms
  - Stable detonations → curvature
  - Unstable detonations → suppresses growth of instability
- S & M criterion for unstable detonation $d_c \sim 13\lambda$



Sequence of schliren photographs of a planar detonation emerging from a tube into unconfined space in (A) the subcritical case and (B) supercritical case

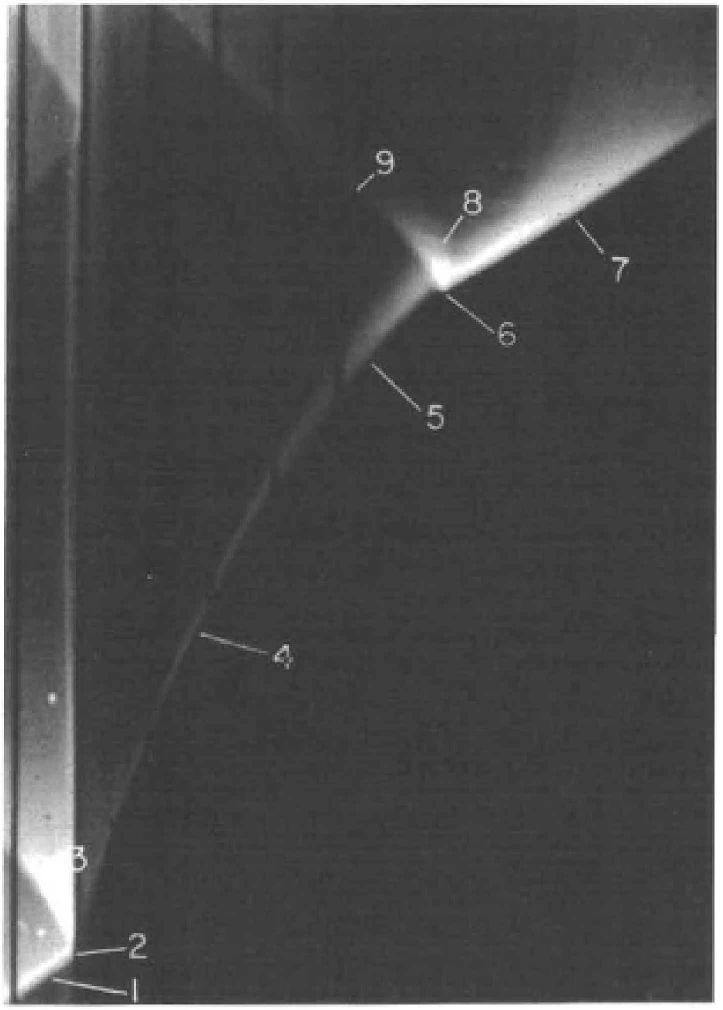
Courtesy of R.I. Soloukin

- Stable detonation $d_c > 13\ \lambda$ $\mathrm{d_c} \simeq 40\lambda$
- Effect of wall
  - Acoustic absorbing walls $d_c \simeq 6\lambda$
  - Readily deformable wall $d_c \simeq 5\lambda$
  - Rough wall → quasi detonation

$$0.3V_{\mathrm{CJ}} \le V_{\mathrm{D}} \le V_{\mathrm{CJ}}$$

Transition from Deflagration to Detonation DDT

- Flame acceleration phase subsequent to ignition
- Mechanisms of flame acceleration:
    - Flame folding
    - Turbulence
    - Instability
    - Acoustic-flame interaction
    - Metastable deflagration



Typical streak photograph of the abrupt transition to detonation via a jet of hot combustion products

Lee et al. 1996

- Mechanisms of flame acceleration (continued) :
    - Explosion centers
    - Growth of instability
    - Transverse acoustic amplification
    - Onset of detonation
    - Effect of wall roughness
    - Obstacles Schelkin spiral