Internal combustion engine: physics and numerical modelling

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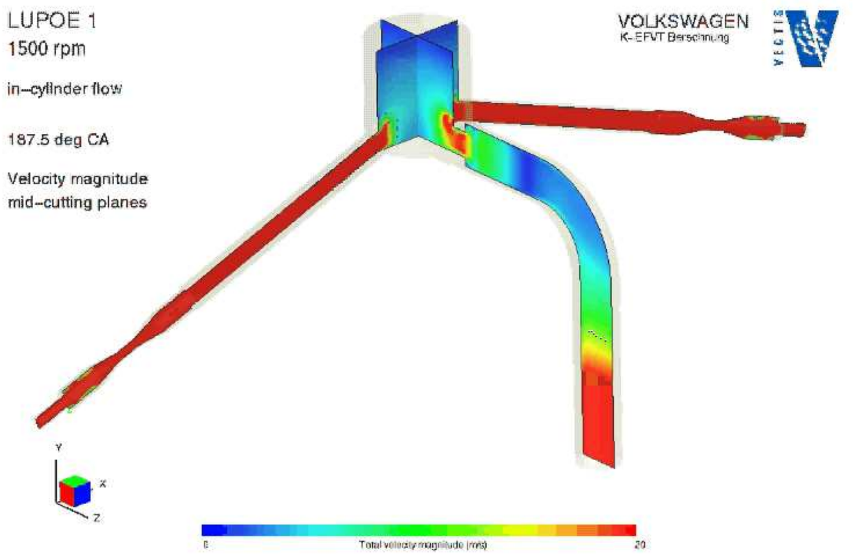
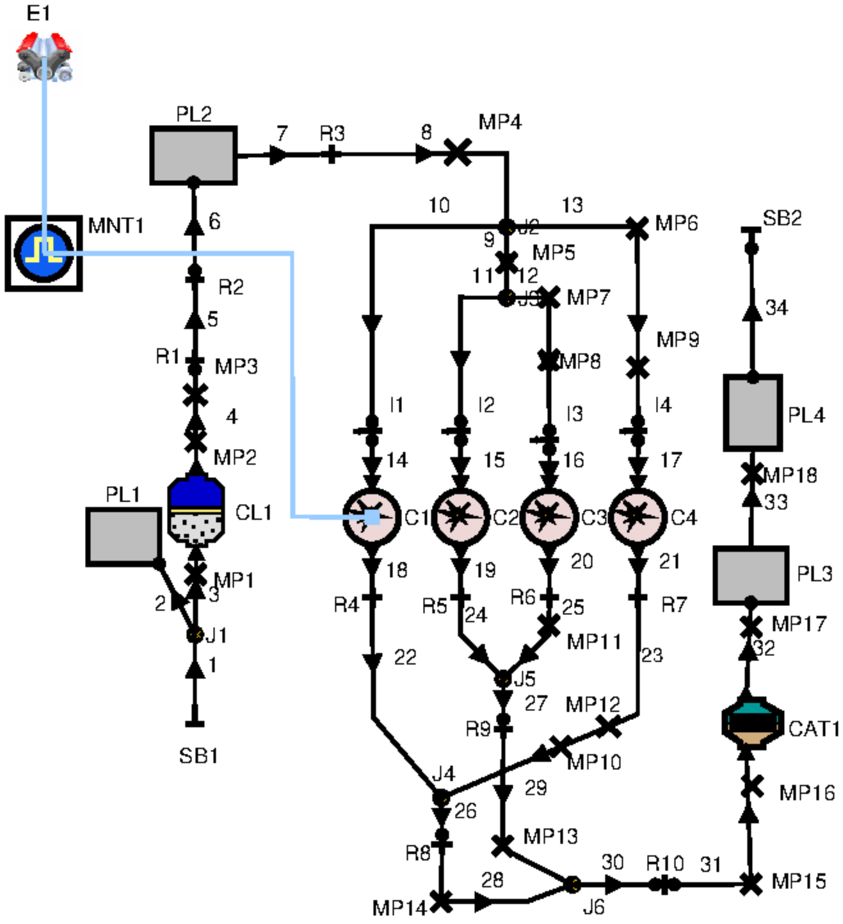
Two main approaches: CFD vs. "thermodynamic" modelling





The Computational Fluid Dynamics (CFD) resolves the flow details in individual engine elements, e.g. inside the combustion chamber. Well-known examples of CFD codes particularly suitable for engines are AVL FIRE or CONVERGE CFD.

The "thermodynamic" modelling represents the engine as a network of zero, e.g combustion chamber or manifolds, or one-dimen-sional, e.g. ducts, elements. Software implementing this type of modelling are AVL BOOST or GT-Power from Gamma technologies.

An accurate prediction of the rate of combustion is crucial for either method.

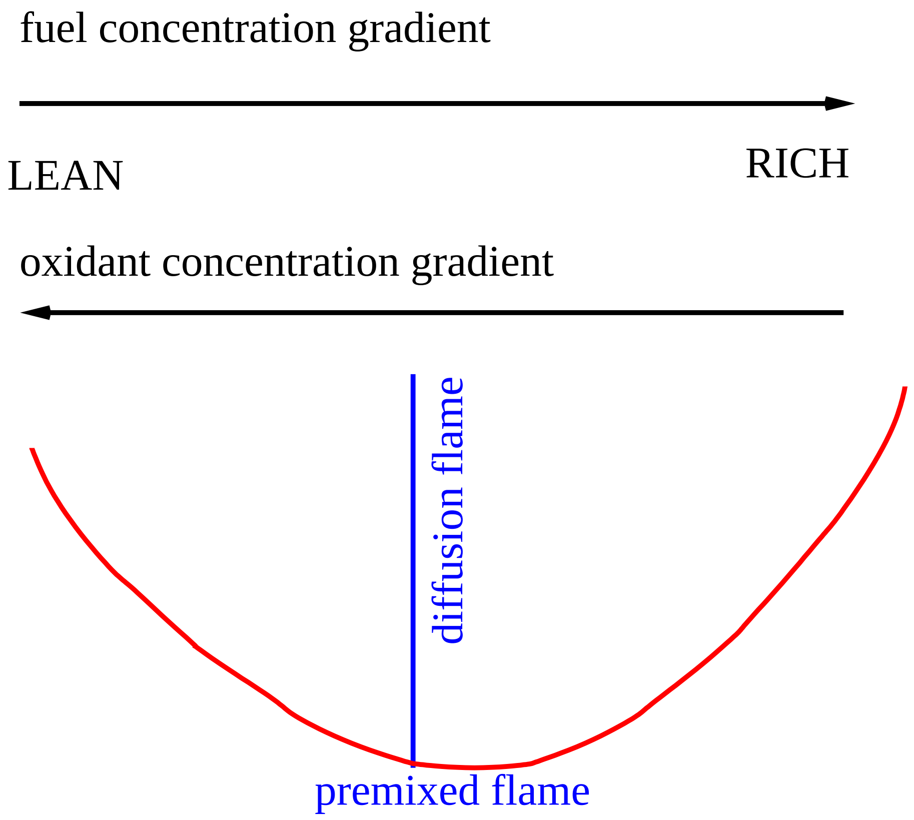
Principles of the thermodynamic engine modelling

The adopted approach consists in splitting of a time step into several pseudo-steps with individual physical processes, in the following sequence: blow-by flow, heat exchange, combustion, thermal expansion of the products, and, finally, the piston motion. The last three steps employ an iterative procedure to find new volumes and temperatures of fresh and burnt zones as well as the new pressure.

Process	Burnt gas	Fresh charge
Piston motion	Isentropic compression	
Constant volume combustion	Total internal energy is constant and the burnt zone internal energy is increased in proportion to the amount of the mass burnt	Constant temperature
Thermal expansion of products – pressure equalisation	Total internal energy is constant	Isentropic compression
Heat loss	The internal energy of the zone is reduced by a known amount	
Blow-by	For mass loss – constant temperature and the decrease of mass by a known amount; for the mass gain occurring at later stages in the working stroke - the returning gas has the wall temperature and the fresh charge composition	Constant temperature, the mass is decreased by a known amount

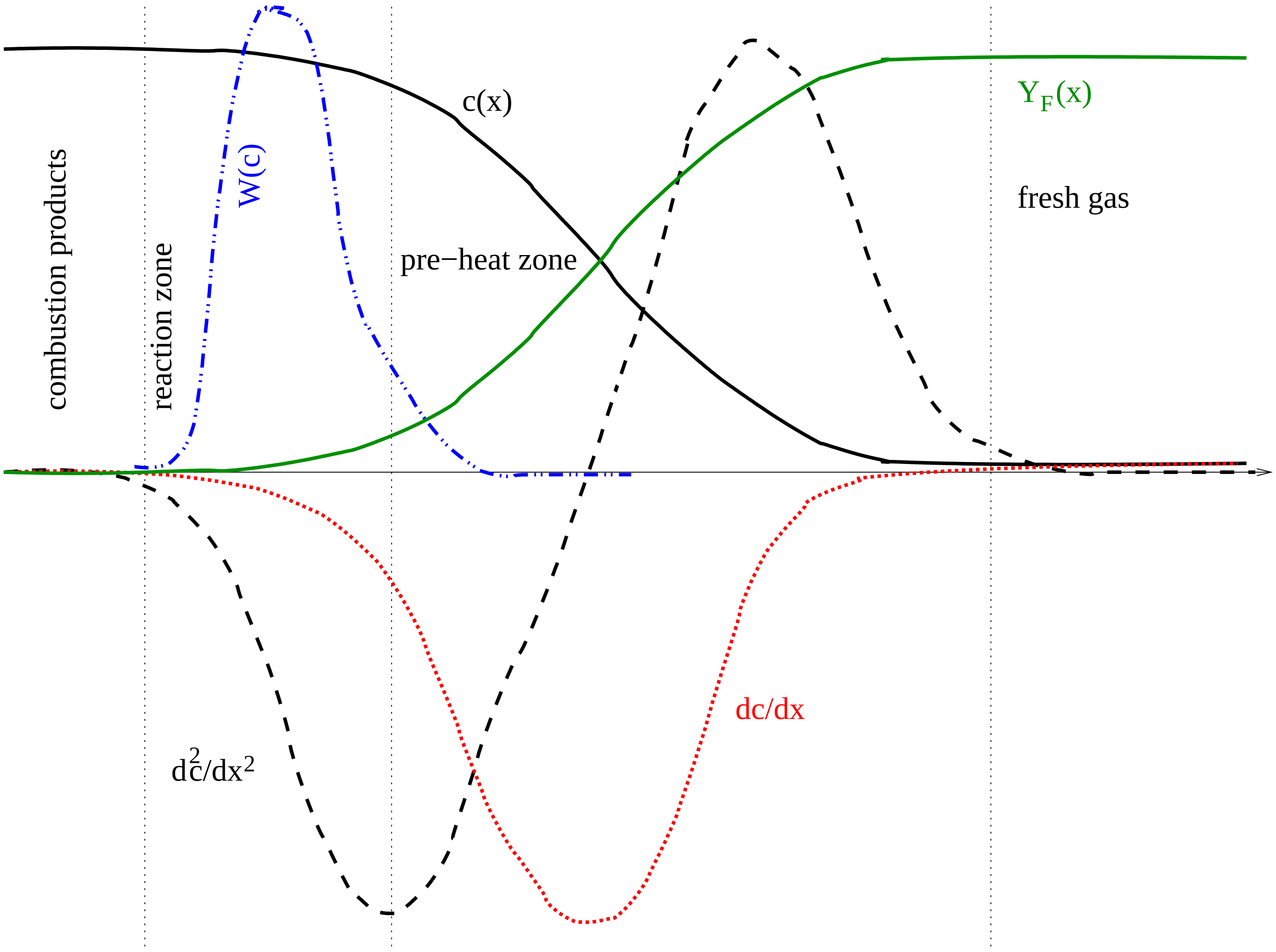
Different combustion regimes

It is remarkable that the same transport equations and reaction rates may lead to a great variety of very different combustion regimes. When the fuel and oxidant are perfectly well mixed together before the reactions begin then the combustion occurs as a **propagating wave**; this wave is known as a **premixed flame**. This is a common situation in most spark ignition engines. When the combustion happens between the distinct and separate flows of fuel and oxidant (air), the flame sits at the boundary between those. Combustion between unmixed reactants is known as **non-premixed** or **diffusion flame**.



When the flows are not perfectly mixed, a large number of scenarios may arise, e.g. some **stratified flames**, or **triple flame** which is a bow of premixed flame ranging from rich to lean side with a diffusion flame joining it at the stoichiometric point.

Propagation of premixed planar laminar flame.



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Laminar flame speed

Zel'dovich-Semenov-Frank-Kamenetski derived the speed u_n of planar, unperturbed, premixed flame speed assuming constant density:

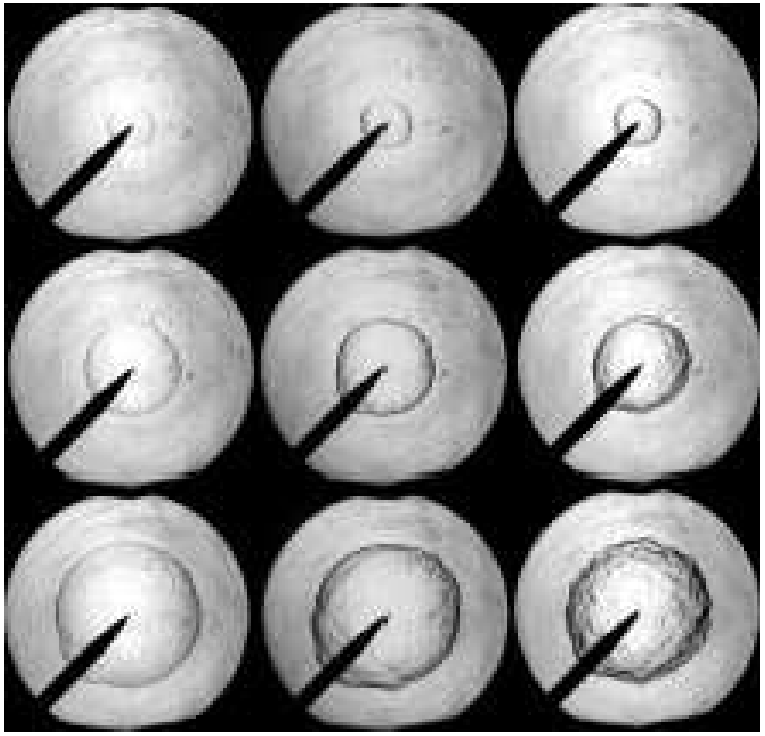
$$u_n = \left[2\kappa \int_0^1 W\left(c'\right) dc' \right]^{1/2}$$

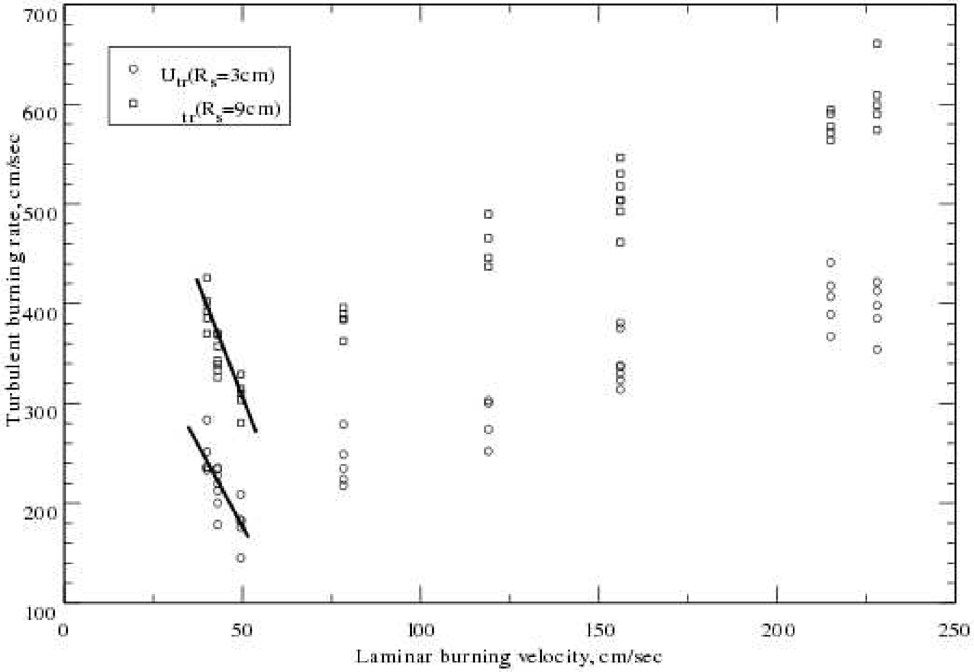
This is a major result of the ZSFK theory; it demonstrates that u_n depends solely on κ and **the integral of the reaction rate profile**. It is very remarkable that the flame speed **does not** depend upon a particular character of the reaction rate dependency upon the temperature and concentration; it depends only on the chemical times scale defined as

$$\tau_c = \left[\int_0^1 W\left(c'\right) dc' \right]^{-1} \qquad u_n = \left(\frac{2\kappa}{\tau_c} \right)^{1/2} \tag{1}$$

If should be noticed that the flame speed depends strongly upon the molecular transport coefficients; when some of the assumptions underlying ZSFK are not fulfilled, then the mathematical analysis becomes quite complicated. When the mass diffusivity of the deficient reactant D is greater than the thermal diffusivity κ, the flame speed becomes proportional to the ratio κ/D. However, when $D \leq \kappa$ then the propagation of flame with a constant speed is unstable and the flame propagation exhibits oscillations of its speed or simply does not exist.

Stability of premixed flame: cellular flames





Bomb measurements. Left: Appearance of the cellularity in lean $H_2 - CO$ flame when the initial pressure is increased from 0.5atm to 1.5 atm. Right: Response of the turbulent burning rate to variation of the laminar flame speed. Fugures taken from [5].

The pressure promotes the flame instability so that **no hydrocarbon flame is stable** at the pressures above 20 atm. in IC engines or gas turbine combustion chambers. The usual combustion models assume that increase of u_n leads to faster turbulent combustion - this is not so not when u_n is varied with pressure.

Non – premixed, or diffusion, flame

Consider a situation where fuel and oxidiser are not premixed. Obviously in this case, for the chemical reactions to proceed, the reactants have to mix first at the molecular level, and if the chemistry is fast enough, which is very often the case, then it will be this molecular mixing – diffusion that controls the rate of combustion. In this case, the flame separates the mixture of fuel and products on one side, and air (oxidiser) on the other side.

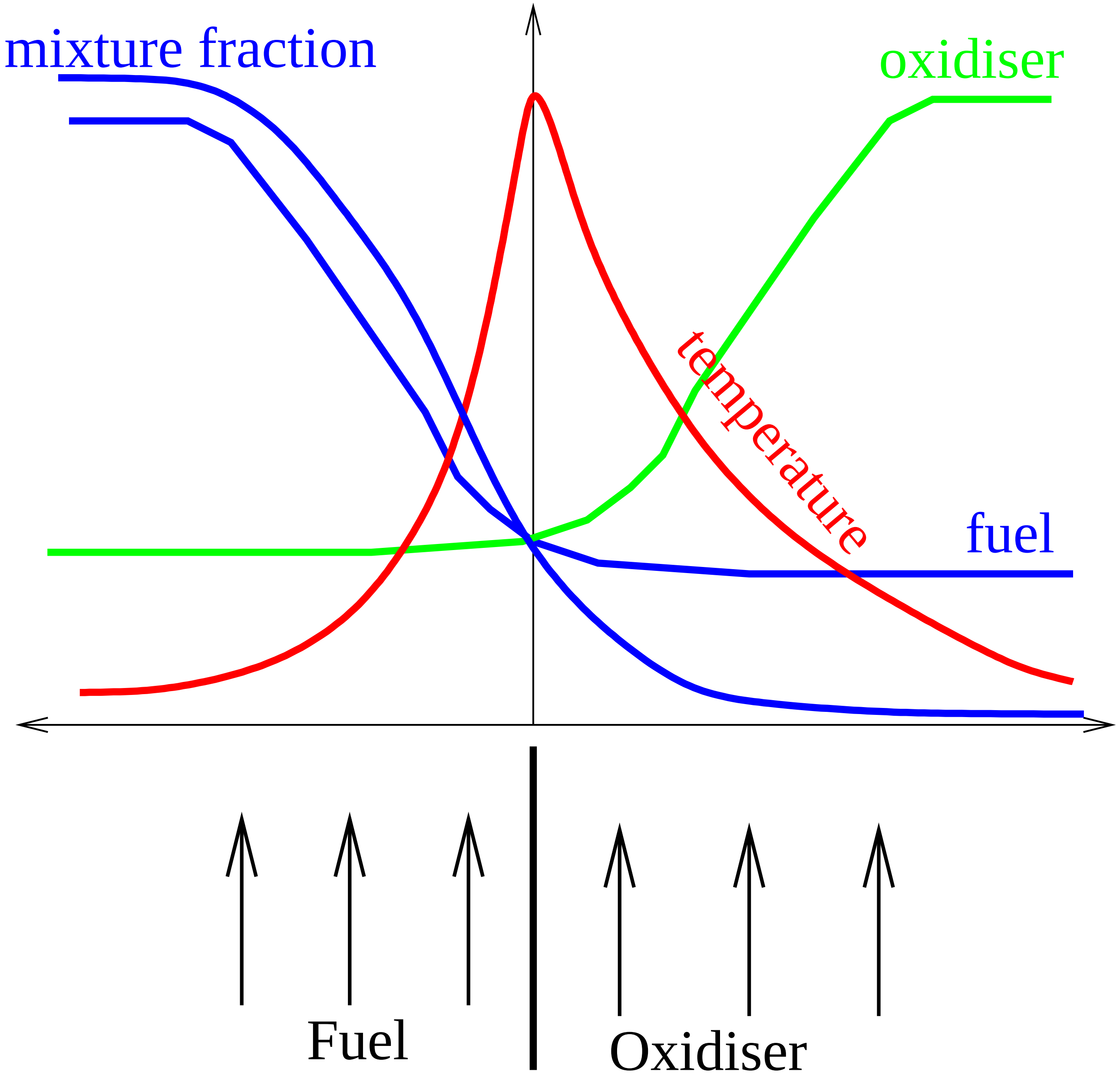
The examples of this regime are: flame of a candle, fire in a domestic stove or combustion in a Diesel engine. It is also very often thought that the diffusion flame is esablished around ablating solid or vaporising liquid fuels; all common fuels, except char or pure carbon, e.g. as charcoal, char or graphite, burn in the gaseous phase.

For a simplified analysis of a diffusion flame, suppose that the chemical reactions may be represented in a simplified form:

$$\nu_1 A_1 + \nu_2 A_2 \rightarrow \nu_3 A_3$$

where ν_i are the stoichiometric coefficients.

Non – premixed, or diffusion, flame



Non – premixed, or diffusion, flame

Brilliant in its simplicity, and one of the most insightful and fundamental observations in the entire combustion theory was made by Burke & Schumann in 1928, that is that if to substract the equation for $\left(-\frac{c_1}{\nu_1}\right)$ from that for $\left(-\frac{c_2}{\nu_2}\right)$ then the reaction rate disappears:

$$\left[\frac{\partial}{\partial t} + \vec{u} \cdot \nabla \ - D_i \,\mathrm{div}\ (\nabla\ )\right] \left[\frac{c_1}{\nu_1} - \frac{c_2}{\nu_2}\right] \ = \ 0 \tag{2}$$

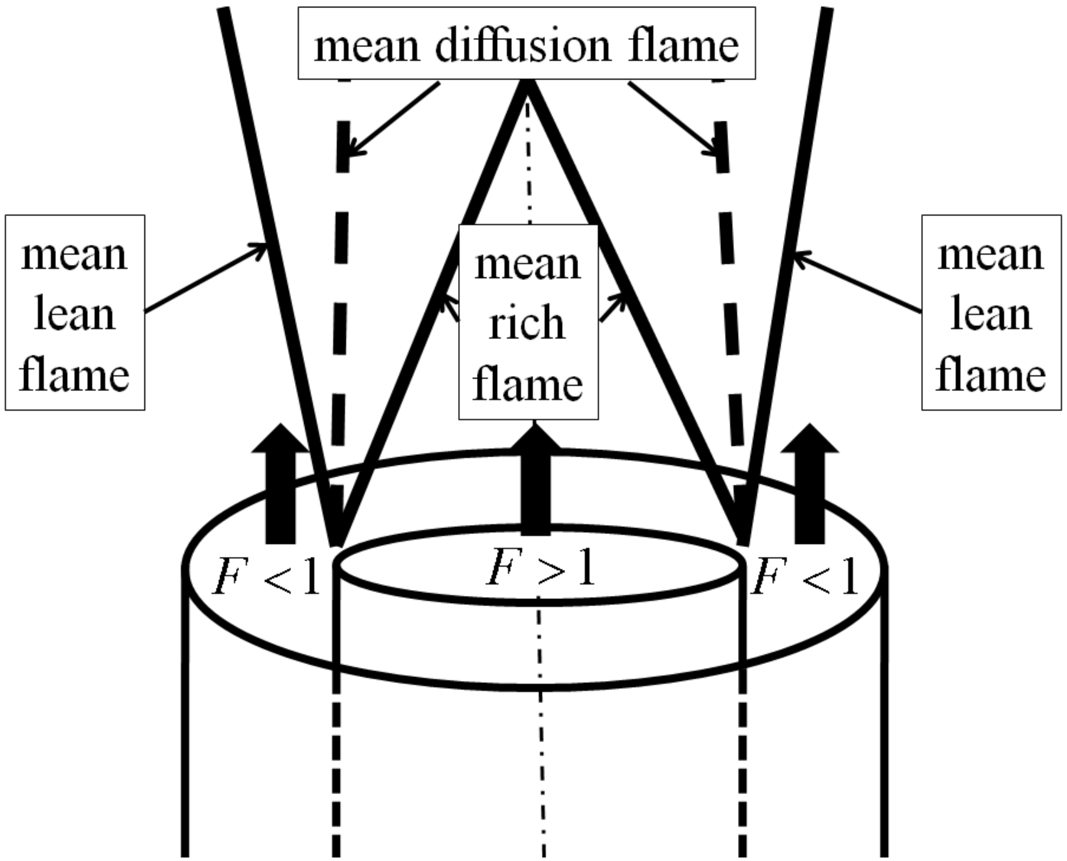
Because its transport equation does not have a source term caused by chemical reactions, the combination $\left[\frac{c_F}{\nu_F} - \frac{c_{ox}}{\nu_{ox}}\right]$ is called a **passive, that is chemically inert, scalar**. Quite often, it is also termed **the mixture fraction**. In addition to the mixture fraction, it is possible to construct another combination of concentrations, e.g. c_1 and c_2, and temperature which will also be a passive scalar, e.g.

$$\eta = Const_1 \ \left[Const_2 \frac{c_1}{\nu_1} + (1 - Const_2)\,\frac{c_2}{\nu_2} + \frac{c_p}{Q}\,(T - T_O)\right] \tag{3}$$

This, or any other similar combination, is known as a **Schwab – Zeldovich variable**.

In order to commence the analysis of a dissusion flame structure, it is expedient to assume that the chemical reactions are very fast. In this case one may conclude that either fuel or oxidiser should be zero at any given point in the flow, i.e. they cannot co-exist. It will also mean that the surface where $\eta = 0$ will represent the surface of the flame where both fuel and oxidiser disappear.

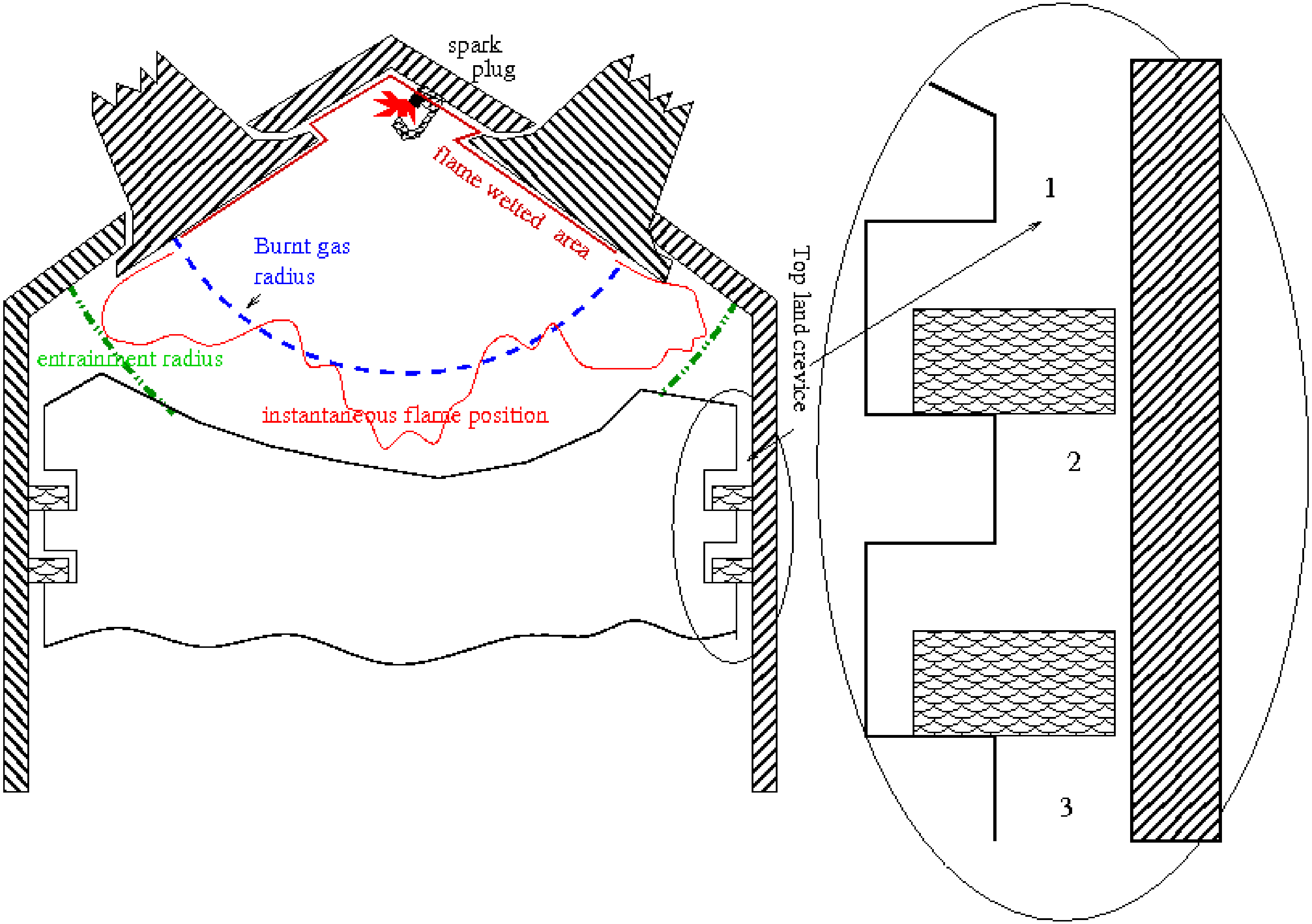
Partially premixed flames.



Taken from [6]

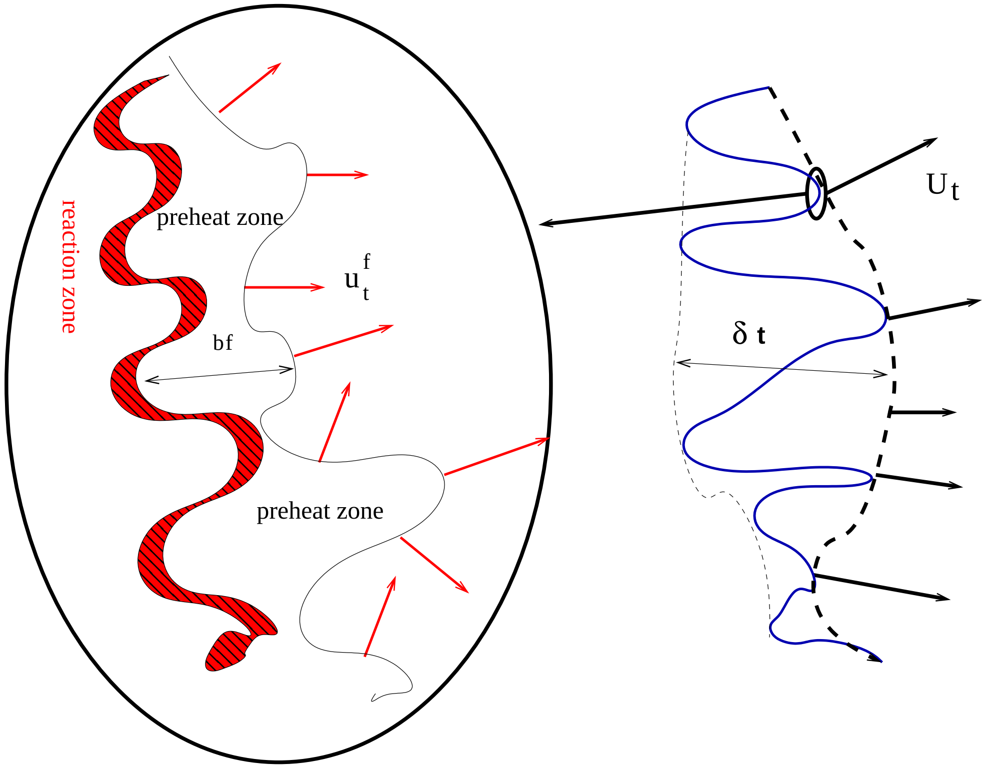
Quite a common flame configuration is when a diffusion flame, where the fluxes of oxidiser and fuel meet at stoichiometric proportions, appears on the boundary between rich and lean premixed flames.

Combustion in SI engine.



The principal combustion regime in SI engine is a propagating turbulent premixed flame. It may be either homogeneous, e.g. a PFI engine, or stratified, e.g. a late injection GDI engine.

Turbulent premixed combustion



Turbulent premixed combustion is the mechanism of the energy conversion in spark-ignition engines and most, if not all, modern gas turbines. Similar to a laminar flame, turbulent premixed combustion occur as a propagating wave, however, determination of the speed and internal structure of this wave is far from trivial. So, both the average burning velocity U_t related to a partilar postion with the flame brush and the instantaneous flame front velocity u_t^f are fluctuating quantities.

One very important step to understanding turbulent premixed combustion has been accomplished with the classification [3] of different regimes of turbulent premixed combustion in terms of ratios of turbulence rms velocity u' to the laminar flame speed u_n and turbulent integral length scale l_t to the laminar flame thickness δ_n.

Direct Numerical simulations of $H2$-air flame: heat release

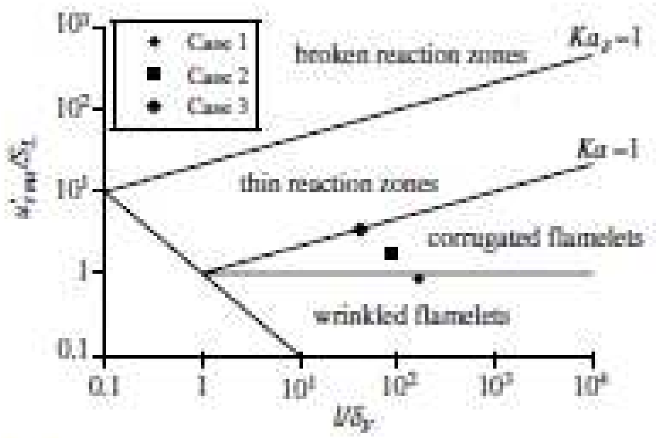


Figure 2. Turbulence combustion diagram.

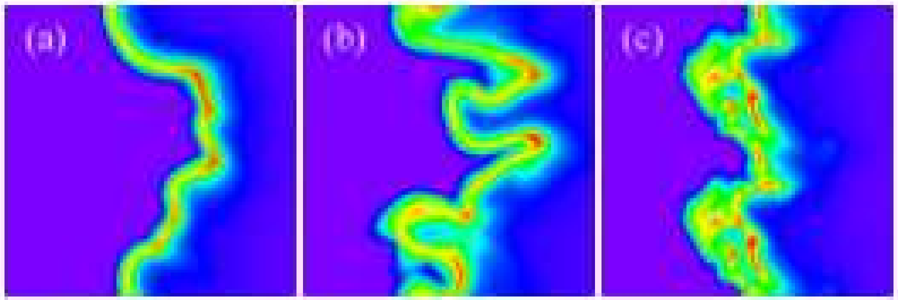
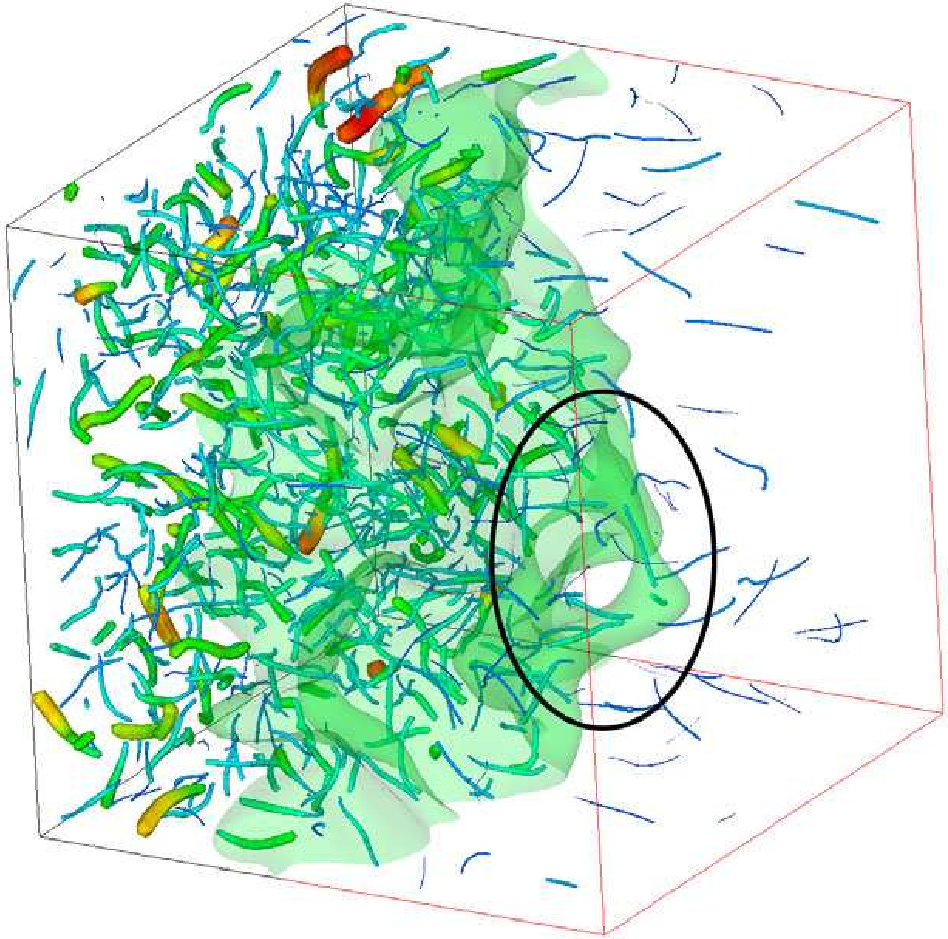


Figure 3. Distributions of the heat-release rate on a typical x–z plane for cases 1(a), 2(b) and 3(c).



Taken from Y. Nada , M. Tanahashi & T. Miyauchi (2004) Effect of turbulence on characteristics on local flame structure of H2-air premixed flames, Journal of Turbulence, 5, N16

Direct Numerical simulations of H_2-air flame: O radical

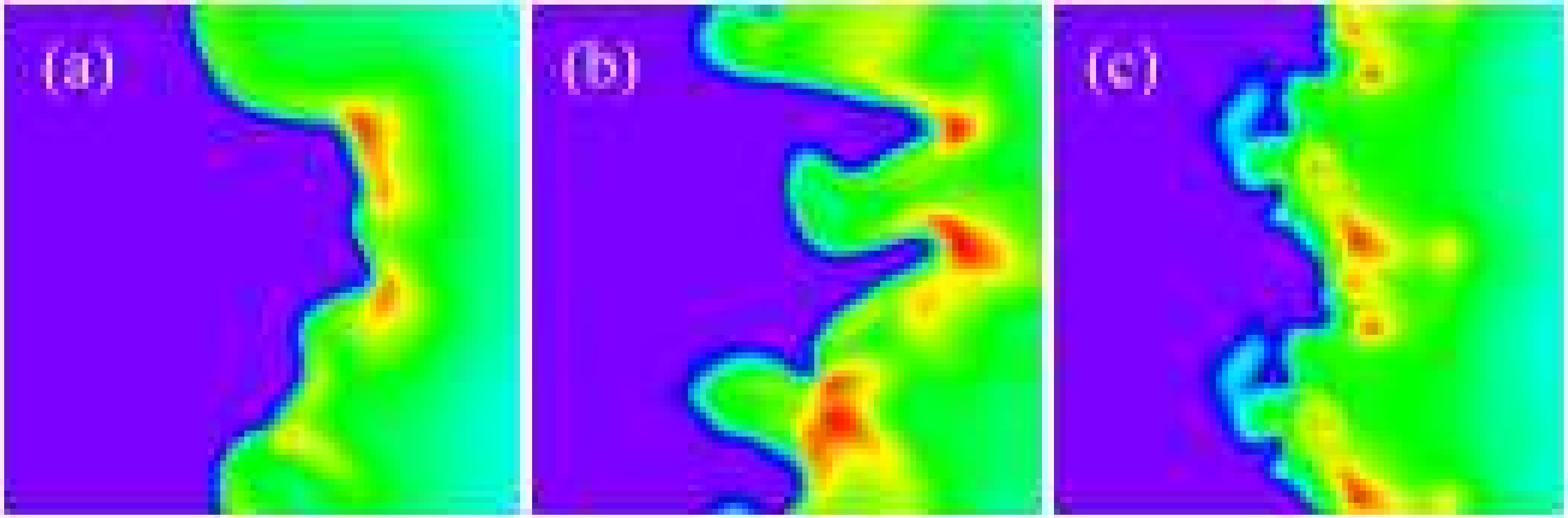


Figure 4. Distributions of the mass fraction of O atom on a typical x-z plane for cases 1(a), 2(b) and 3(c).

Taken from Y. Nada , M. Tanahashi & T. Miyauchi (2004) Effect of turbulence on characteristics on local flame structure of H2-air premixed flames, Journal of Turbulence, 5, N16

Turbulent premixed combustion - equilibrium

Very recently, two papers of monumental proportions [7, 8] (featuring 350 and 571 referred papers, respectively) presented a comprehensive review of turbulent premixed flames properties and physical variables defining these properties. Some of these variables, such as laminar flame speed u_n or molecular heat diffusivity κ are determined by the mixture composition, pressure and temperature, some, such as turbulence properties, are dependent on flow and flame geometry.

The first review argued that, under most circumstances, determination the velocity and the thickness of the turbulent flame should include the flame development effects. The flame development means that the turbulent flame brush thickness grows with time from igntion, as in a SI engine, or the distance from the flame-holder as in gas turbine, in the same way as grows turbulent mixing layer. The turbulent flame speed also grows reflecting the fact that wider flame brush can accommodate larger area of the wrinkled flame:

$$U_t = \left\langle \frac{A}{A_0} \right\rangle u_t^f \sim \frac{\delta_t}{b_t^f} u_t^f$$

At the present it is not entirely clear whether a turbulent flame velocity and thickness grow indefinitely, i.e. an infintiely large flame has an infinite velocity or there are some mechanism which limit this growth and sturate both flame speed and thickness.

Turbulent premixed combustion - Zimont-Lipatnikov model

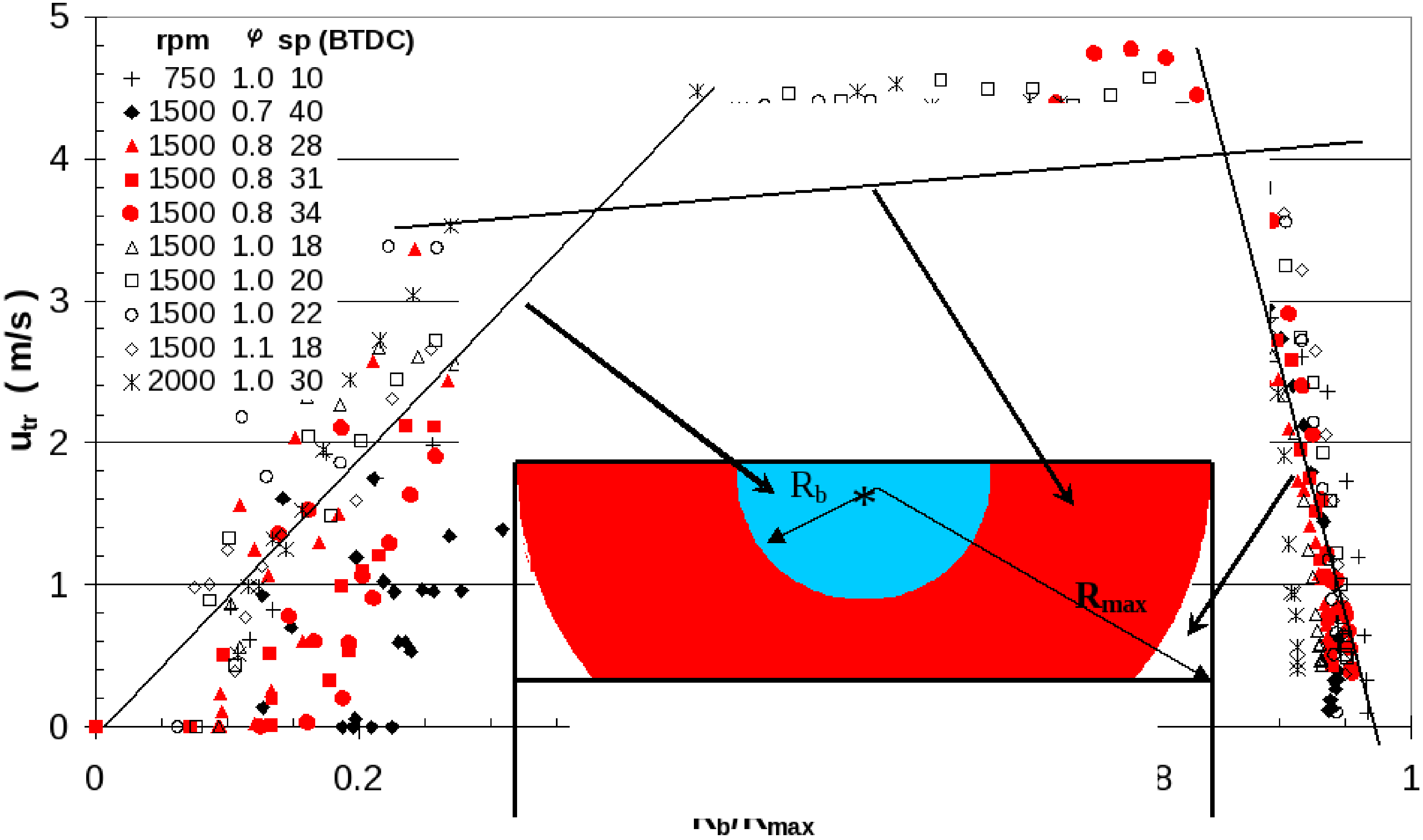
It is quite interesting that a very large body of experimental measurements are well represented with a very successful Zimont-Lipatnikov model, also referred to in some CFD packages, e.g. Fluent, as Turbulent Flame Speed Closure, [11, 7]. This model postulates that eventually an equilibrium is reached between a progressive entrainment of the fresh gas into the front by the small-scale turbulence and the own flame propagation. Quoting [11], the flame will reach "*static equilibrium between the increase in the surface area of the front because of turbulent pulsations and its diminution because of displacement of the combustion front relative to the medium*".

At this equilibrium:

$$U_t \approx u' \cdot Da^{1/4} = Const u'^{3/4} l_t^{1/4} u_n^{1/2} \kappa^{1/4}$$

However, the review [7] concluded that dependency of the burning rate U_t upon the integral length-scale l_t cannot be established without ambiguity because of controversy and paucity of available experimental data. It is also appropriate to mention that the remarkable success of Zimont-Lipatnikov model applied for very diverse flame configurations [7], indicates that the effects of the integral scale are likely to be weak, because this model assumes that $U_t \sim l_t^{1/4}$.

Flame development in SI engine



Experimental observations clearly show that in engines the flame speed is first increasing, then attains some more or less constant value and then the flame slows down when approaching the walls.

Models of unsteady flame development

Zimont-Lipatnikov model

Growth of flame kernel is similar to the Taylor turbulent diffusivity, so:

$$U_t = U_t^0 \left(1 + \frac{\tau_t}{t}\left(\exp\left(-\frac{t}{\tau_t}\right) - 1\right)\right)^{1/2}$$

According to the same hypothesis, a turbulent flame should also have a growing thickness, such that at long times $\delta_f(t) \sim t^{1/2}$:

$$\delta_f \; = \; \sqrt{2} l_t \cdot \left[\frac{t}{\tau_t} - 1 + \exp\left(-\,\frac{t}{\tau_t}\right)\right]^{1/2}$$

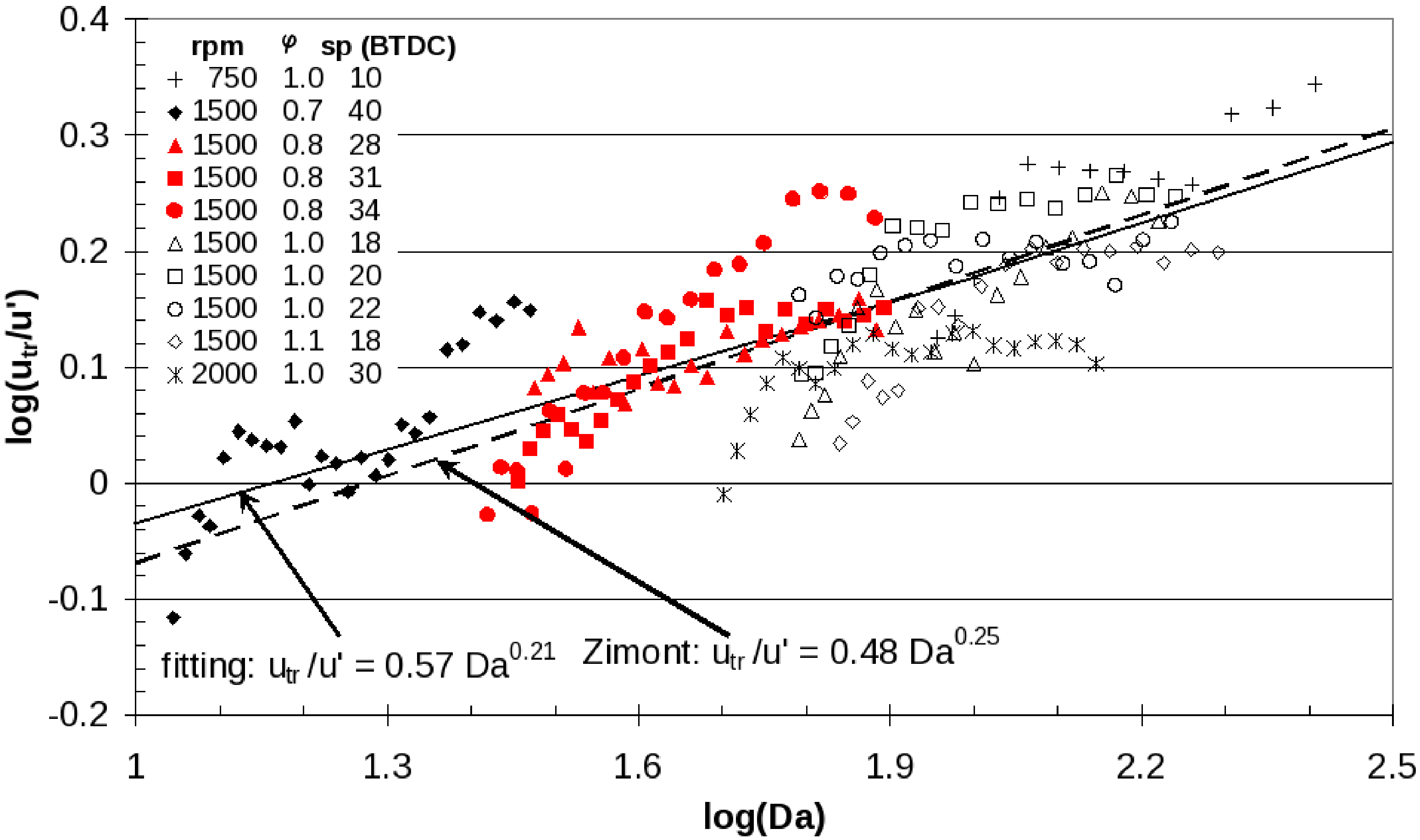
It is important to emphasize that virtually any flame one may encounter in an SI engine is a developing one.

Asymptotic value for $t \to \infty$ U_t^0 may be calculated from some other model. One such model proposed originally by Zimont:

$$U_t^0 = A u'^{0.75} u_n^{0.5} \kappa^{-0.25} l_t^{0.25}$$

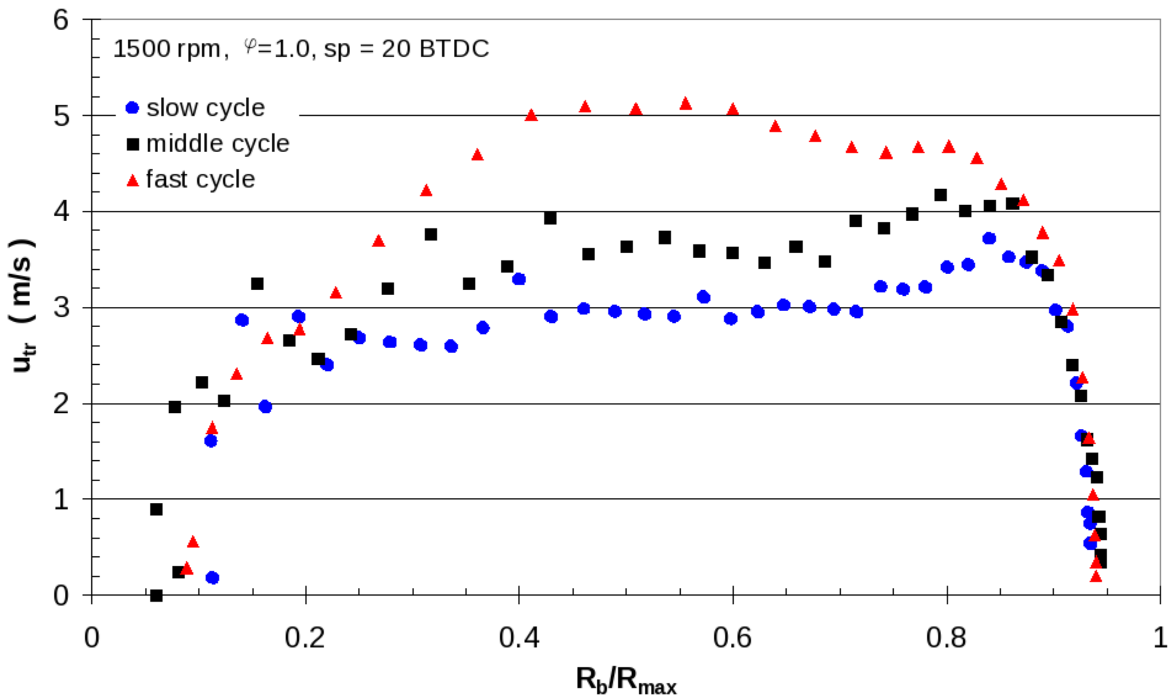
where u_n is the laminar flame speed, κ is the heat conductivity, l_t is the integral length scale of turbulence.

Asymptotic value of the flame speed in an SI engine



It can be seen that both turbulence and the molecular transport, that is thermal and mass diffusivity, affect the flame propagation rate [9]. **The aim is to organise the main combustion event in such a manner that virtually all charge is consumed by the propagating flame BEFORE the spontaneous self-ignition of the end gas sets on.**

Flame deceleration by the wall



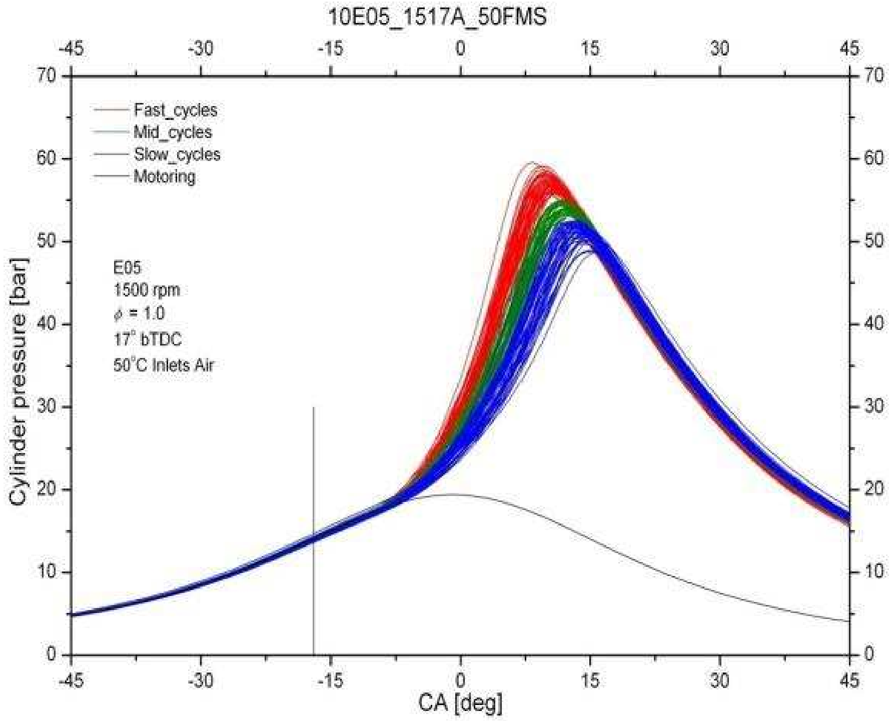
For engine applications, an additional factor has to be introduced in order to take into account the deceleration of a flame approaching the chamber side wall. To derive an expression for the deceleration, use is made of the self-similar spatial profile of the mean flame progress variable:

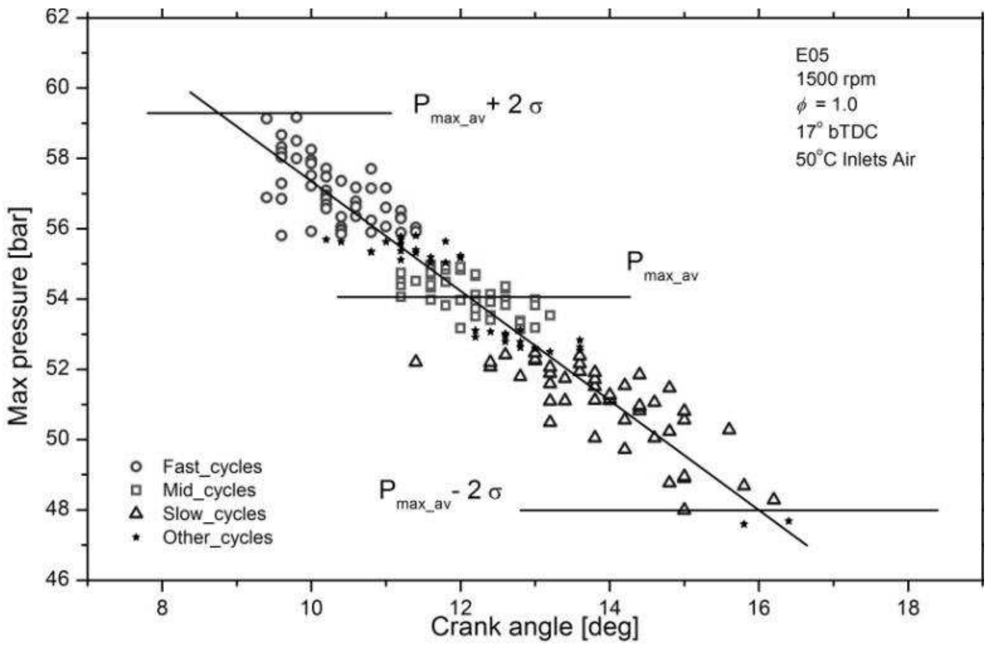
$$c\left(r,t\right) = \frac{1}{2}\left(1 - \mathrm{erf}\left(\frac{r - r_{fe}}{\delta_f\left(t\right)}\right)\right)$$

Validity of this profile in the engine conditions is confirmed experimentally [9]. Using it:

$$\frac{U_{te}}{U_{te}^0} = 2 \cdot \mathrm{erf}\left(\frac{R_w - r_{fe}}{\delta_f\left(t\right)}\right) - 1$$

Cyclic variability.





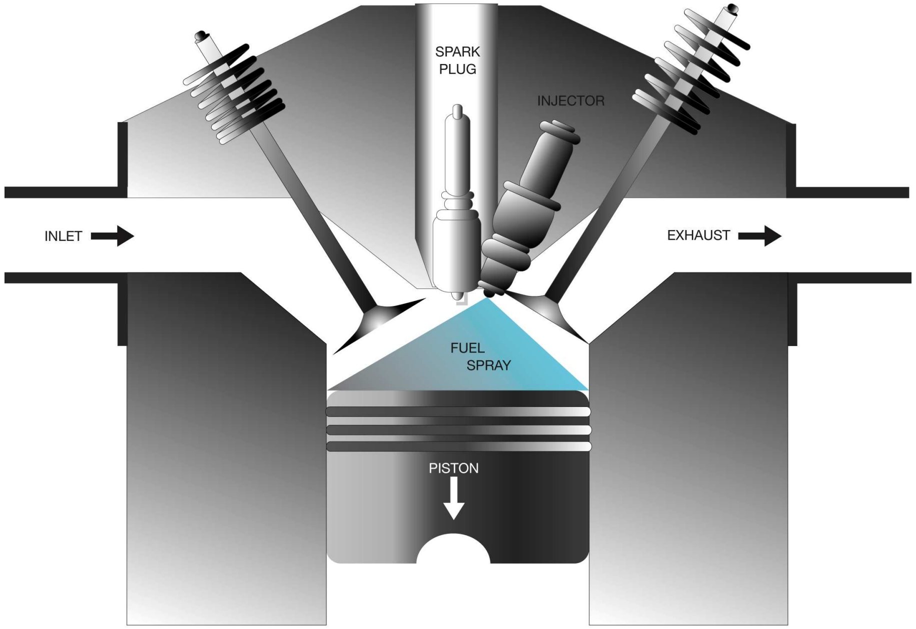
There are various potential sources of cyclic variations which can be divided into two groups. The first group includes sources which their contribution to cyclic variations could be eliminated or minimised when precise equipment associated with feedback control is used. Those are:

(a) variability in the trapped quantities of fuel, and residual and/or EGR, which imperfectly mix with the fresh charge.

(b) non-homogeneity of the mixture strength, especially in the vicinity of the spark plug.

(c) variability in the spark timing and its discharge characteristics, such as breakdown energy, initial flame kernel shape, size and random displacement.

Gasoline DI engines: early injection



DIRECT INJECTION - HOMOGENEOUS MIXTURE
SPRAY GUIDED SYSTEM

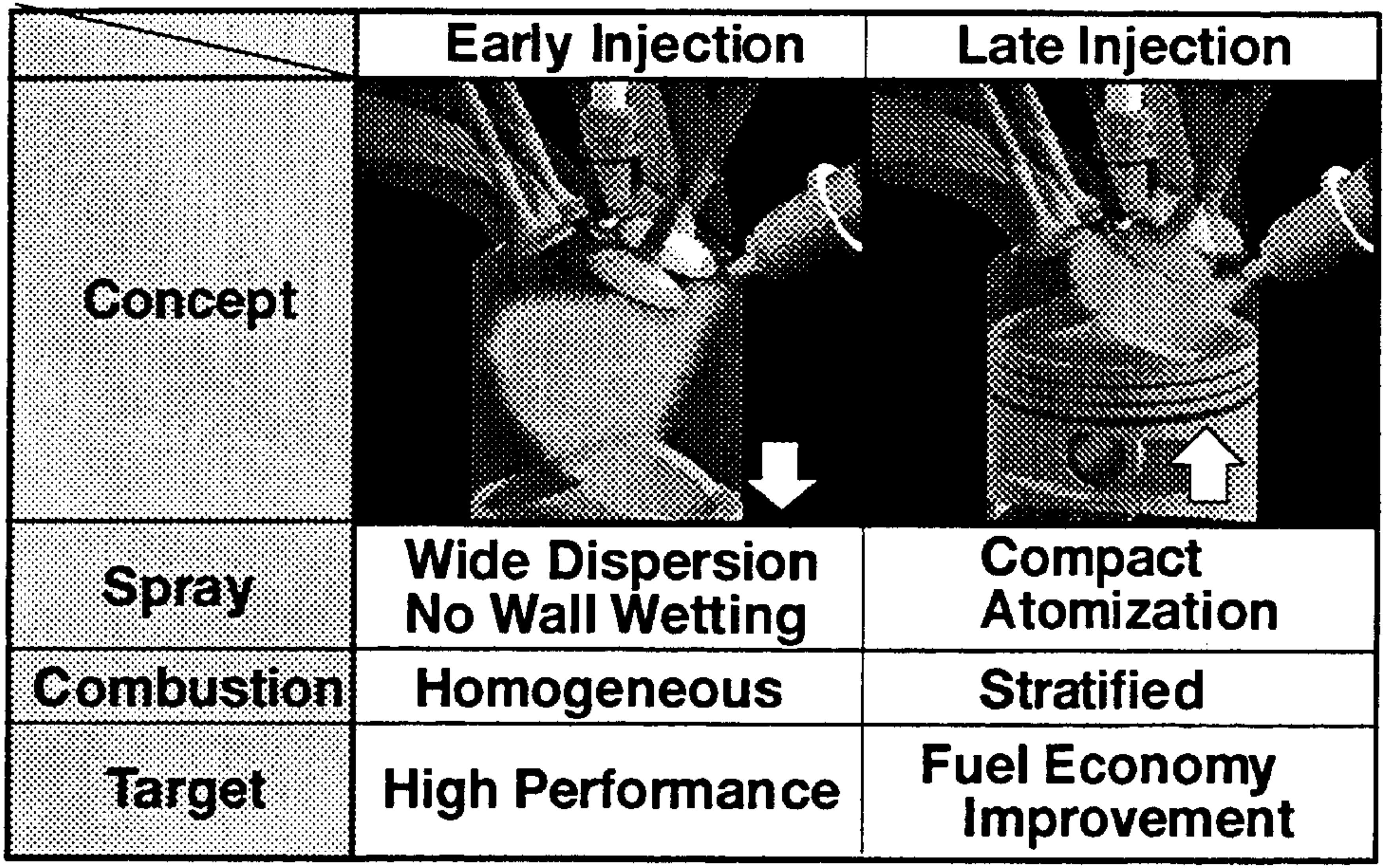
The first Gasoline Direct Injection (GDI) system was pioneered by Mitsubishi in 1997. Since then every major engine OEM has an active R& D program in GDI systems.

In a homogenous GDI combustion system, i.e one employing injection directly into the combustion chamber, early in the beginning of a compression stroke, fuel has an ample time to vaporise and mix with air so that at the moment of ignition there is virtually no stratification. Aftertreatment is simple: no need for NO_x trap, and possibility of up to 10% improvement in fuel economy has been reported as compared to PFI systems.

GDI is well suited to downsized engines. With a fully variable valve train (VVT), this is an extremely attractive concept. VVT reduces throttling losses, while GDI still yields major benefits: target is 15-18% improvement in fuel economy.

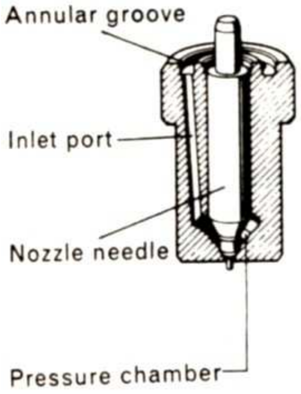
Absence of the fuel film on walls of the intake manifold or runners means more accurate fuel metering, hence potentially lower cyclic variability. Latent heat of evaporation comes from the charge, the cooling of which means better resistance to self-ignition and knock.

GDI: late vs. early injection



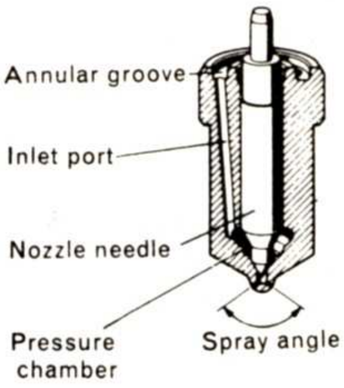
	Early Injection	Late Injection
Concept		
Spray	Wide Dispersion No Wall Wetting	Compact Atomization
Combustion	Homogeneous	Stratified
Target	High Performance	Fuel Economy Improvement

Fuel injection systems

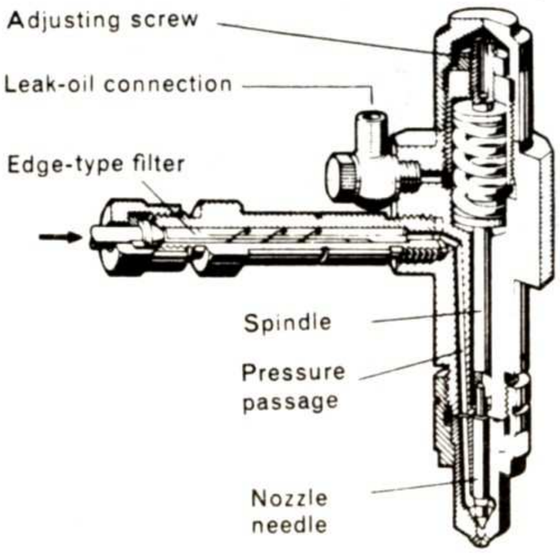


Pintle nozzle closed

Pintle nozzle open



Multihole nozzle open



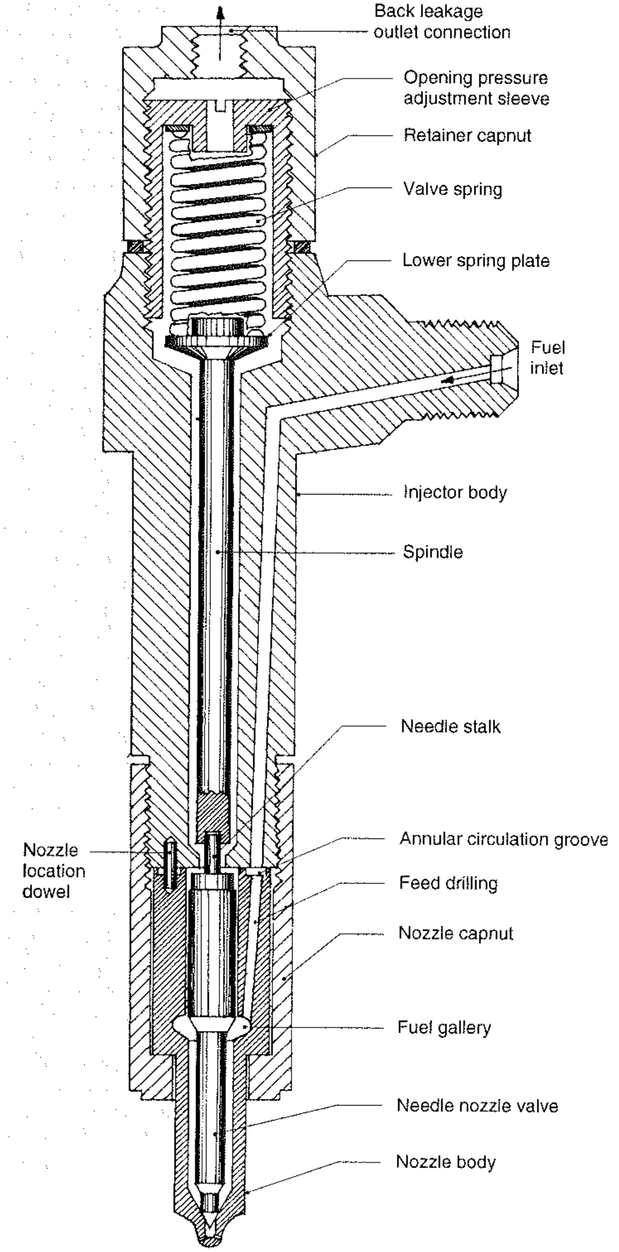
Nozzle-holder assembly with nozzle

For a typical four cylinder, four stroke, car engine with a rated full load power of 100 bhp and running at an engine speed of 2,400 rpm, there are 288,000 separate injections of fuel per hour. Each injection must deliver about 60 mm^3 of fuel. (This is the volume of two raindrops).

This same fuel injector must be capable of delivering, with high precision, quantities of 5 mm^3 under idling conditions and 1 mm^3 when pre-injection is used.The nature of the spray at any instant has a direct effect on combustion and emissions. In diesels, fuel is injected near to TDC into a very high pressure medium and injection continues during much of the combustion process.

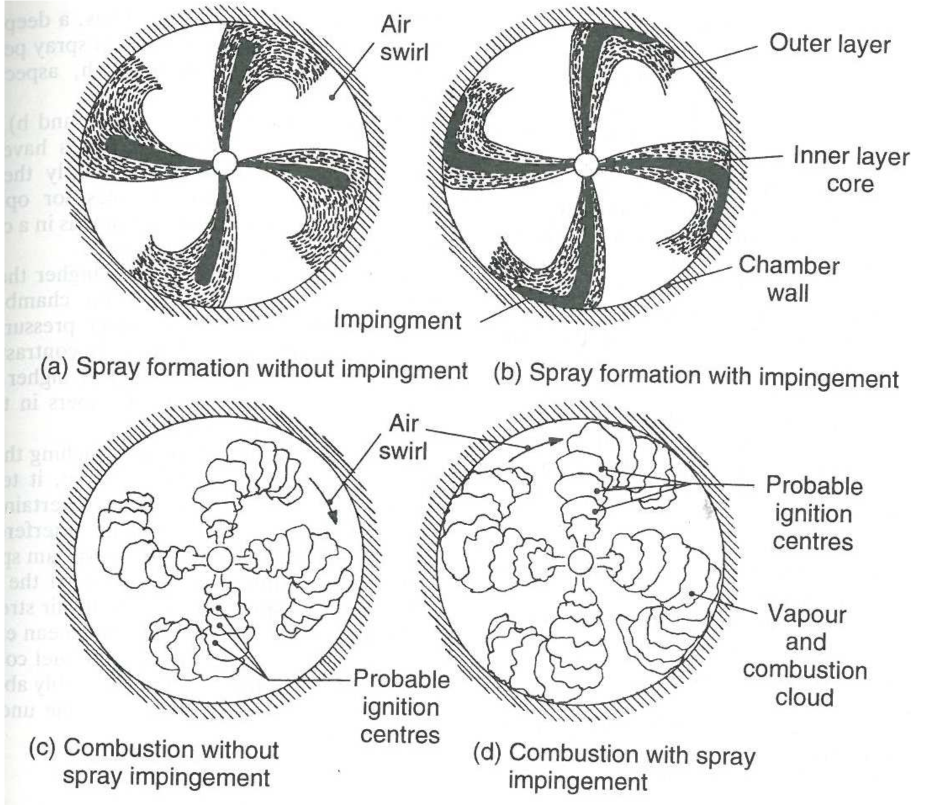
Because of a large back pressure and very agressive high temperatures diesel fuel injectors are much more complex (and expensive) than those for spark ignition. **The fuel injection system of a passenger car diesel engine may cost more than the entire spark ignition engine.**

Multi-hole injector



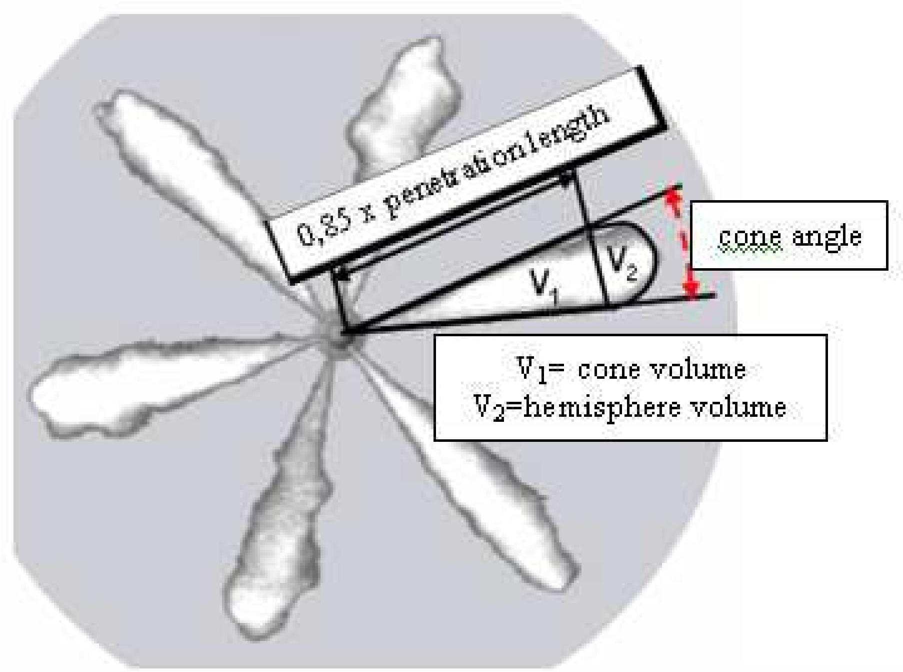
Because it is difficult to design a system where one spray jet spreads over large volume, it is common to employ another type of injectors where the spray comes through a number of tiny holes sat radially through the injector tip. The number of holes is an essential parameter for the mixture formation and combustion, it is closely interlinked with injection pressure. An increase in the number of holes improves the fuel distribution in the circumferential direction of the combustion bowl, but the decreased penetration of a liquid jet with smaller diameter needs to be compensated for by higher rail pressure. The number of nozzle holes will increase from currently 6 to at least 8, possibly 12 in the near future. Subsequently the hole diameter, cuurently around 0.1mm, will decrease and, to facilitate suitable penetration and the appropriate hydraulic flow, the rail pressure will increase. Nozzle hole coking currently is one of the limiting parameters with regard to the reduction of the hole diameter.

Multi-hole injection



(a) Spray formation without impingment (b) Spray formation with impingement

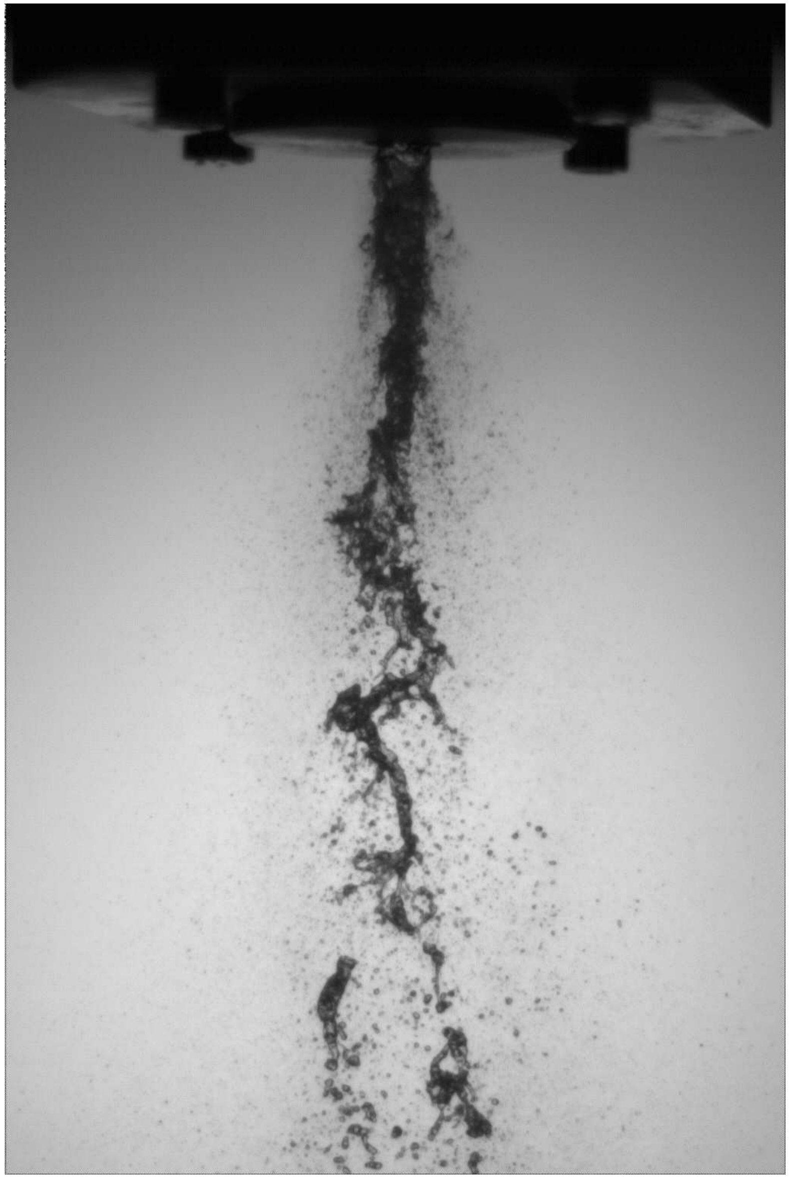
(c) Combustion without spray impingement (d) Combustion with spray impingement



The pictures are taken from: *S. Heisler Advanced engine technology and F. Atzler et al., Modern Diesel injection systems and combustion technologies, 2005.*

Very often the multi-hole injection in diesel engines is accompanied with the large-scale swirl of the flow created by profiling of the intake ports. The resulting pattern of the diffusion flames is then determined by the interaction of the two main flows, one induced by injection and the bulk swirl.

Fuel injection systems



The main factors determining the mixture formation are:

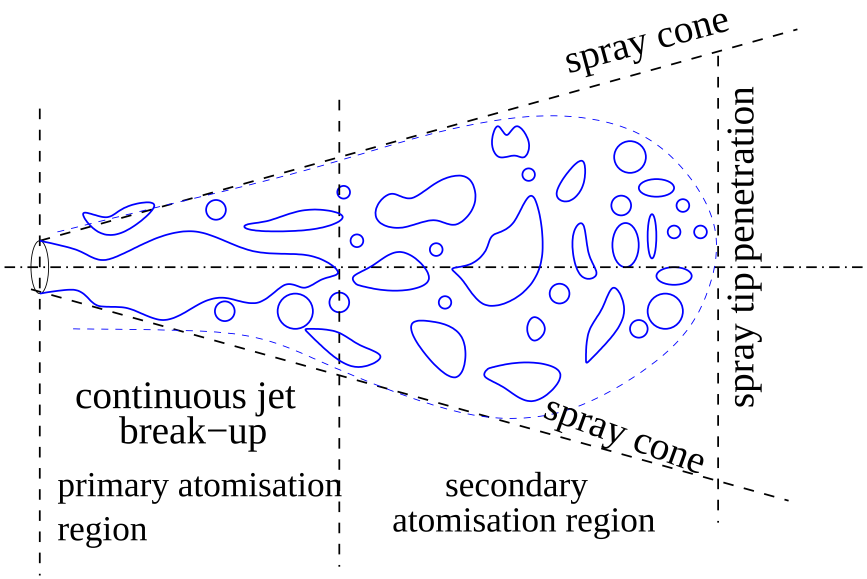
- ⋆ the injector and nozzle geometry
- ⋆ fuel properties, e.g. surface tension, and delivery pressure,
- ⋆ the charge motion and its density and composition (EGR),
- ⋆ the combustion chamber geometry.

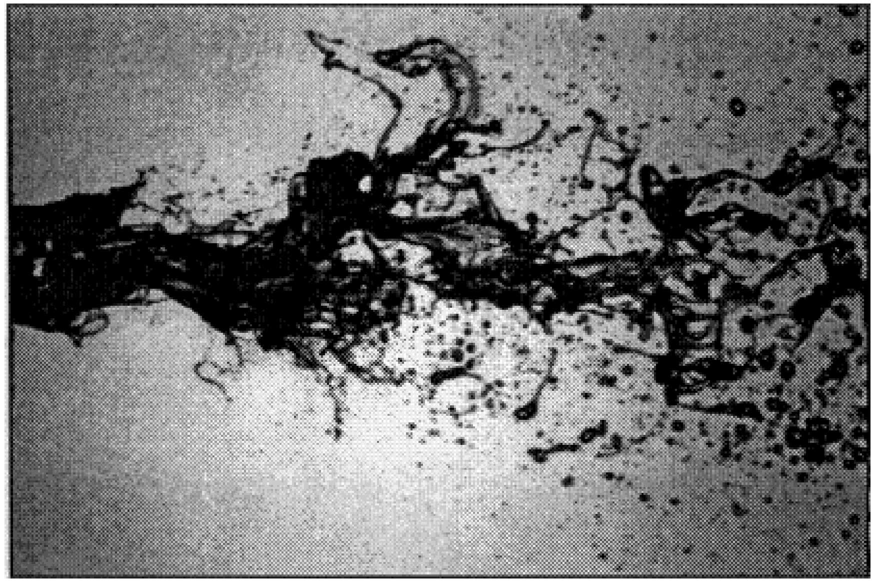
The main stages in the mixture formation are:

- ⋆ atomisation, i.e. breakdown of the injected continuous liquid jets into progressively smaller parcels and drops
- ⋆ vaporisation, e.g phase transition liquid-to-vapour
- ⋆ mixing, turbulent at large scales and mole-cular diffusion at the much smaller scales

Combustion is only possible in the gas phase.

Atomisation of fuel jets





Atomisation of the fuel spray arises in many processes, from aerosol paint to mazoute (residual heavy black oil) burner; both Reynolds and Weber numbers are (very) large. Liquid forms ligaments of various shapes and sizes In engines liquid phase pattern matters little, rather it is gas-liquid heat and mass average exchange rates which is important. These rates are defined by the average liquid surface area. Pressure, temperature and mean flow pattern, e.g. swirl, and turbulence effects are important. No universal empirical correlation has yet been established for atomisation quality embracing all injectors. Weber number

$$We = \frac{\rho u^2 r_d}{\sigma}$$

where σ is the surface tension, is indicator of the relative importance of the convective and the superficial tension energies per unit volume. **The key to a fine spray is a large relative velocity between the liquid and surrounding gas/air.**

Atomisation mechanism

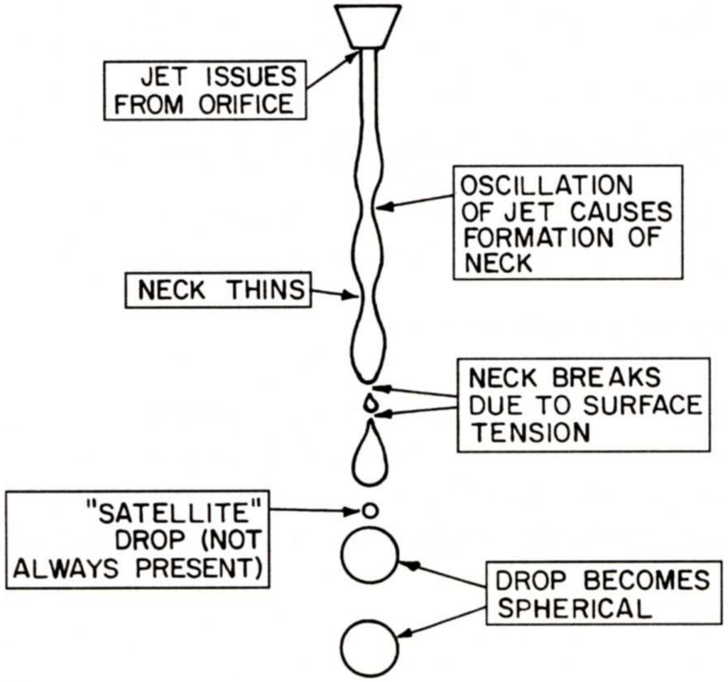


Figure 6-1 Breakup of a plain circular jet.

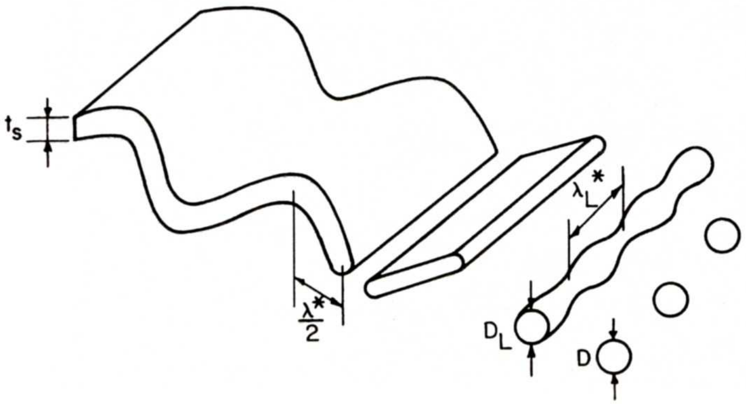


Figure 6-3 Successive stages in the idealized breakup of a fuel sheet [8].

Rayleigh instability: round jet breaks up when the amplitude of the perturbation equals its radius; the unstable wavlength is then $9r_{jet}$.

Small disturbances, either within or on the surface of a fuel jet or sheet promote the formation of waves on the surface; these lead to disintegration into ligaments and then drops. Drop diameter decrease with relative gas-liquid velocity from nearly 2 jet diameters downstream.

With a further increase in jet velocity, drop-lets are produced by the rapid (unstable) growth of small waves on the jet surface caused by interaction between the jet and the surrounding air. These waves become detached from the jet surface to form ligaments which disintegrate into drops. Drop diameters are typically much smaller than the initial jet diameter.

At very high velocities atomization occurs rapidly, close to the nozzle. Mean diameters are ranging from few to few tens of microns, usually less than 50 μm

Atomisation modelling

Lagrangian approach:

- ⋆ the liquid phase is described as an ensemble of some statistical particles often thought as “droplets”
- ⋆ employed in more than 99% of modelling studies
- ⋆ primary atomisation, that is breakdown of continuous liquid jet, cannot be described in terms of a discrete particles ensemble

Sectional approach and multi-moments models:

- ⋆ transport equations are formulated and solved for several $n_d(\hat{r})$ for different size classes, where momentum, mass and heat gas-liquid exchange rates are usually derived from dependencies for an isolated drop for the lack of better formulations
- ⋆ complicated (if at all possible) description of:
- • primary atomisation
- • droplet collisions in a turbulent flow

Eulerian methods based on **front tracking (VOF)**:

- ⋆ heavy computational demands for turbulent flow
- ⋆ surface tension effects require non-local descriptions

Atomisation modelling II

Entirely Eulerian model of Borghi et al. [10, 1]

- ⋆ The two-phase mixture is treated as a single continuum:
- ⋆ a single continuity equation without source terms
- ⋆ Quality of atomisation is described in terms of the average area of the liquid surface. This area is determined from its own transport equation
- ⋆ a single pressure (so algorithms similar to SIMPLE or PISO can be used)
- ⋆ momentum exchange between gas and liquid may appear only in turbulent stresses transport equations
- ⋆ Both Reynolds and Weber numbers are large:
- ⋆ the dispersion of liquid by turbulence depends neither on viscosity nor on surface tension; this dispersion can therefore be described as the turbulent diffusion of a species

The outcome of these assumptions is that the atomisation is described, from the first principles, in terms of the two transport equations only, one for **the liquid mass fraction** Y_{liq}, and the other - for **the average area of the liquid surface per unit volume**.

Practical formulation of the model also invokes an idea that if a liquid is immersed for a long, may be an infinite, time into a turbulent flow with constant properties, then it will form a monodisperse spray. The drop size in this monodisperse spray will be such that an equilibrium is attained between surface tension (capillary) action and factors causing drop break-up, e.g. viscous stress at the drop surface or drop collisions.

$Y_{liq} - \sigma$ model

Entirely Eulerian approach proposed by Borghi [10] treats a two-phase medium as a single continuum where the dense phase is described similarly to a specie in a multi-component reactive mixture. The transport equation for the liquid mass fraction $\widetilde{Y}_{liq}$, that is the mass of liquid phase *per unit mass of two-phase media*, is [10]:

$$\frac{\partial \bar{\rho} \widetilde{Y_{liq}}}{\partial t} + \frac{\partial \bar{\rho} \widetilde{u}_j \widetilde{Y_{liq}}}{\partial x_j} = \frac{\partial}{\partial x_j} \bar{\rho} \frac{D_T}{Sc_{liq}} \frac{\partial \widetilde{Y_{liq}}}{\partial x_j} - \dot{m}_{vap} \bar{\rho} \sigma \tag{4}$$

where D_T is the turbulent diffusivity, Sc_{liq} is the turbulent Schmidt number kept as a constant $Sc_{liq} = 0.7$, and $\dot{m}_{vap}$ is the rate of vaporisation per unit surface area of the liquid. Key quantity determining the vaporisation rate is the average surface area of the gas-liquid boundary *per unit mass of two-phase media* σ, the transport equation for which is:

$$\frac{\partial \bar{\rho} \tilde{\sigma}}{\partial t} + \frac{\partial \bar{\rho} \widetilde{u}_j \tilde{\sigma}}{\partial x_j} = \frac{\partial}{\partial x_j} \bar{\rho} \frac{D_T}{Sc_\sigma} \frac{\partial \tilde{\sigma}}{\partial x_j} + \frac{\bar{\rho} \tilde{\sigma}}{\tau_c} \left[1 - \frac{\tilde{\sigma}}{\sigma_{eq}} \right] + S_{\sigma,vap} \tag{5}$$

where $Sc_\sigma = Sc_{liq}$, and $S_{\sigma,vap}$ is the source term caused by the vaporisation. The liquid phase pattern tends to the state of a monodisperse spray characterised with the drop size r_{eq} where the droplet coalescence compensates the break-up, and this asymptotic equilibrium liquid surface is:

$$\begin{aligned} \sigma_{eq} &= \frac{3\widetilde{Y}_{liq}}{\rho_{liq} r_{eq}} \\ r_{eq} &= C_r \cdot \left(\frac{\bar{\rho} \widetilde{Y_{liq}}}{\rho_{liq}} \right)^{2/15} \frac{\eta^{3/5}}{\varepsilon^{2/5} \rho_{liq}^{3/5}} \end{aligned} \tag{6}$$

where $C_r = 0.23$.

Non-premixed, or diffusion, combustion

Invariably, description of turbulent diffusion flames is based upon introduction of a passive scalar, typically, the mixture fraction, or a Shwab-Zeldovich variable. In a turbulent flow concentrations, temperature, flow velocity etc. at a point are fluctuating; because of this engineering methods of turbulent flow description employ averaged transport equations. It has been shown [2] that an appropriate description of turbulent non-premixed combustion should involve the average and root-mean-square (rms) values of the mixture fraction.

Typically, **the Favre, i.e. density-weighted, averaging** is considered: $\overline{\rho\xi} = \bar{\rho}\tilde{\xi}$. Let the Favre-averaged value of the mixture fraction ξ be denoted as $\tilde{\xi}$, its deviation as ξ'' and its rms value as

$$\left(\widetilde{\xi''2}\right)^{1/2} = \left(\widetilde{\xi^2} - \left(\tilde{\xi}\right)^2\right)^{1/2}$$

The transport equation for $\tilde{\xi}$ can be obtained applying Favre averaging to a transport equation for mixture fraction written for variable density case:

$$\frac{\overline{\partial\rho\xi}}{\partial t} + \overline{\underset{\rightarrow}{u} \cdot \text{grad}\ \ \rho\xi} - \overline{D\ \text{div}\ \rho\,(\text{grad}\ \ \xi)}\ = \ \frac{\partial\bar{\rho}\tilde{\xi}}{\partial t} + \bar{\rho}\left(\underset{\rightarrow}{\tilde{u}} \cdot \text{grad}\right)\tilde{\xi}\ +\ \bar{\rho}\ \text{div}\ \left(\widetilde{\underset{\rightarrow}{\text{u}''}\xi''}\right) = 0 \qquad (7)$$

where the molecular diffusion fluxes are neglected in comparison with the turbulent diffusion grad $\widetilde{\underset{\rightarrow}{\text{u}''} \cdot \xi''}$; this is owing to the fact that the turbulent-to-molecular diffusivity ratio is proportional to the turbulent Reynolds number Re_t and is much greater than one. Also neglected were correlations with the density fluctuations; the reasons for doing so are discussed in [2].

Mixture fraction fluctuations

The transport equation for the intensity of the mixture fraction fluctuations $\xi\tilde{''}2$ can be obtained with multiplying transport equation for mixture fraction by ξ and applying the averaging procedure after that:

$$\underbrace{\frac{\partial \bar{\rho}\widetilde{\xi''^2}}{\partial t}}_{I} + \underbrace{\bar{\rho}\left(\underset{\rightarrow}{\tilde{u}} \cdot \text{grad}\right)\widetilde{\xi''^2}}_{II} + \underbrace{\bar{\rho}\ \text{div}\ \widetilde{\underset{\rightarrow}{\text{u}}''\xi''^2}}_{III} + \underbrace{\bar{\rho}\ \text{grad}\ \tilde{\xi} \cdot \widetilde{\underset{\rightarrow}{\text{u}}''\xi''}}_{IV} = \underbrace{-2\overline{\rho D\left(\text{grad}\ \xi'' \cdot \text{grad}\ \xi''\right)}}_{V} \tag{8}$$

where the terms, in order of their apprearance describe:

I accumulation (unsteadiness),

II convection by the mean velocity,

III turbulent diffusion, i.e. convection by the fluctuating velocity,

IV generation by the mean concentration gradient, and,

V (the term on the right-hand-side), **the dissipation of the concentration fluctuations by molecular diffusion.**

The last term in Eq.(8) makes appear explicitly the scalar dissipation:

$$\tilde{\chi} = 2\overline{D\text{grad}\ \xi'' \cdot \text{grad}\ \xi''} \tag{9}$$

which plays a very important role in determining the rate of combustion.

Average rate of non-premixed combustion

The cornerstone of the method proposed by R.W. Bilger [2] in the late 1970s is the assumption that concentrations (mass fractions) of all species Y_i as well as the temperature and density in a turbulent flame can be found assuming that they are **the equilibrium functions of the mixture fraction**:

$$Y_i(\underset{\rightarrow}{x}, t) = Y_i^{eq}\left(\xi(\underset{\rightarrow}{x}, t)\right), \quad T(\underset{\rightarrow}{x}, t) = T^{eq}\left(\xi(\underset{\rightarrow}{x}, t)\right)$$

This method can be illustrated, for example with determination of the average rate of consumption of k-th species, as follows. If the mass fraction Y_k depends only on the mixture fraction ξ, then its transport equation written for variable density:

$$\frac{\partial \rho Y_i}{\partial t} + \operatorname{div}\left(\rho \vec{u} Y_i - D_i \operatorname{div} \rho\left(\operatorname{grad}\ \mathrm{Y_i}\right)\right) - W_i = 0 \tag{10}$$

will lead to:[†]

$$\frac{dY_i^{eq}}{d\xi} \cdot \left[\frac{\partial \rho \xi}{\partial t} + \operatorname{div}\left(\rho \vec{u} \xi\right) - D \operatorname{div} \rho\left(\operatorname{grad}\ \xi\right)\right] = \frac{d^2 Y_i^{eq}}{d\xi^2} \cdot \left[\rho D \operatorname{grad}\ \xi \cdot \operatorname{grad}\ \xi\right] + W_i$$

where the expression in the square brackets on the left hand side is zero by virtue of Eq. (7). Thus:

$$\frac{d^2 Y_i^{eq}}{d\xi^2} \cdot \left[\rho D\left(\operatorname{grad} \xi \cdot \operatorname{grad} \xi\right)\right] = -W_i$$

[†] Notice that

$$\nabla(\bullet) = \frac{d(\bullet)}{d\xi} \nabla(\xi)$$

where, obviously,($\bullet$) may denote scalar, vector or even a tensor.

and, applying averaging and invoking the definition of the scalar dissipation χ, one obtains:

$$\bar{W}_i = \frac{1}{2}\bar{\rho}\tilde{\chi} \cdot \frac{d^2 Y_i^{eq}}{d\xi^2} \tag{11}$$

which shows that the average rate of chemical reactions is proportional to the scalar dissipation. The Eq. (11) underlies a number of combustion models, known as Eddy-Break-Up model, mixing-controlled reactions, fast reactions etc

The “fast chemistry” approximation replaces the problem of calculating various average reaction rates for multiple species to determination of only one quantity, that is the dissipation of the passive scalar fluctuations. One may derive a transport equation for this latter quantity, however, very often, this latter quantity is simply taken as proportional to the square of the rms scalar fluctuation, e.g.:

$$\tilde{\chi} \approx Const \cdot \frac{\widetilde{\xi''^2}}{\tau_t}$$

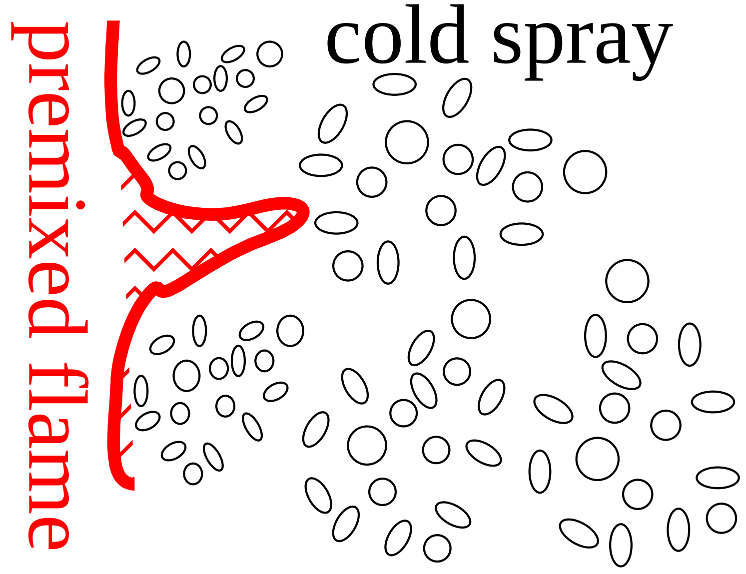
where τ_t is the integral time-scale of turbulence.

Two-phase flame

The two-phase flames surrounding the sprays may exist in a variety of regimes. The classical regime studied since 1950's is the combustion of an isolated drop in an infinite gas environment. When a diffusion flame surrounds a drop there is an equilibirum between the fuel flux from the drop surface to the flame and the heat flux from the flame to the drop surface supplies the heat required for vaporisation. When the drop moves then the flame may adopt various shapes and become detached from the drop surface. It is obvious that in a diesel engine charge drops and liquid parcels move and there are large variations from one point to another in amount fo the fuel in the vapour and liquid state, spacing between the drops, $l_d \approx n_d^{1/3}$ where n_d is the droplet number density, droplet shapes and sizes etc. A number of possible configurations of a two-phase flame may be envisaged depending on the ratio of the characteristic times of turbulent mixing, drop vaporisation and chemical reactions. The following cursory analysis follows Chapter 9 of [4] which should be consulted for further details.

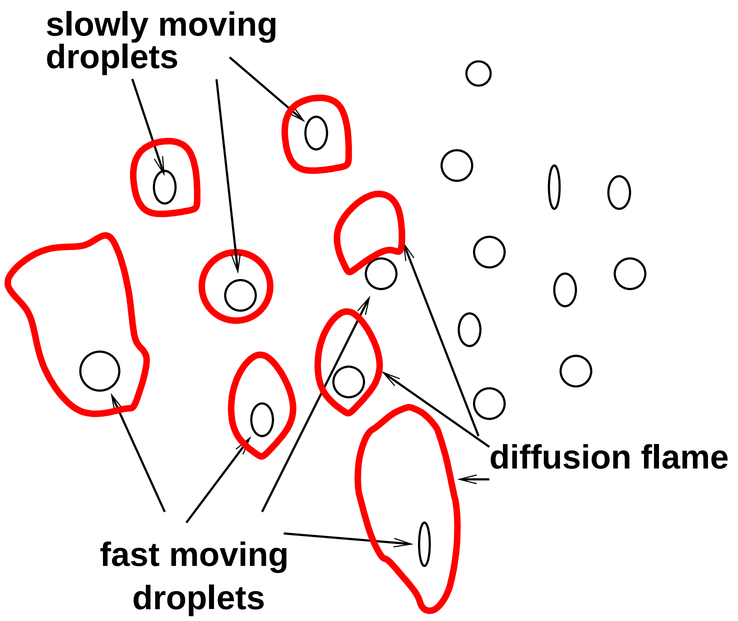
The first configuration of a turbulent spray, which may be referred to as "pre-vaporised flame", corresponds to the case of very small droplets and very fast turbulent mixing.

Two-phase flame configurations

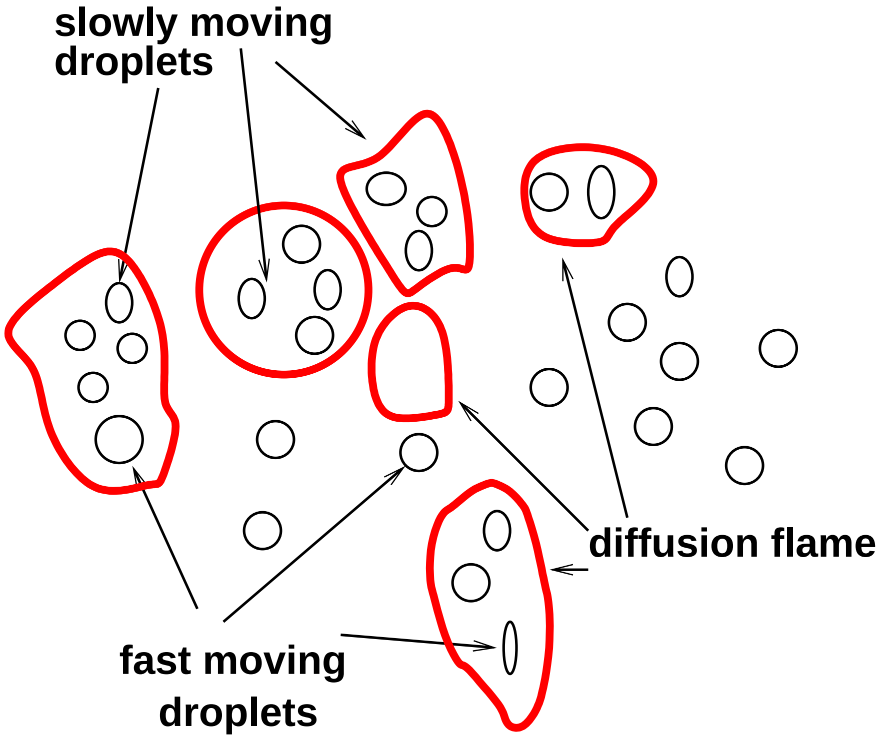


If the drops completely evaporate in the preheat zone and the vapour mixes with the air before the reactions occur then one may envisage existence of a premixed flame propagating into spray. Obviously, to sustain the premixed flame propagation, the amount of liquid per unit mass of the two-phase mixture must be such that the vapour-air mixture in the preheat zone is within the inflammability limits. The speed of propagation of such a flame is the same as the turbulent premixed flame speed under the local turbulence conditions, i.e. presence of the liquid does not affect the rate of combustion.

Another extreme two-phase flame configuration is the case of a very dilute spray where $r_d << n_d^{1/3}$ where the composition of the gas phase is below the lean inflammabality limit. If the gas phase and the drops were stationary then each drop may sustain a diffusion flame surrounding it. In the absence of the gravity this flame would be spherical; buoyancy and the relative motion of the drops and the gas will lead to non-spherical flames. If the velocity of the drop relative to the gas exceeds a certain value, the flame may blow out to the downwind side of the drop and burn in the drop wake.



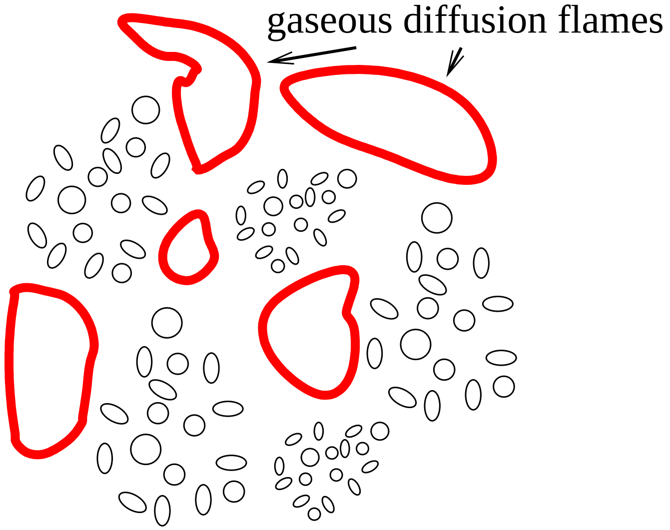
Two-phase flame configurations - group combustion



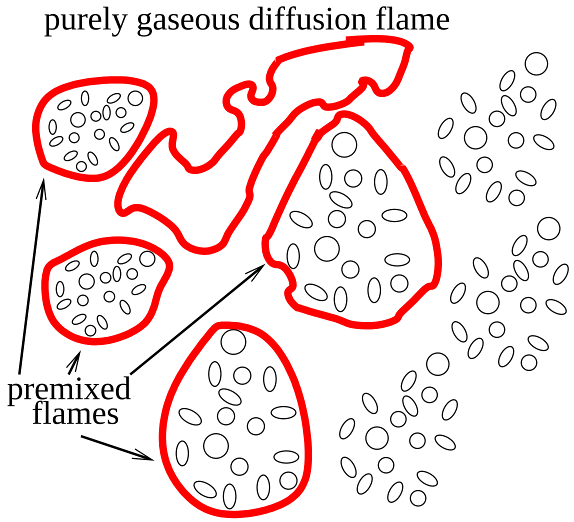
When a diffusion flame surrounds an isolated drop flame, the distance d_F between the drop and the flame may not be arbitrary but is a function of the vapour diffusivity, flame temperature and other factors. If the average distance between the drops is less than this flame "stand-off" distance, then the diffusion flames between isolated drops will coalesce. So, the diffusion flames may now encircle several liquid parcles in the regime known as **group** combustion. In a turbulent flame one may expect that a random number of liquid parcels may be enclosed in flame envelopes, and to complicate things further, the wake flames formed behind moving drops may "capture" and englobe neighbouring liquid parcels.

Two-phase flame configurations - pockets and percolations

When the ratio of the flame stand-off distance d_F to the droplet spacing $n_d^{1/3}$ is increasing further, i.e the spray becomes denser still, then it becomes impossible for the flame to encircle the drops. The diffusion flames in this “pocket combustion” regime are now separated by the regions of the dense spray where the flame cannot penetrate. Following the arguments of [4], transition to this “pocket combustion” regime occurs when $d_F \cdot n_d^{1/3} \approx 0.7$ In this regime, the oxidant comes from the gas pockets encircled by the flames



For the intermidiate ratios of the flame stand-off distance d_F to the droplet spacing $n_d^{1/3}$ one may envisage the combustion regime where the diffusion flames surround relatively large clusters of the liquid fule parcels and there are also relatively large diffusion flames surrounding oxygen-rich areas with some combustion products. This combustion regime, referred to as the “percolation” combustion [4], may exist when $0.5 \leq d_F \cdot n_d^{1/3} \leq 0.75$.



Possible configurations of two-phase flame depend not only on local properties of the mixture but also on their CORRELATION PATTERNS over distances comparable to flame dimensions and wide range of turbulence scales. As yet, there are no fully satisfactory theoretical apporaches to describe them.

Conclusions

- ⋆ Efficiency of energy storage in chemical bonds of a liquid fuel is not likely to be matched any time soon by any other form of energy storage, including electrical storage; therefore the rumours of combustion engine death are somewhat exaggerated.
- ⋆ Combustion in any engine of practical value is invariably turbulent; interaction of turbulence with molecular transport and chemistry is the key physical factor determining engine performance.
- ⋆ Combustion in any engine of practical value occurs invariably at high pressures; in combustion, high pressure often leads to necessity of taking into account instabilities and extrapolation of laboratory data obtained at low pressure may be problematic.
- ⋆ While the existing modeeling approaches focussed on the **average** rate of combustion, local or global, combined action of turbulence and instabilities gives rise to strong fluctuations of the burning rates. Understanding and modelling of these fluctuations is in its infancy.
- ⋆ There are good reasons to believe that appoach based on transport equation for liquid surface may have stronger predictive capability compared to the currently widely used methods based on instability analysis of laminar liquid jet.
- ⋆ *There are more things in heaven and earth, Horatio,*
  Than are dreamt of in your philosophy.
  W. Shakespeare, Hamlet

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