Aerospace Combustion

Lectures 9:

Combustion Theory: Premixed Flames

Content

- Basic Features
  - Flammability Limits,
  - Activation Energy,
  - Ignition,
  - Extinction)
- Premixed Flames
  - Deflagration & Detonation (Infinite, plane, steady-state 1-D flows with exothermic reactions (Hugoniot, Chapman, Jouguet))
  - Laminar Premixed Flames
  - Turbulent Premixed Flames

Basic Features

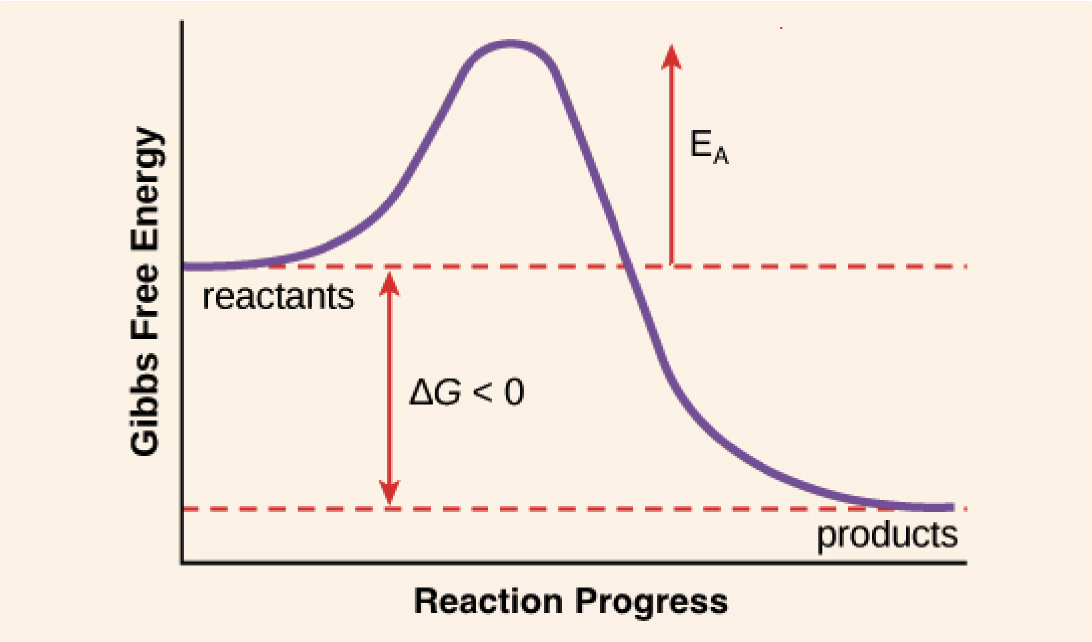
Prior to going into details we have to mention a few basic features first which are characteristic for all combustion processes

- Activation Energy: Energy necessary for the initiation of a chemical reaction, typically a radical generation process. Hence, this is a characteristic for a certain molecule.

Arrhenius form $$k = Ae^{\frac{-E_a}{RT}}$$

k; reaction rate
A; pre-exponential faction (collision probability)
E_a; activation energy
R; general gas constant
T; temperature

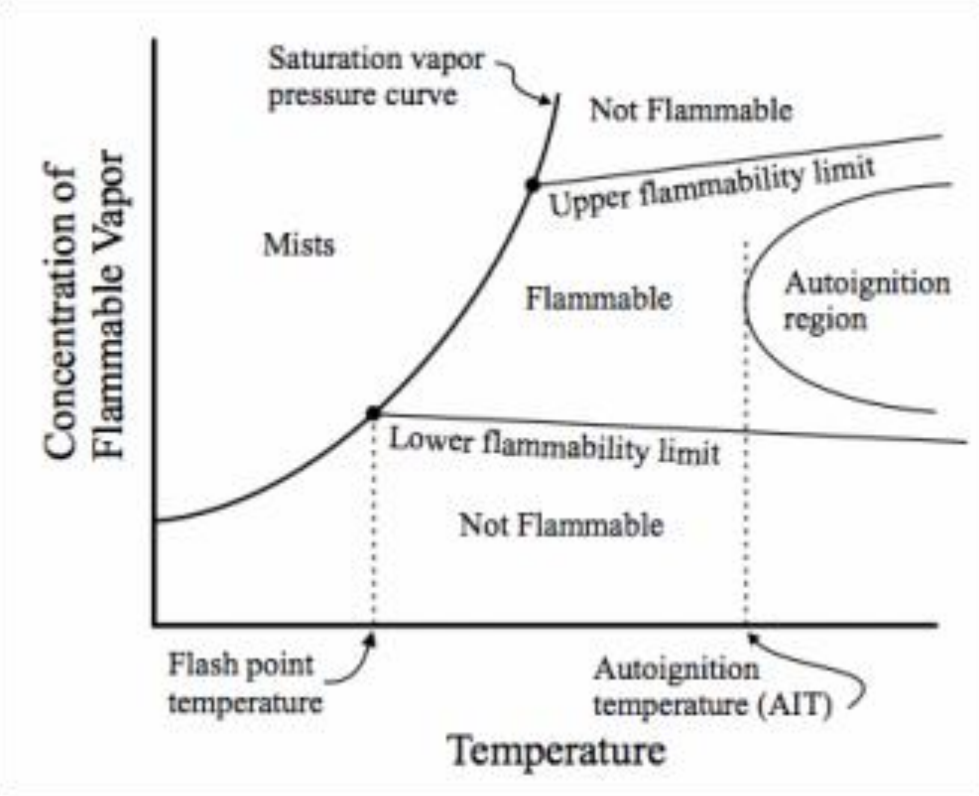
Exothermal reaction



Basic Features

Prior to going into details we have to mention a few basic features first which are characteristic for all combustion processes

- Auto-ignition temperature: Temperature at which a mixture of fuel and oxidizer ignites
- Flammability limits: range of propellant mixture for which auto-ignition occurs. Typically, for fuel-rich or lean conditions the auto-ignition temperature increases

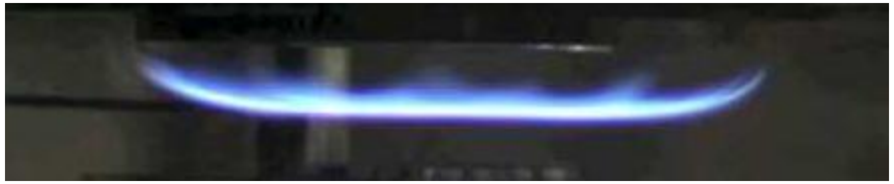


Basic Features

Prior to going into details we have to mention a few basic features first which are characteristic for all combustion processes

- Extinction: flame extinguishes due to different reasons

1. Stretch, strain may cause extinction: an argumentation based on Damköhler reasoning where the convective time scale is smaller than the chemical one
2. Heat losses, in particular near cooled walls may overcome the local heat release due to chemical reactions
3. Flame front reaches flammability limits, local heat release to small to compensate preheating losses



Extinction of a counter-flow diffusion flame due to strain

Characterization of Combustion Processes

There are many ways combustion processes can be characterized. Generally, people distinguish between

- premixed,
- non-premixed,
- and partially premixed combustion

However, there are many applications where heterogeneous processes are involved such as

- spray combustion in internal combustion engines, gas turbines or rocket engines
- or combustion in coal-fired power plants or in solid rocket motors.

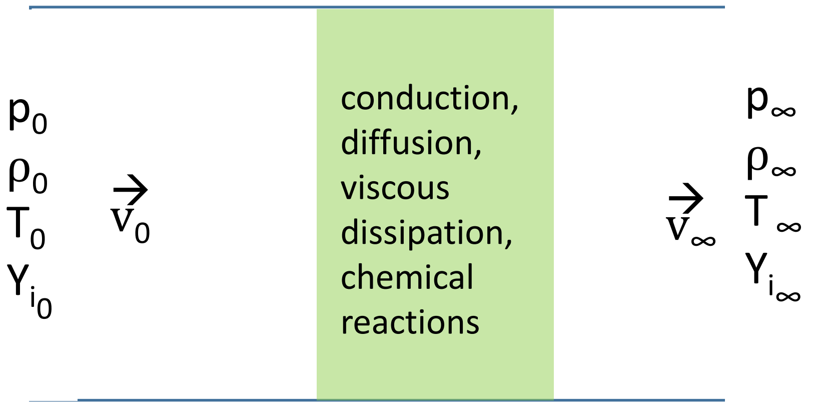
The heat release may occur in a

- deflagration mode with flame velocities ranging from *cm/s* - *m/s*
- or detonation mode with flame velocities in the *km/s* range. Propagation is faster in liquid and solids than in gases.

Detonation/Deflagration

Assumptions:

plane, steady, 1-D flow with exothermal reactions with uniform properties far away from the reaction zone.



steady, 1-D

$$\frac{D}{Dt} = \cancel{\frac{\partial}{\partial t}} + v\frac{\partial}{\partial x};$$

$$\frac{d}{dx}(\rho v) = 0;$$

$$\frac{d}{dx}(\rho v) = \frac{dp}{dx} + \frac{4}{3}\mu\frac{d^2 v}{dx^2};$$

$$\frac{d}{dx}(\rho v h) = v\frac{dp}{dx} + \frac{4}{3}\mu\left(\frac{dv}{dx}\right)^2 - \frac{dq}{dx};$$

$$\frac{d}{dx}(\rho v Y_i) + \frac{d}{dx}(\rho Y_i V_i) = \omega_i; \qquad i = 1,2,..N$$

$$p = \rho R T / W$$

$$\Longrightarrow$$

$$\rho v = const.;$$

$$p + \rho v^2 - \frac{4}{3}\mu\frac{dv}{dx} = const.;$$

$$\rho v\left(h + \frac{1}{2}v^2\right) - \frac{4}{3}\mu v\frac{dv}{dx} + q = const.;$$

$$\frac{d}{dx}(\rho v Y_i + \rho Y_i V_i) = \omega_i;$$

Detonation/Deflagration

Assumptions:

plane, steady, 1-D flow with exothermal reactions with uniform properties far away from the reaction zone.

$$[\rho v]_{-\infty}^{+\infty} = 0;$$

$$\left[p + \rho v^2 - \cancel{\frac{4}{3}\mu\frac{dv}{dx}}\right]_{-\infty}^{+\infty} = 0$$

$$\left[\rho v\left(h + \frac{1}{2}v^2\right) - \cancel{\frac{4}{3}\mu v\frac{dv}{dx}} + \cancel{q}\right] = 0$$

$$\left[\frac{d}{dx}\left(\rho v Y_i + \cancel{\rho Y_i V_i}\right)\right]_{-\infty}^{+\infty} = [\omega_i]_{-\infty}^{+\infty}$$

$$q = -\lambda\frac{dT}{dx} + \sum_{i=1}^{N}\rho Y_i h_i^0 V_i; \quad h = \sum_{i=1}^{N} Y_i h_i^0 + \int_{T^0}^{T} c_p\,dT$$

$$\rho Y_i V_i = -\rho D_i\frac{dY_i}{dx}; \; p = \rho\frac{RT}{W}$$

p_0, ρ_0, T_0, Y_{i_0} $\quad \vec{v}_0$

conduction, diffusion, viscous dissipation, chemical reactions

$\vec{v}_\infty$ $\quad$ p_∞, ρ_∞, T_∞, Y_{i_∞}

steady, 1-D

$$\frac{D}{Dt} = \cancel{\frac{\partial}{\partial t}} + v\frac{\partial}{\partial x};$$

$$\Longrightarrow$$

$$\rho_0 v_0 = \rho_\infty v_\infty;$$

$$p_0 + \rho_0 v_0^2 = p_\infty + \rho_\infty v_\infty^2;$$

$$h_0 + \frac{1}{2}v_0^2 = \frac{1}{2}h_\infty v_\infty^2;$$

$$\omega_{i_0} = \omega_{i_\infty} = 0; \quad i = 1,2,.., N$$

$$p_0/\rho_0 T_0 = p_\infty/\rho_\infty T_\infty = R/W$$

$$R/W = \frac{\gamma - 1}{\lambda}c_p$$

Detonation

Detonation is a type of combustion where a supersonic shock wave propagates in front of the combustion zone. First attempts to describe the phenomenon theoretically are from D. Chapman and E. Jouguet.

Rayleigh line equation
$$\frac{\frac{p_2}{p_1}\text{-1}}{\frac{\rho_1}{\rho_2}\text{-1}} = -\frac{m^2}{p_1 \rho_1};$$

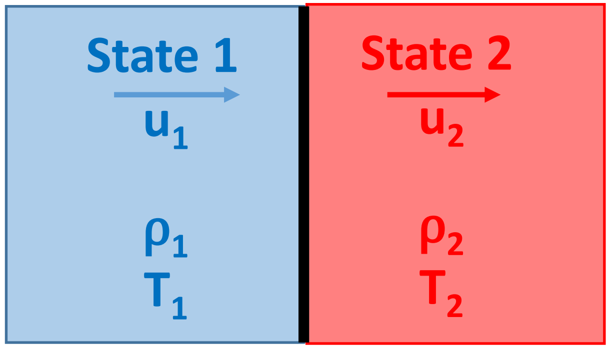
Hugoniot curve equation
$$\frac{p_2}{p_1} = \frac{\left[2q\frac{\rho_1}{p_1} + (\gamma+1)/(\gamma-1)\right] - \frac{\rho_1}{\rho_2}}{\left[(\gamma+1)/(\lambda-1)\right]\frac{\rho_1}{\rho_2} - 1}$$

are obtained from Rankine-Hugoniot relations which describe the relationship between both sides of a shock wave or combustion wave for an ideal gas of constant specific heat and molecular weight.

from mass and momentum conservation follows that
$$\frac{p_2\text{-}p_1}{1/\rho_2 + 1/\rho_1} = -m^2;$$

and the energy equation yields
$$h_2 - h_1 = \frac{1}{2}\left(\frac{1}{\rho_2} + \frac{1}{\rho_1}\right)(p_2 - p_1);$$

assuming constant specific heat
$$h_2 - h_1 = -q + c_p(T_2 - T_1);$$

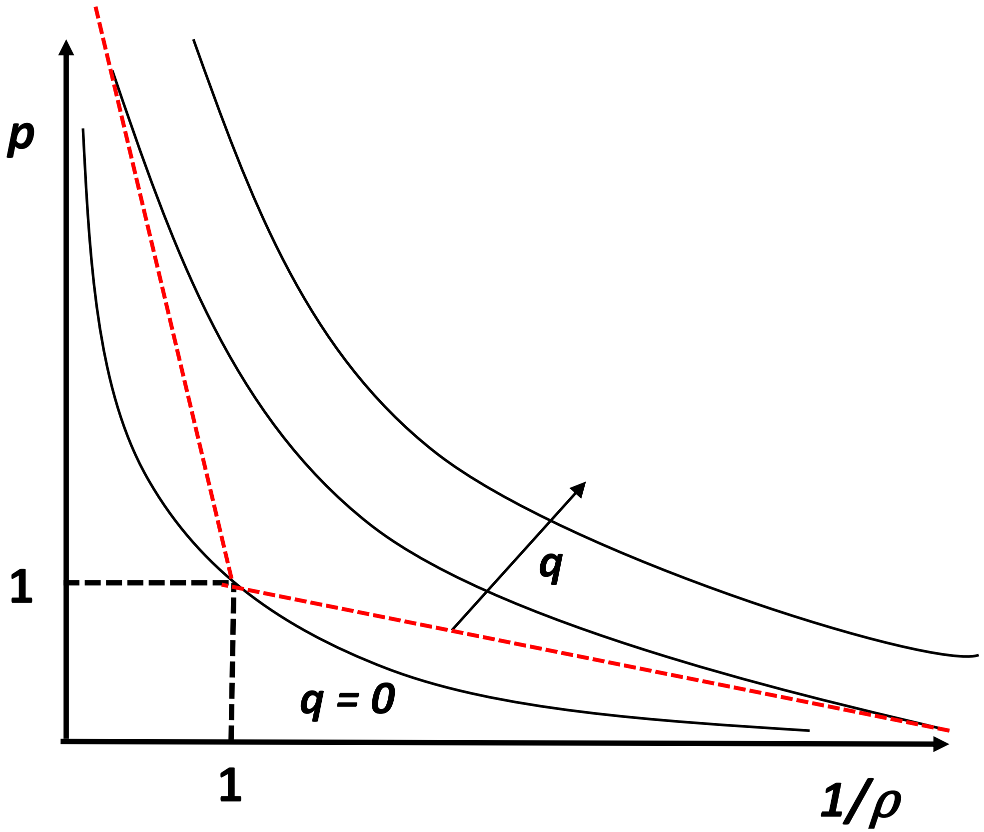


Premixed Flames

Detonation

Chapman – Jouguet Graph

Black solid lines are is the Hugoniot curves for different heat releases and the red dashed lines are Rayleigh lines.



Hugoniot curve is a hyperbola which asymptotes to

$$\frac{1}{\rho} = \frac{\gamma - 1}{\lambda + 1} \text{ for } p \to \infty \quad \text{and}$$

$$p = -\frac{\gamma - 1}{\lambda + 1} \quad \text{for } 1/\rho \to \infty;$$

Solutions are restricted to:

$$\frac{\gamma - 1}{\gamma + 1} \le \frac{1}{\rho} \le 2q + \frac{\gamma + 1}{\lambda - 1};$$

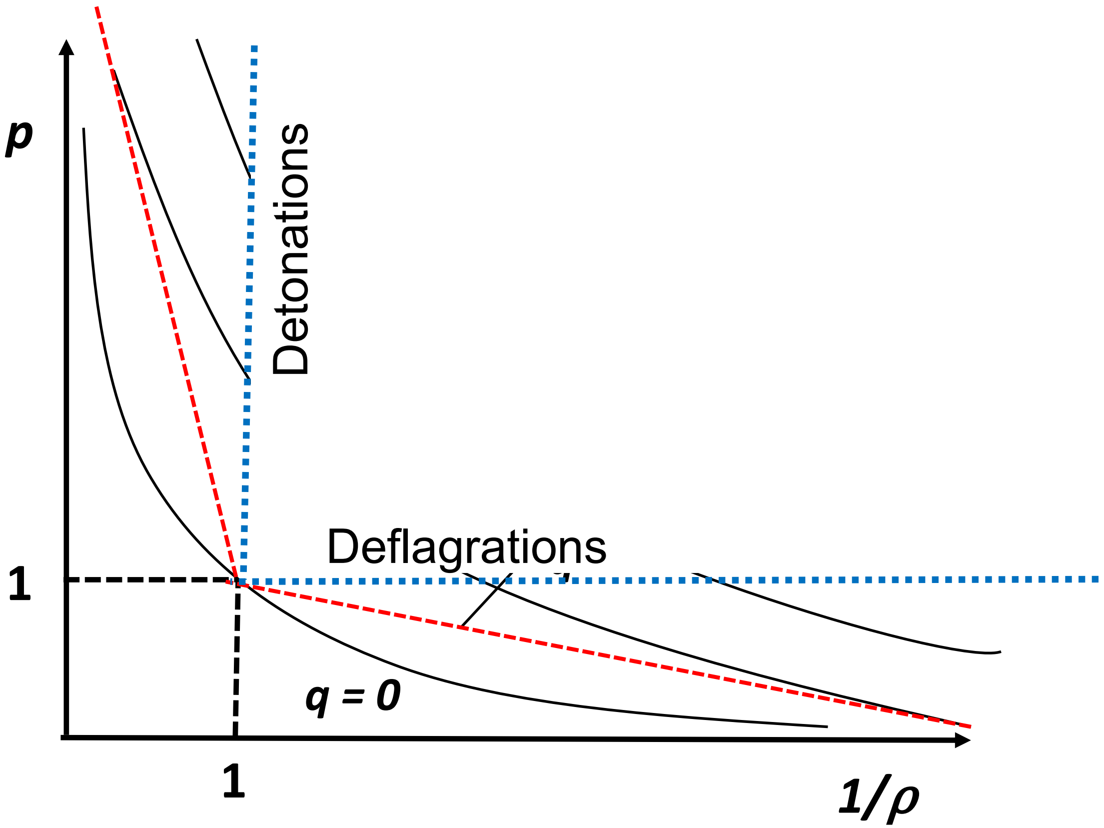
$$0 < p < \infty;$$

Premixed Flames

Detonation

Chapman – Jouguet Graph

Black solid lines are is the Hugoniot curves for different heat releases and the red dashed lines are Rayleigh lines.



Rayleigh lines always go through (1,1) have negative slopes and solutions are further restricted to

$$\frac{\gamma-1}{\gamma+1} \le \frac{1}{\rho} < 1 \quad \text{and} \quad 1+(\lambda-1)q \le p \le \infty;$$

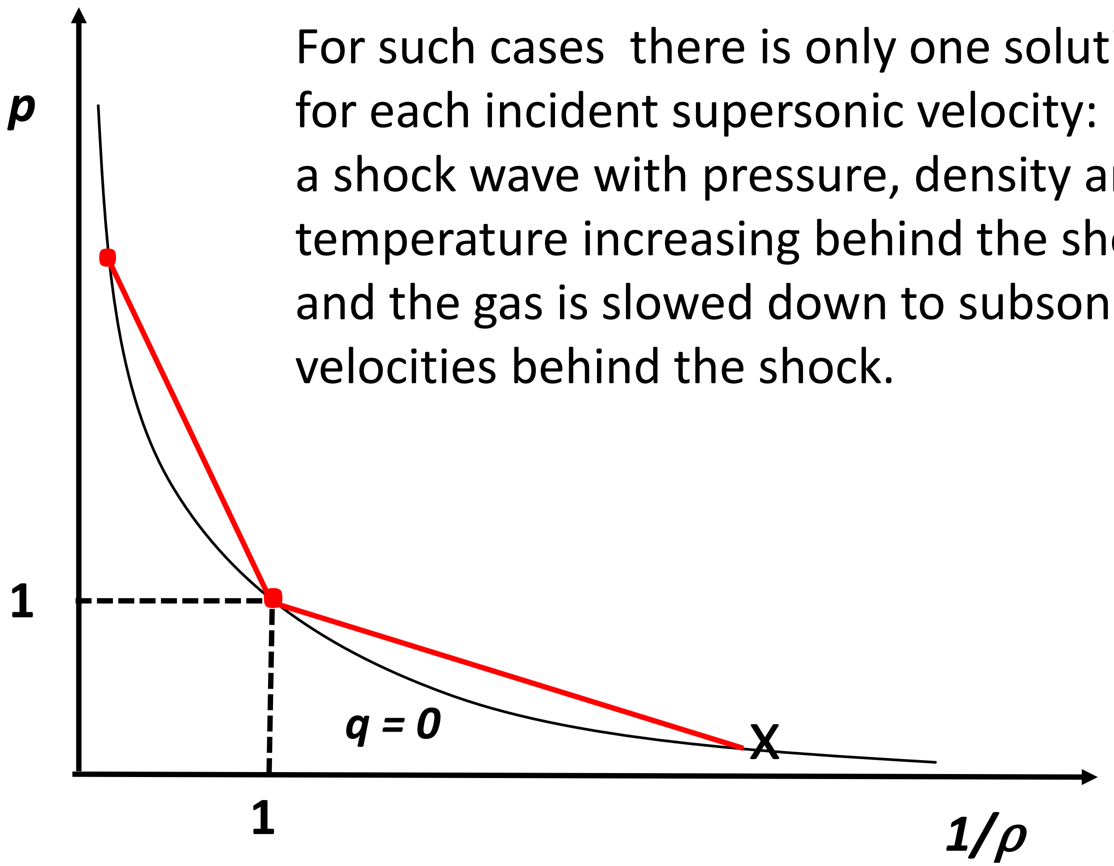
$$1+\frac{\lambda-1}{\lambda}q < \frac{1}{\rho} < 2q+\frac{\gamma+1}{\gamma-1} \quad \text{and} \quad 0 \le p < 1;$$

Detonation

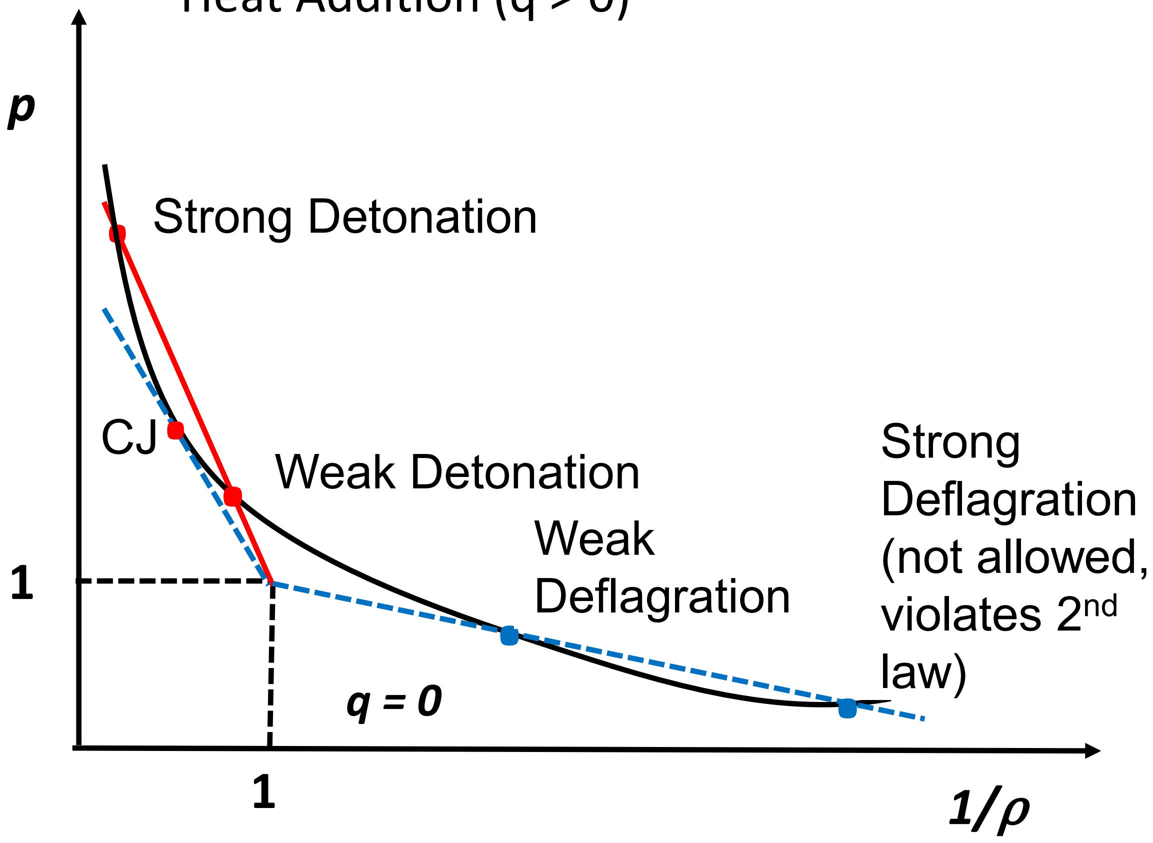
Chapman – Jouguet Graph

No Heat Addition (q = 0)

For such cases there is only one solution for each incident supersonic velocity: a shock wave with pressure, density and temperature increasing behind the shock and the gas is slowed down to subsonic velocities behind the shock.



Heat Addition (q > 0)



Premixed Flames

Deflagration

1. there is a maximum value of $\frac{m^2}{p_1 \rho_1}$ and, as a consequence, a maximum wave speed corresponding to Chapman-Jouguet (CJ) deflagration;

2. for $\frac{m^2}{p_1 \rho_1} < \left.\frac{m^2}{p_1 \rho_1}\right|_{\mathrm{CJ}}$

there are two solutions, weak and strong deflagration

3. When passing through a deflagration wave
   - the gas velocity increases
   - the gas expands
   - the pressure decreases

Detonation

1. there is a minimum value of $\frac{m^2}{p_1 \rho_1}$

and, as a consequence, a minimum wave speed corresponding to Chapman-Jouguet (CJ) detonation

2. for $\frac{m^2}{p_1 \rho_1} > \left.\frac{m^2}{p_1 \rho_1}\right|_{\mathrm{CJ}}$

there are two solutions, strong and weak detonation

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3. When passing through a detonation wave
   - the gas slows down
   - it is compressed
   - and the pressure increases

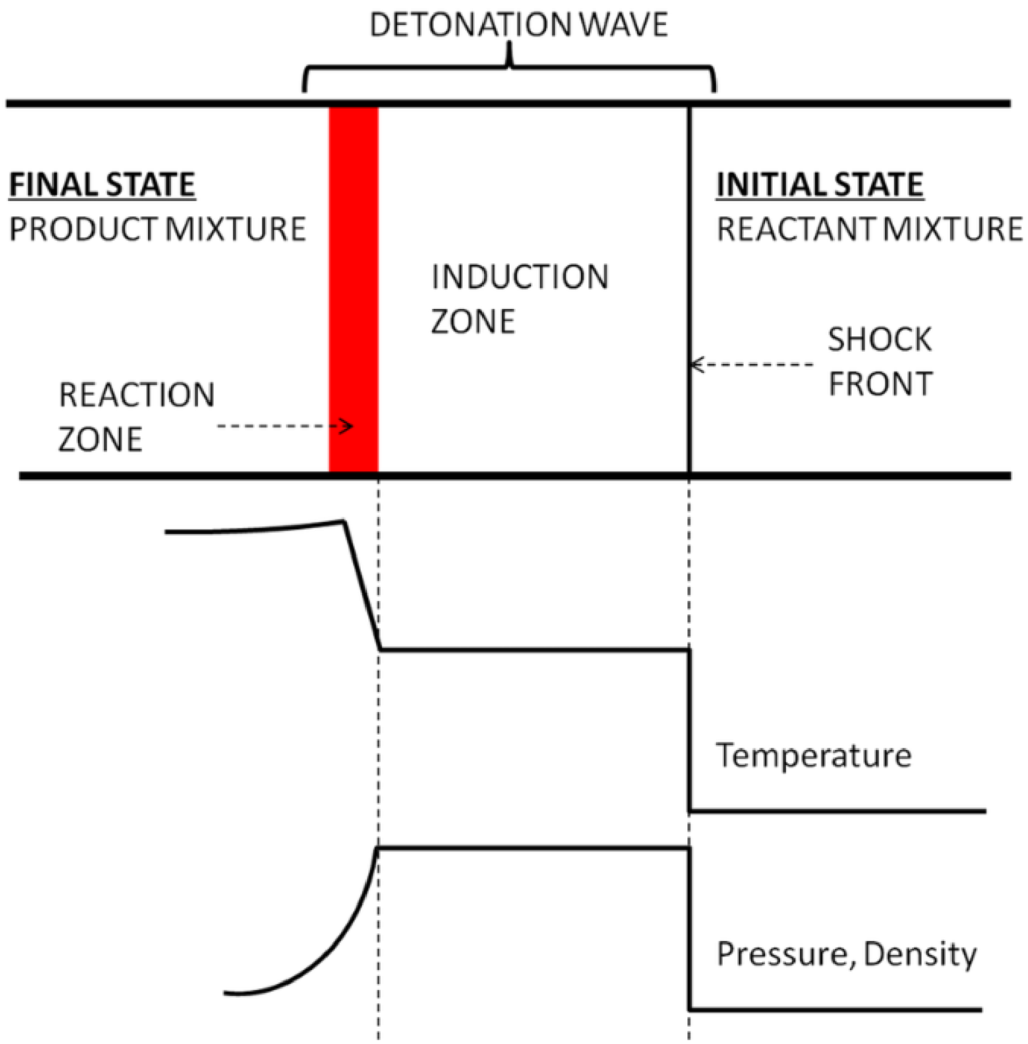
Zeldovich, von Neumann, Döring Detonation Model

Molecular collisions precede chemical reactions

- Characteristic times of collisional momentum transfer (< 1 ns)
- Characteristic time of chemical reactions (> 1µs)

Detonation is leading shock followed by reaction zone

- Shock yields raise of pressure and temperature
- Subsonic situation behind shock
- Auto-ignition after reactant-specific ignition delay
- Heat release yields temperature increase and pressure reduction (similar to deflagration)



Premixed Flames

Laminar Premixed Flames

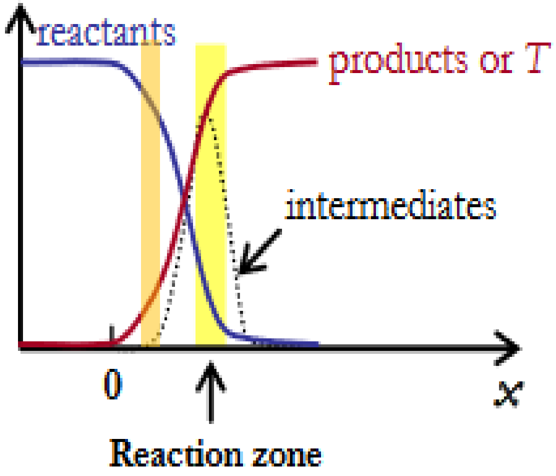
Such flames hardly exist in technical applications, however their analyses help for a better understanding of basic flame phenomena.

- Flame speed and thickness
- Importance of heat and mass transfer

Processes involved are heat and mass transfer driven by concentration and temperature gradients (Fick, Soret, Dufour is usually neglected). Reactants, intermediates and products form a multi-component system.

Characteristics of laminar premixed flame:

- Flame has finite thickness
- Diffusive transport (mass and heat) are very important
- Radical and intermediate species diffuse and may initiate chemical reactions
- Reaction take place all over the flame thickness
- Maximum heat release at low temperature



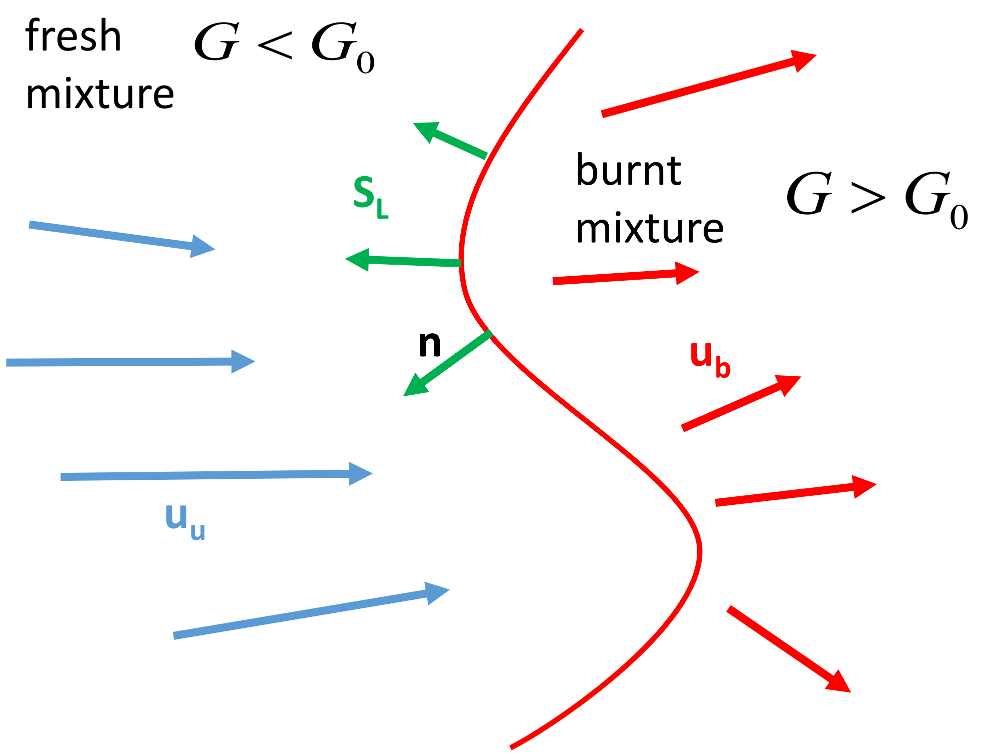
In case of hydrogen combustion, the diffusive zone is thicker due to the Soret effect.

Laminar Premixed Flames

How to describe flame position ?

- displacement velocity of flame front $\frac{du_f}{dt}$
- flow velocity of unburnt mixture u_u
- burning velocity $S_{L,u}$

$$\frac{du_f}{dt} = u_u + S_{L,u}$$



With a vector **n** normal to the flame

$$\frac{dx_f}{dt} = u + S_L \mathbf{n}; \qquad \mathbf{n} = -\frac{\nabla G}{|\nabla G|}; \qquad \nabla = \left(\frac{\partial}{\partial x_i} \right)$$

with x_f, the vector describing the position of the flame and dx_f/dt, the flame propagation velocity

$G(x,T) = G_0$; represents the flame surface;

$G > G_0$ the burnt region

$G < G_0$ and the fresh mixture.

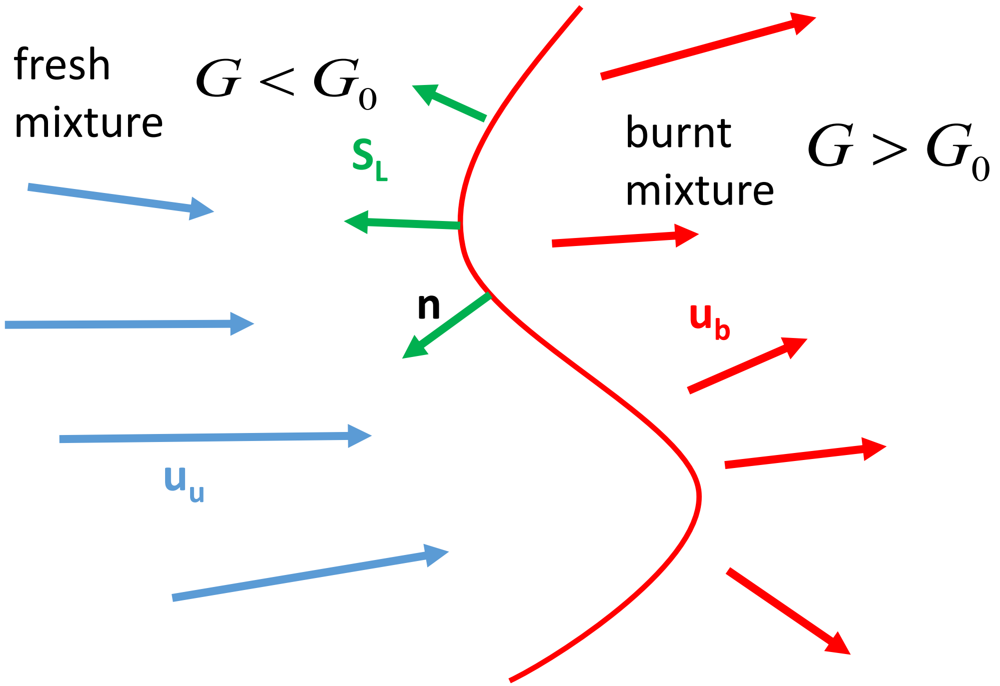
Premixed Flames

Laminar Premixed Flames

Derivation of level set equation for the propagating flame → differentiation of $G(x,T) = G_0$;

$$\frac{\partial G}{\partial t} + \nabla G \cdot \frac{\partial x}{\partial t}\Big|_{G=G_0};$$ with $$\frac{dx_f}{dt} = u + S_L \mathbf{n};$$

$$\Longrightarrow \quad \frac{\partial G}{\partial t} + u \nabla G = S_L |\nabla G|;$$

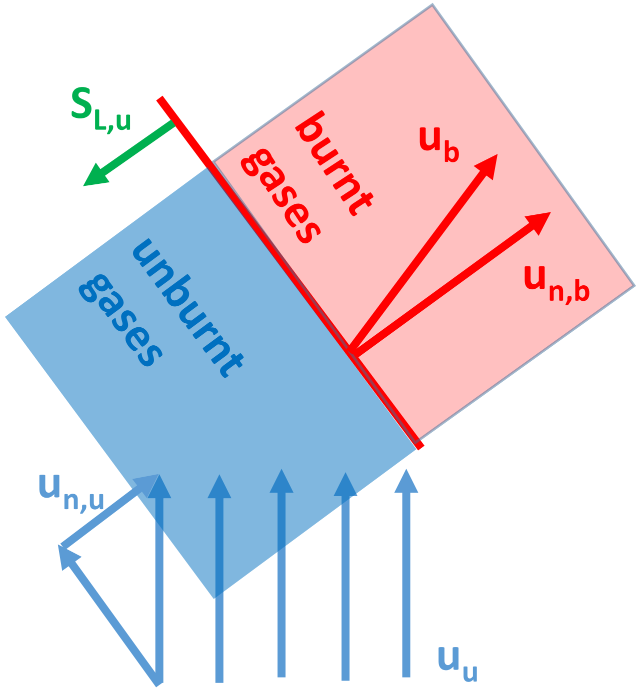


Even an originally smooth flame front will in a quiescent flow form cusps and eventually become flatter over time. (compare with Huygens' principle from optics)

Premixed Flames

Laminar Premixed Flames
Slot Burner

Flow Visualization of Slot burner flame:
→ fluid moves away from flame



$$S_{L,u} = u_{n,u} = u_u \sin\alpha$$

<u>Interesting Result:</u>
Velocity component normal to flame front $u_{n,u}$ is locally equal to the propagation velocity of the flame front, the laminar burning velocity $S_{L,u}$.

Across flame front we find a large temperature increase and a drastic density decrease while pressure stays nearly constant.

Laminar Premixed Flames

Slot Burner

At the tip of the Bunsen flame, there is a different situation:

The burning velocity is equal to the one of the unburnt mixture and by a factor of 1/sin(α) larger than the normal flame velocity. The reason for this higher velocity is the fact that there is increased pre-heating from the lateral parts of the flame front.

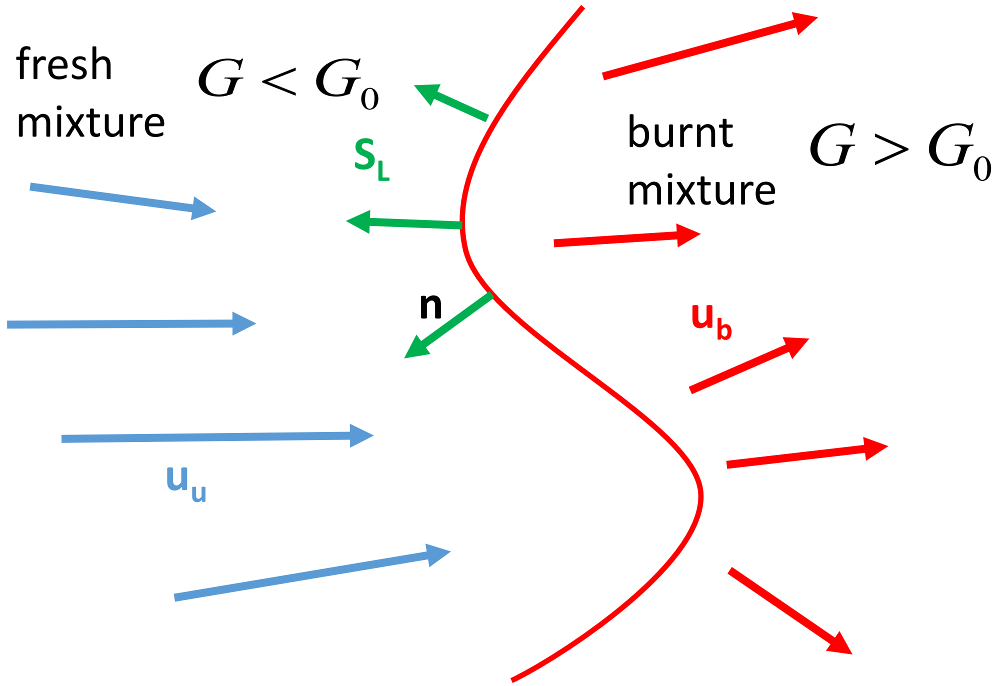
The Lewis number, the ratio of thermal diffusivity to mass diffusivity. For simplification, generally average quantities are used.

$$\mathrm{Le} = \frac{\bar{\lambda}}{\bar{\rho}\bar{D}_m\bar{c}_p} = \frac{\mathrm{Sc}}{\mathrm{Pr}}$$

Quite often Le ~ 1, however when hydrogen is present, thermal diffusivity can't be neglected.

In order to get the exact flame form at the tip one has to modify the flame velocity due to a curvature effect. This leads to the concept of flame stretch.

Flame Stretch



Two contributions due to

- Curvature of the flame
- Divergence of flow (strain)

Assumptions:

- 1-step reaction (reactants → products) with large activation energy (negligible reaction in the fresh mixture)
- Constant properties

→ Laminar flame velocity becomes $S_L = S_L^0 - S_L^0 \mathrm{L}\kappa + \mathrm{L}\,\mathbf{n}\cdot\nabla u\mathbf{n};$

S_L^0 Laminar burning velocity for an un-stretched flame

L Markstein length $\quad L \sim O(l_F)$

κ Stretch rate of flame $\quad \kappa = \nabla\cdot\mathbf{n} = -\left(\frac{\nabla G}{|\nabla G|}\right) = -\frac{\nabla^2 G + \mathbf{n}\cdot\nabla(\mathbf{n}\cdot\nabla G)}{|\nabla G|};$

$\mathrm{M} = \frac{l_F}{\delta_F}$ Markstein number

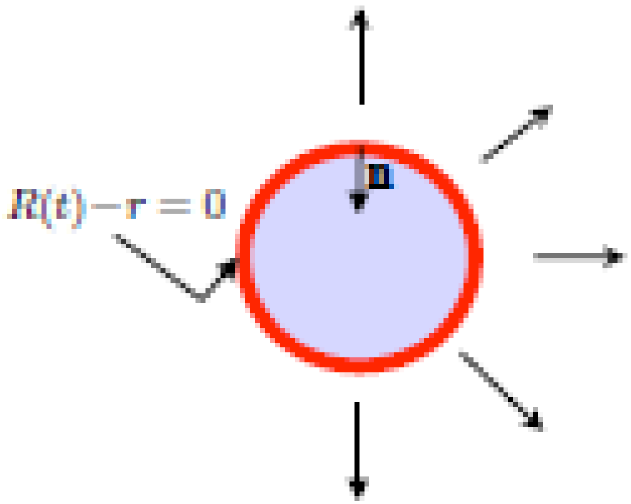
δ_F flame thickness

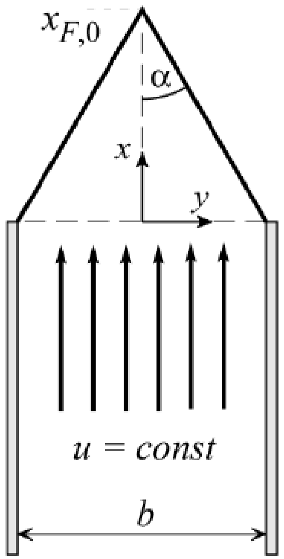
Premixed Flames

Flame Stretch

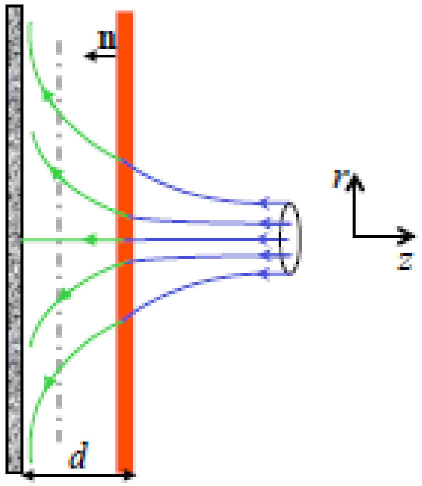
Examples of stretched flames

- Spherical flames (expanding flame: positively stretched; inward propagating flame: negatively stretched (compressed)





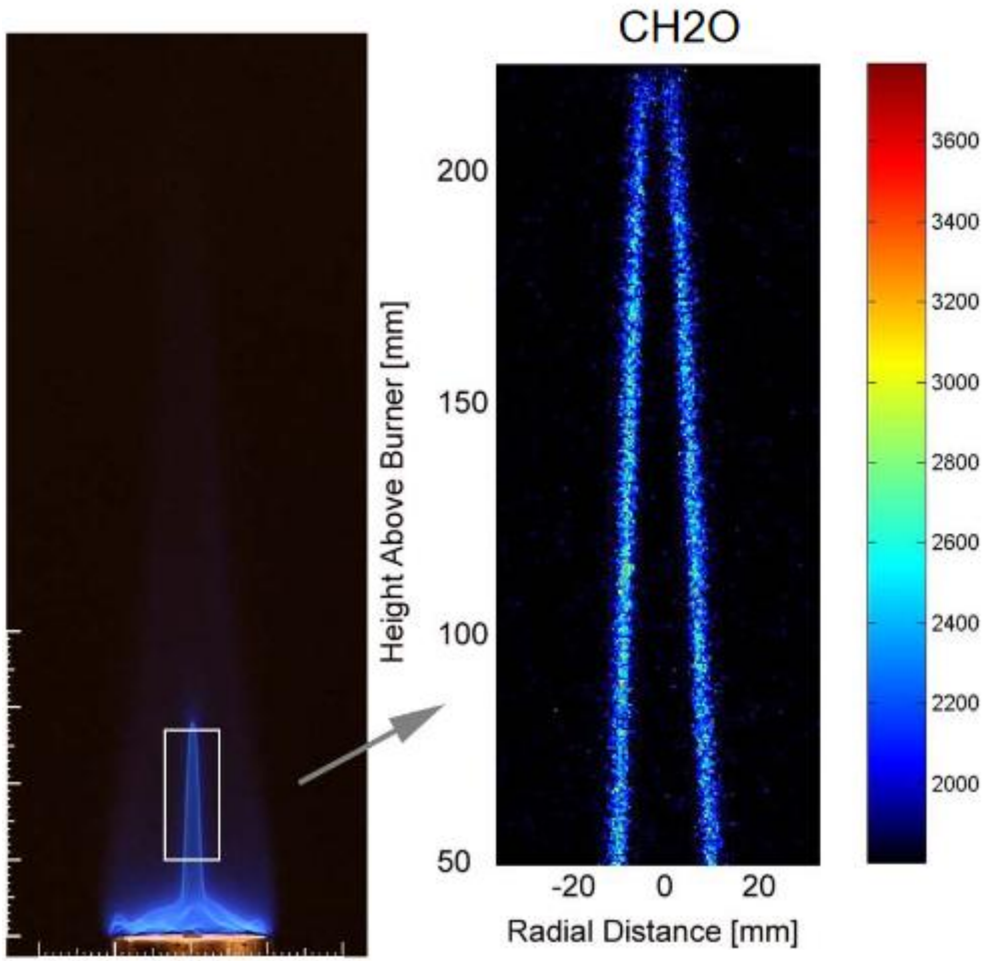
- Stagnation point flow



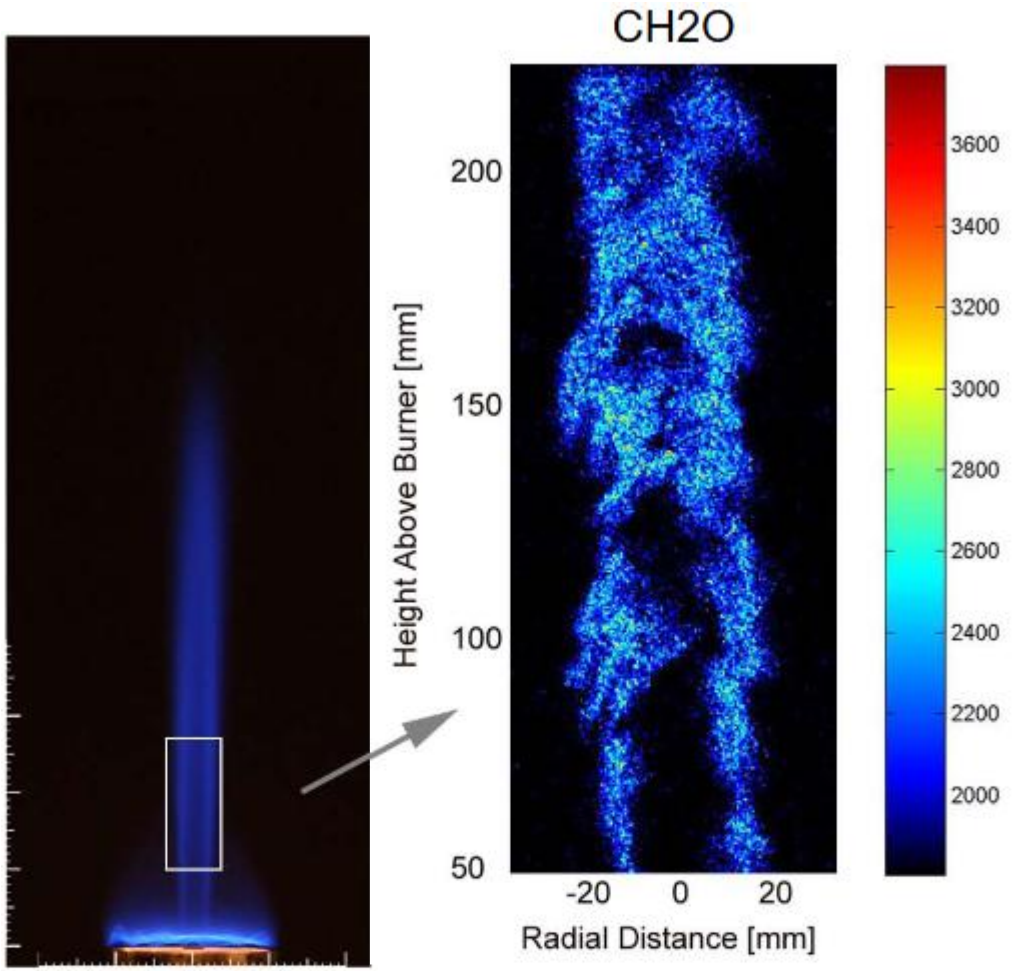
- Bunsen (2D-axisymmetric)
- and Slot Burner (2D)

Premixed Flames

Turbulent Premixed Flames



X.S. Bai, Lund



Laminar Premixed Methane/air Combustion Turbulent

Turbulent Premixed Flames

Turbulent pre-mixed flames may be divided in three regions where different processes dominate

- Preheating area (heat and mass transfer by turbulence and diffusion)
- Reaction region which is generally very thin (chemical kinetics, heat release, propellant consumption)
- Post-flame region (turbulent transport)

The reaction zone is generally highly wrinkled due to

- Turbulent structures
- Intrinsic instabilities
  - Hydro-dynamically instable (Landau-Darrieus)
  - Thermal diffusion instability (Soret)
  - Bouyancy (Rayleigh-Taylor)

While normally $\mathrm{Re} = \frac{ul}{\upsilon};$

where l is a macroscopic length characteristic for the flow geometry

the turbulent $\mathrm{Re}_t = \frac{u' l_0}{\upsilon};$

depends on the velocity fluctuations and the integral length scale, a local quantity

$\mathrm{Re}_t > 1$ **Turbulent**

Turbulent Premixed Flames

Flow Scales

- Mean scales
  - Velocity U, length L, time $t=(L/U)$
- Integral scales
  - Length l_0, Velocity $u_0 = U(l_0)$, time $t_0 = l_0/u_0$
- Kolmogorov scales
  - Length l_K, velocity $u_K = U(l_K)$, time $t_K = l_K/u_K$

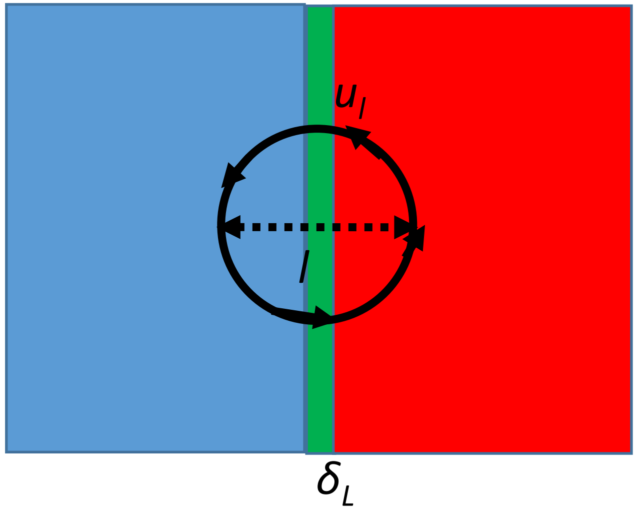
Flame Scales

- Flame speed S_L
- Flame thickness δ_L
- Time scales
  - Flame thickness/flame speed δ_L/S_L
  - Chemical reaction time t_c

Remarks:

- Wrinkled flame structure may complicate the determination of appropriate velocity and length scales
- Chemical time scale of the dominating reactions may not be easy to determine

Turbulent Premixed Flames



Flow Scales

- Size of vortex l
- Molecular mixing time at Kolmogorov length scale l_K $t_K=l_K l_K/D$
- Eddy velocity u_l
- Eddy turnover time $t_e=l/u_l$

Non-Dimensional Numbers

- Reynolds $$\mathrm{Re}_{l0} = \frac{u_0 l_0}{\upsilon};$$
- Karlovitz $$Ka = \frac{t_0}{t_K} = \frac{\delta_L u_K}{S_L l_K} = \left(\frac{\delta_L}{l_K}\right)^2;$$
- Damköhler $$Da = \frac{t_0}{t_c} = \frac{l_0}{u_0}\frac{S_L}{\delta_L};$$
- Turbulence intensity $$TI = \frac{u_0}{S_L};$$

Generally, the turbulence intensity is defined as:

$$TI = \frac{\frac{1}{3}\left(\sum_{i=1}^{3} u_i'^2\right)^{1/2}}{\left(\sum_{i=1}^{3} u_i^2\right)};$$

However, in flames the characteristic velocity of the flow is the integral velocity scale and the reference is the laminar flame speed.

Premixed Flames

Turbulent Premixed Flames

Non-Dimensional Numbers and Borghi Diagram

$$\mathrm{Re}_{l0} = \frac{u_0 l_0}{\upsilon} \propto \frac{u_0 l_0}{D} \propto \frac{u_0 l_0}{S_L \delta_L};$$

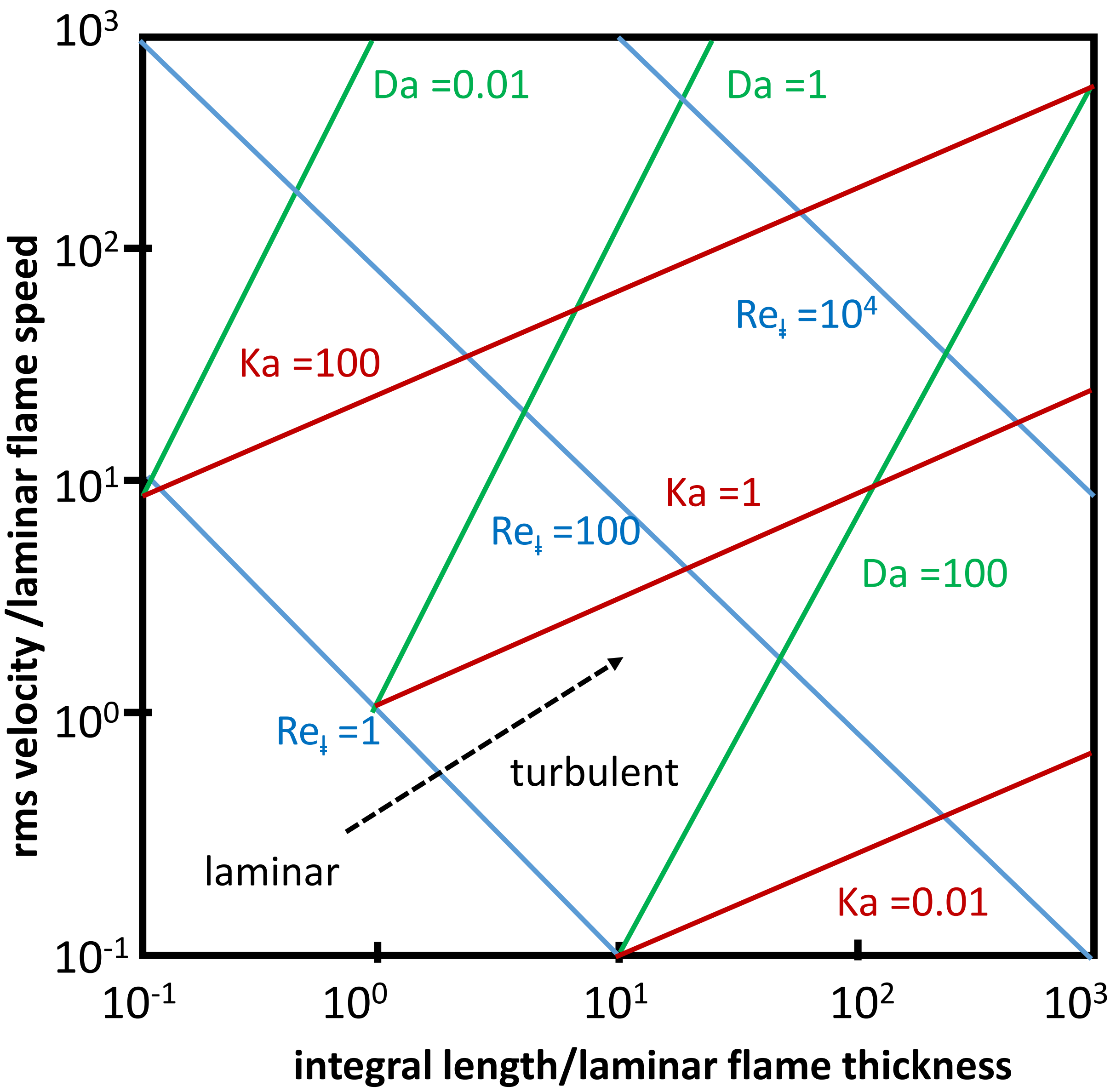
$$\Rightarrow \quad \log\left(\frac{u_0}{S_L}\right) = \log(\mathrm{Re}_{l0}) - \log\left(\frac{l_0}{\delta_L}\right);$$

$$Da = \frac{t_0}{t_c} = \frac{l_0}{u_0}\frac{S_L}{\delta_L};$$

$$\log(Da) = \log\left(\frac{l_0}{\delta_L}\right) - \log\left(\frac{u_0}{S_L}\right);$$

$$Ka = \frac{t_0}{t_K} = \frac{\delta_L u_K}{S_L l_K} = \left(\frac{\delta_L}{l_K}\right)^2;$$

$$\log\left(\frac{u'}{S_L}\right) = \frac{1}{3}\log\left(\frac{l_0}{\delta_L}\right) + \frac{2}{3}\log(Ka);$$



Premixed Flames

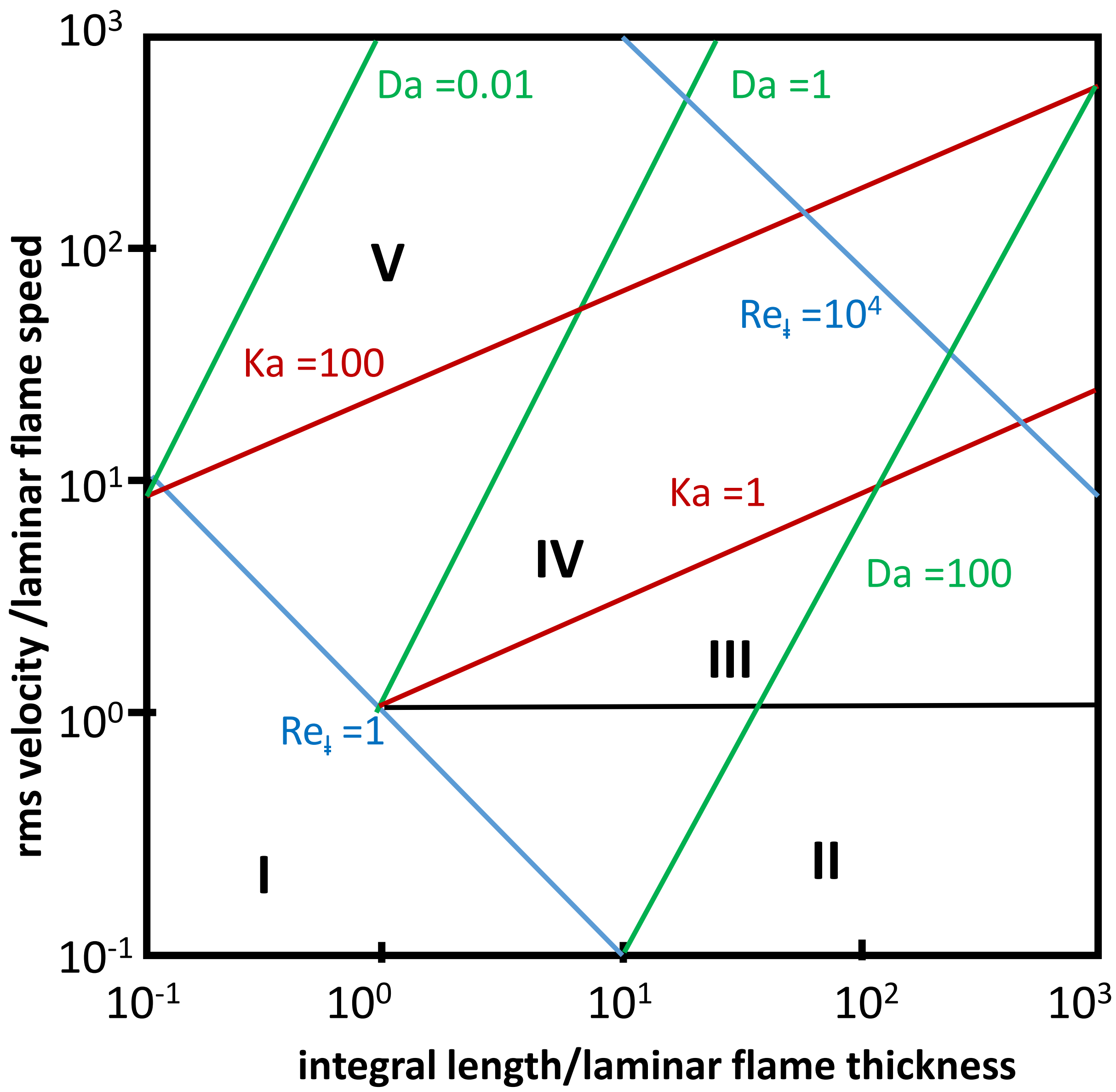
Turbulent Premixed Flames

Borghi Diagram

I	laminar flame regime
II	wrinkled flamelet regime
III	corrugated flamelet regime
IV	thin reaction region
V	distributed reaction region

Nota:

Based on assumption that Lewis number and Schmidt are equal and 1.
Le = Sc = 1



Turbulent Premixed Flames

Borghi Diagram

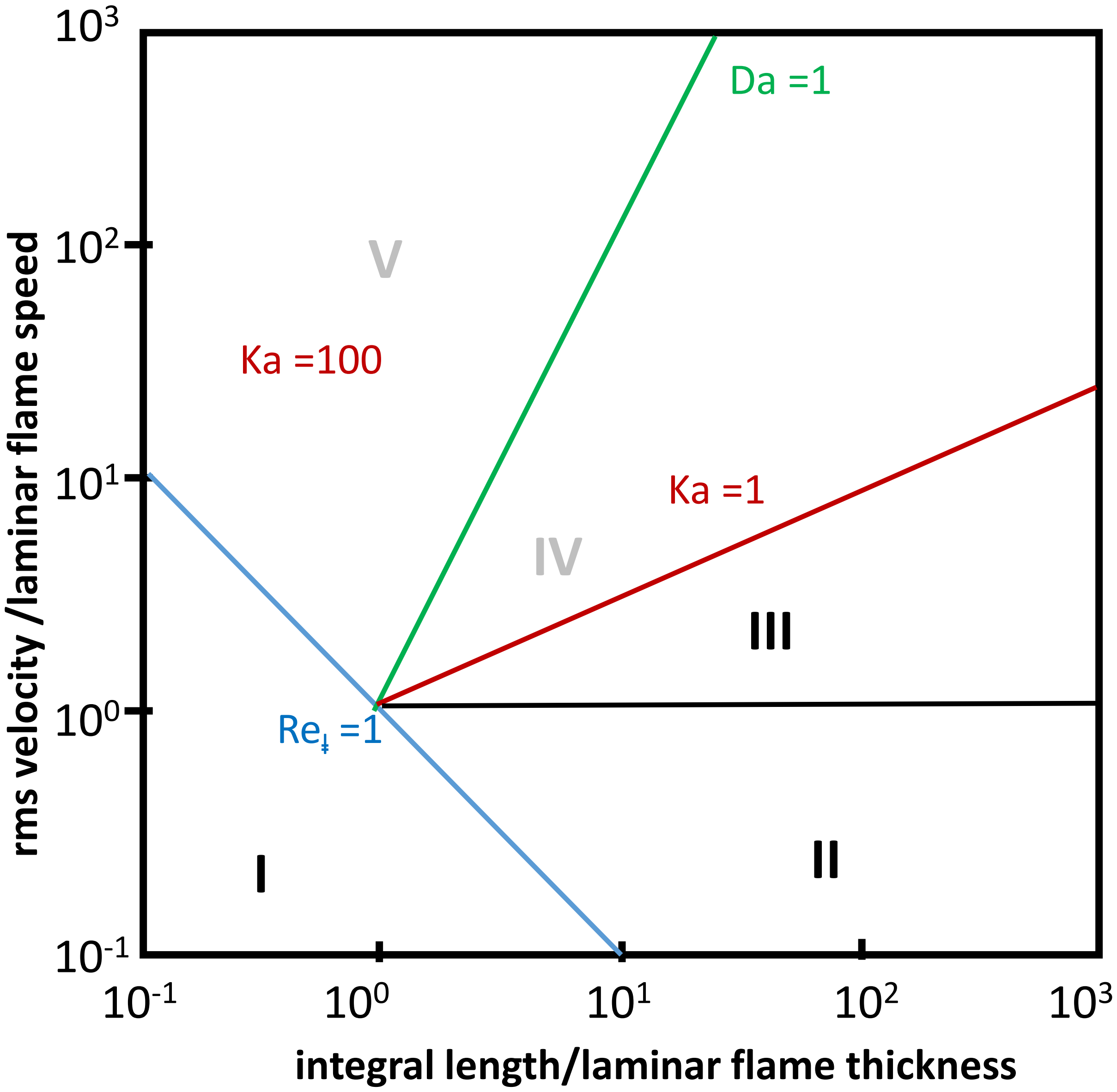
I	laminar flame regime
II	wrinkled flamelet regime
III	corrugated flamelet regime
IV	thin reaction region
V	distributed reactions

For $$Ka = \frac{t_0}{t_K} = \left(\frac{\delta_L}{l_K}\right)^2 < 1;$$

the combined reaction and preheat zones are smaller than the Kolmogorov length l_K

- molecular transport of heat and mass dominates
- flame propagates at laminar speed
- laminar flame thickness

→ **flamelet concept holds**



Premixed Flames

Turbulent Premixed Flames

Borghi Diagram

For $1 < Ka < 100$

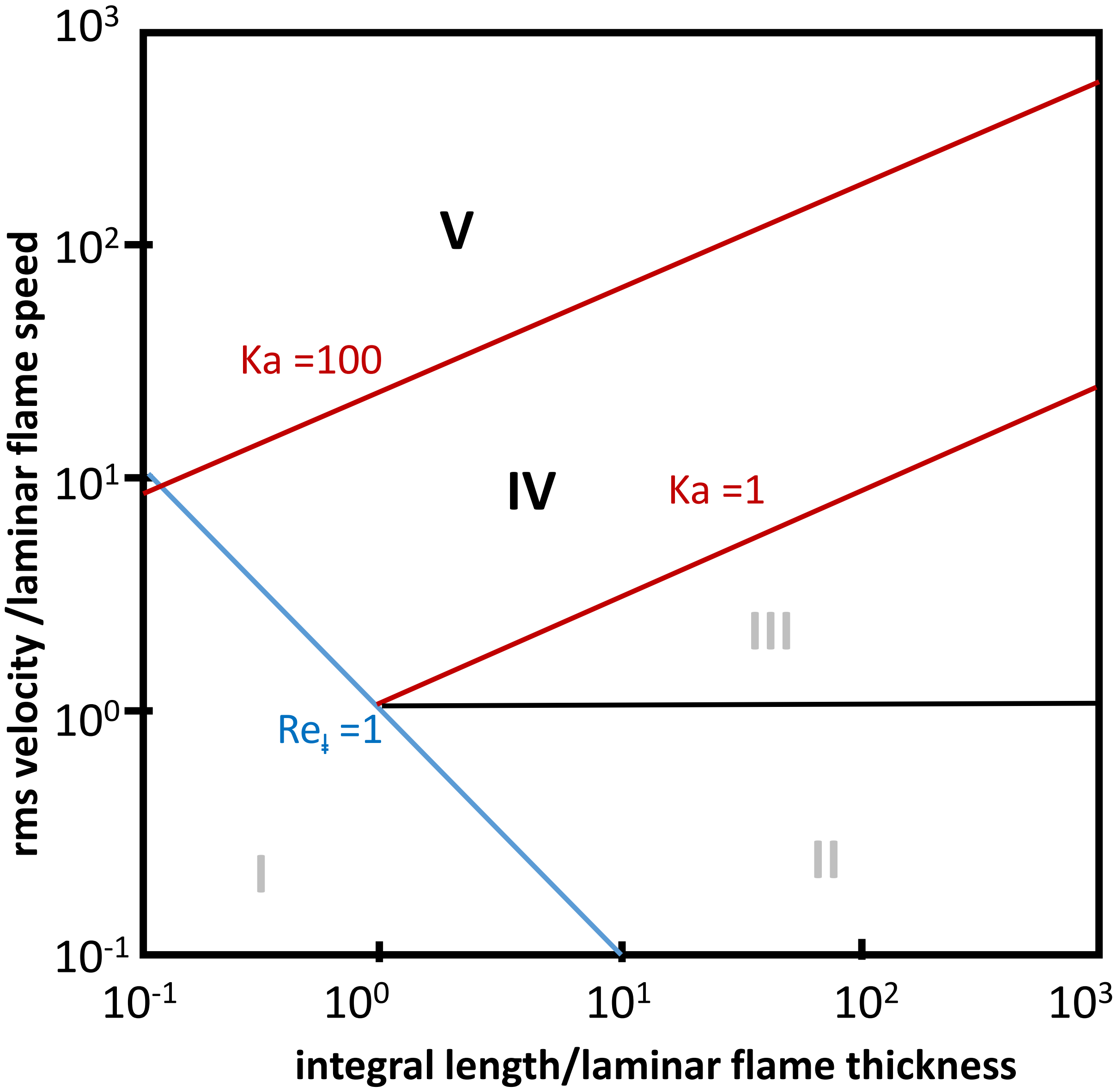
eddies of reactants (eddy diameter << flame thickness) aren't able to pass through the reaction layer but thicken the flame front due to an increase of diffusive transport

→ **Thin reaction zone (IV)**

For $Ka > 100$

eddies of reactants (eddy diameter >> flame thickness) pass through the reaction layer without being fully consumed;
Additional reacting pockets within burned zone

→ **Distributed reaction zone (V)**



Turbulent Premixed Flames

Borghi Diagram

Damköhler dependency:

For Da << 1

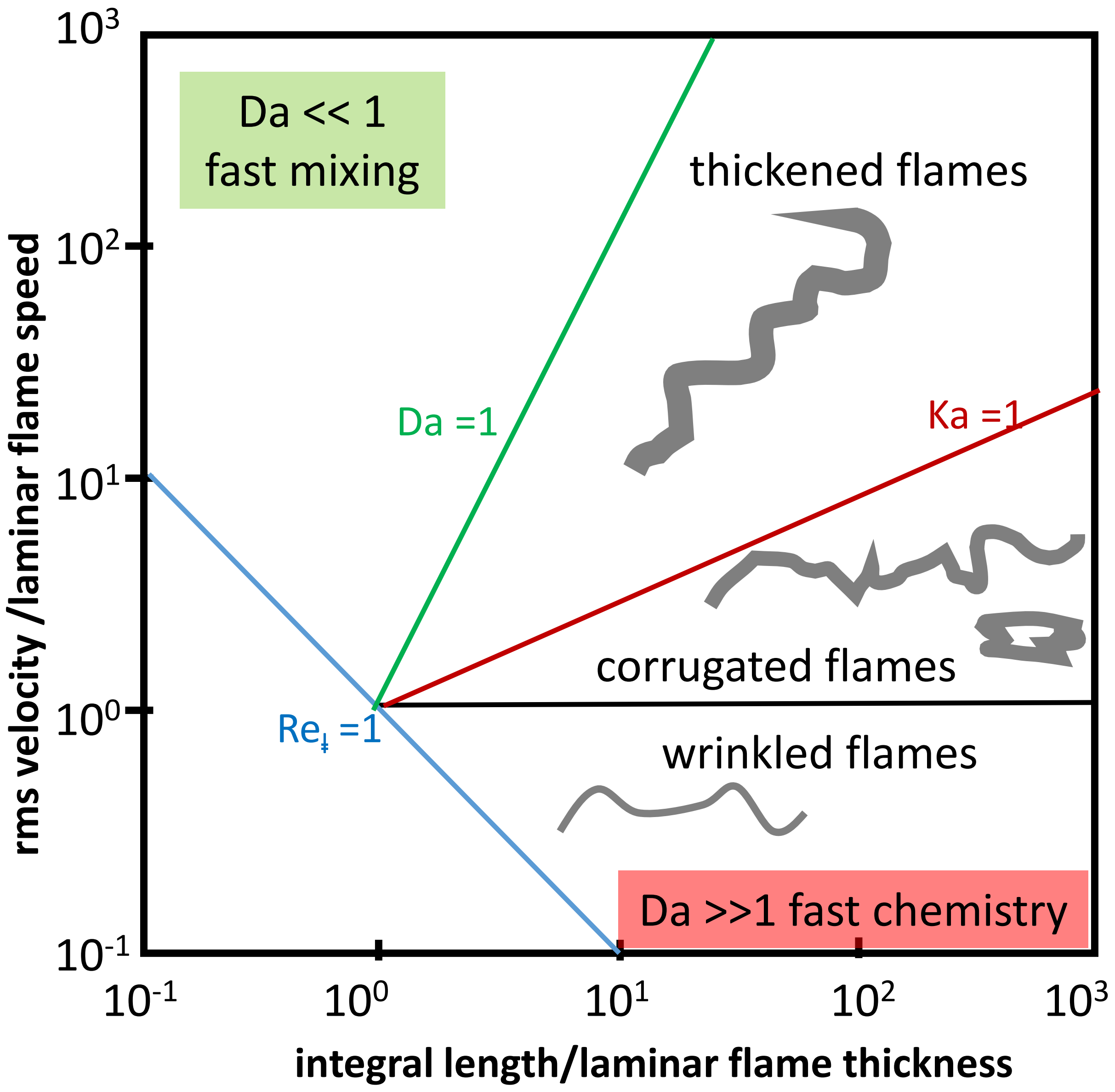
mixing is much faster than chemistry

→ **well-stirred reactor**

For Da >>1

chemistry is much faster than transport

→ **wrinkled laminar flamelet**



Premixed Flames

Turbulent Premixed Flames

Turbulent flame speed depends on

- flame parameters: propellants, mixture ratio, *p, T,* → S_L (laminar burning velocity)
- flow parameters: turbulence intensity, Re_t, Da, …

Damköhler Theory:

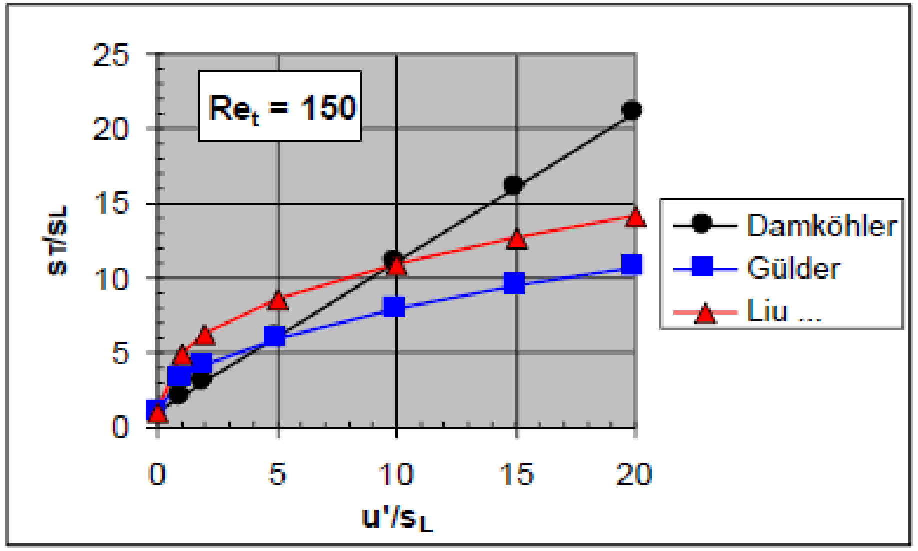
for wrinkled flames, turbulent flame speed proportional to flame surface area

$$\frac{S_T}{S_L} = \frac{A_L}{A_T} = 1 + \frac{u'}{S_L};$$

Many correlations available

$$\frac{S_T}{S_L} = 1 + 0.62\left(\frac{u'}{S_L}\right)^{0.5} (\mathrm{Re}_t)^{0.25}; \text{Gülder}$$

$$\frac{S_T}{S_L} = 1 + 0.435\left(\frac{u'}{S_L}\right)^{0.4} (\mathrm{Re}_t)^{0.44}; \text{Liu}$$



Flamelet region ⟷ thin reaction region

Things you shouldn't forget

- Activation energy, auto-ignition temperature, flammability limits
- Difference between Detonation and Deflagration
- Basics of Chapman-Jouget Graph
- Basics of Laminar-Premixed Flames
- Turbulent Per-mixed Flames (Borghi-Diagram)