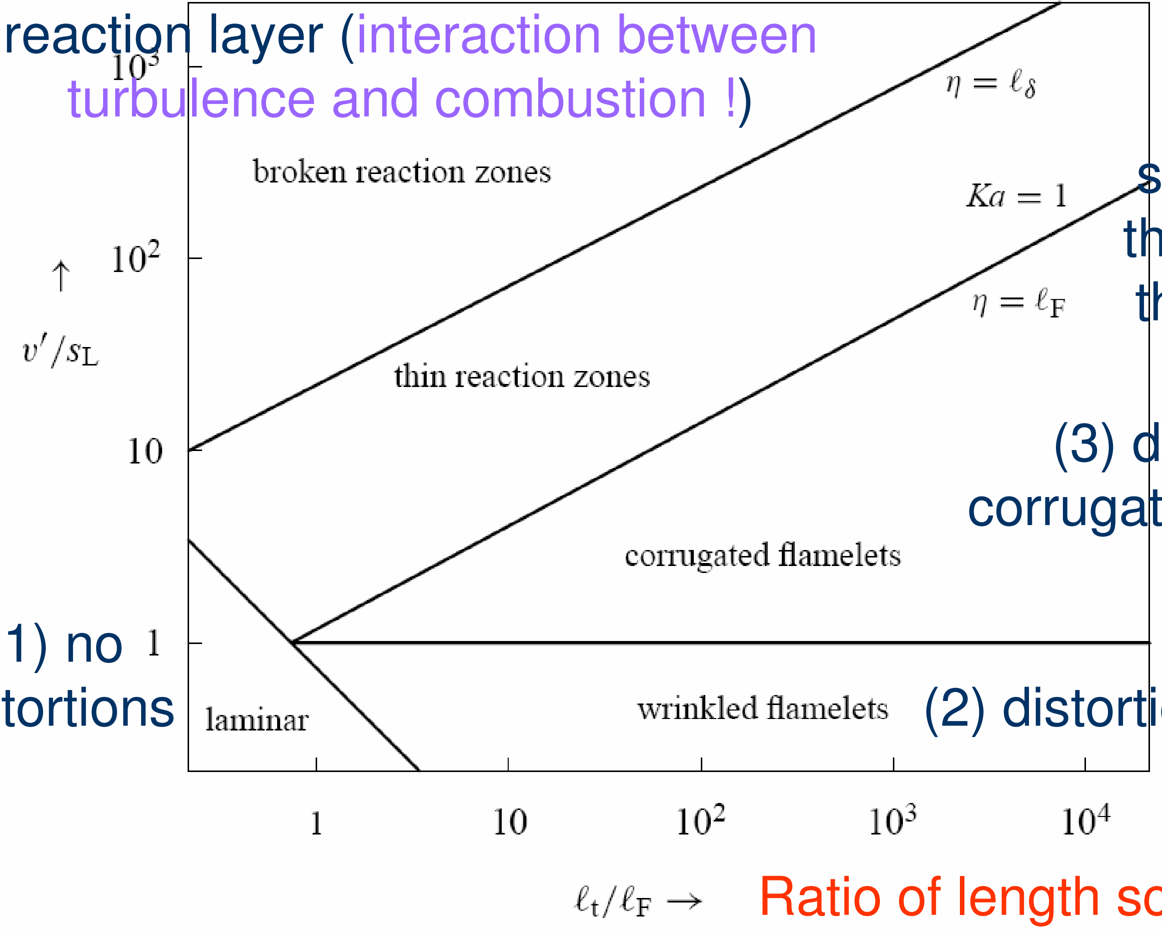
Reactive Mixture Flows: Combustion

	Laminar	Turbulent
Premixed	**LP**	**TP**
Diffusion	**LD**	**TD**

- Depending on the flow type (laminar / turbulent) and the type of premixing (premixed / non–premixed or diffusion), it is possible to distinguish different kinds of combustion regimes, each with its own characteristic features

Premixed Combustion: Main Regimes

(5) smallest flow distortions enter the reaction layer (interaction between turbulence and combustion !)



(4) smallest flow distortions are smaller than flame thickness but larger than reaction layer

(3) distortions are corrugating the flamelets

(2) distortions are dumped

(1) no distortions

Ratio of velocity scales

Ratio of length scales

The modified Borghi-diagram for premixed turbulent combustion.

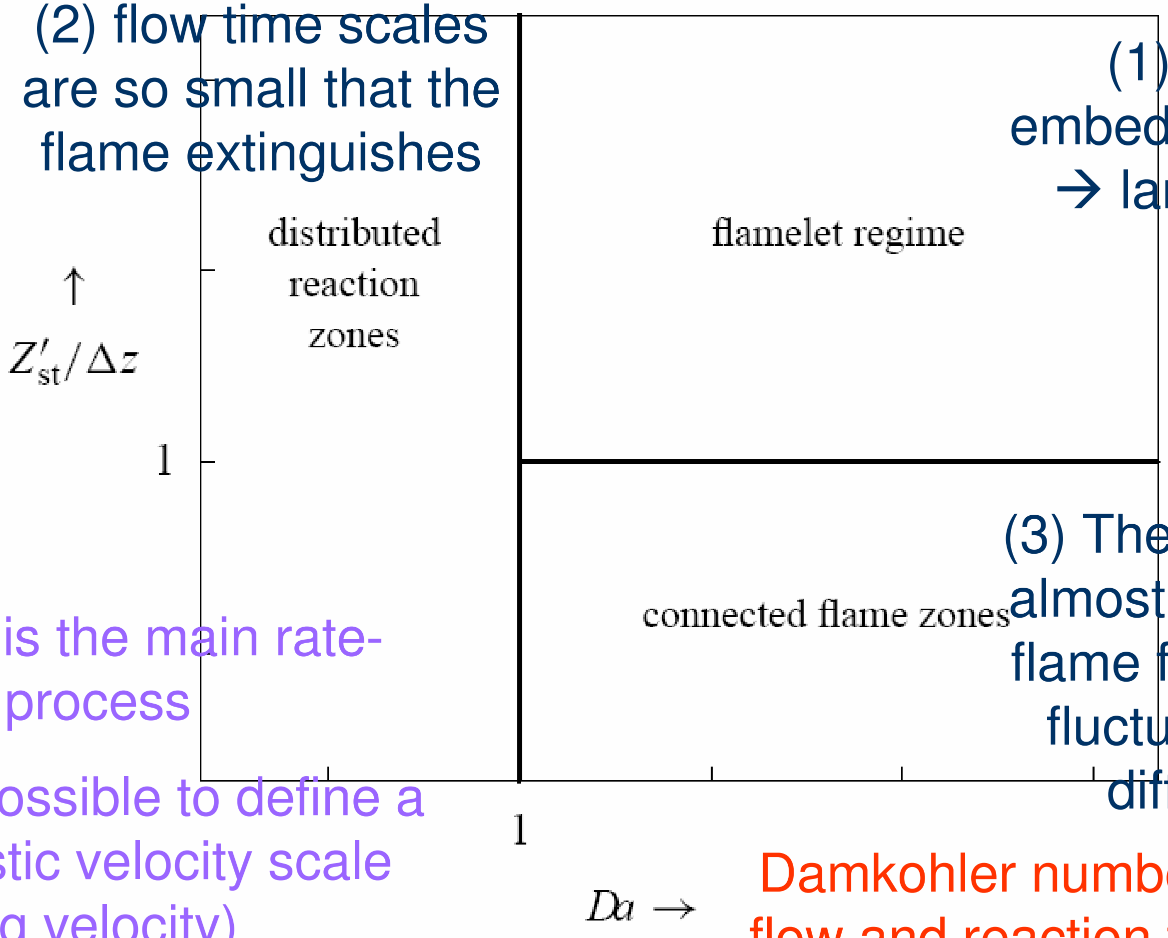
Burning Velocity of Premixed Flames

- The (adiabatic) burning velocity (**s_L^0**) is the speed of a two-dimensional flame front normal to its surface and relative to the unburned gaseous-and-fuel oxidizer mixture in adiabatic conditions (thermal insulation)

$$s_\mathrm{L}^0 = \sqrt{\frac{D}{t_R}} = \sqrt{\rho_\mathrm{u} A D \exp(-E_\mathrm{a}/RT_\mathrm{b})}.$$

  - The unburnt mixture just ahead of the flame front starts reacting only if the gas temperature has increased up to a value very close to the adiabatic burning temperature
  - The exponential decay of the reaction time scale is related to the Maxwellian translational energy distribution in the gas → indicating that only collisions with kinetic energy larger than activation energy threshold can undergo chemical reaction

Non-premixed (Diffusion) Combustion



Regimes in non-premixed turbulent combustion.

(2) flow time scales are so small that the flame extinguishes

(1) thin fronts embedded in the flow → laminar regime

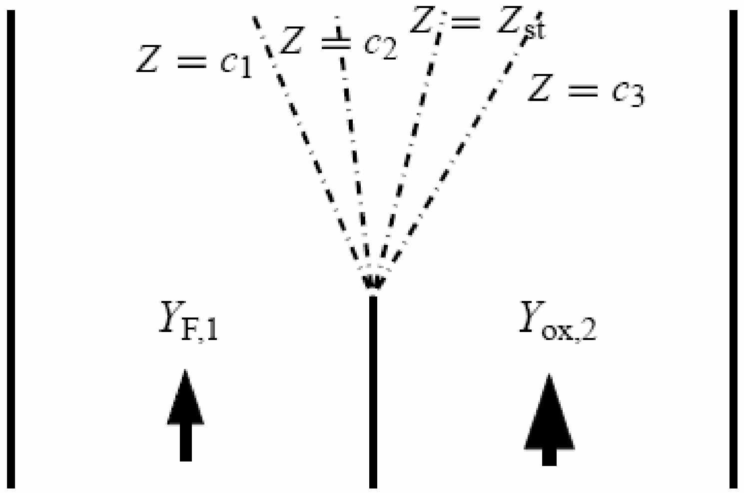
(3) The gasses became almost premixed → the flame front is large and fluctuations connect different zones

Fluctuation in the degree of mixing of fuel and oxidizer

Damkohler number, Ratio of flow and reaction time scales

- Diffusion is the main rate-controlling process
- It is not possible to define a characteristic velocity scale (i.e. burning velocity)

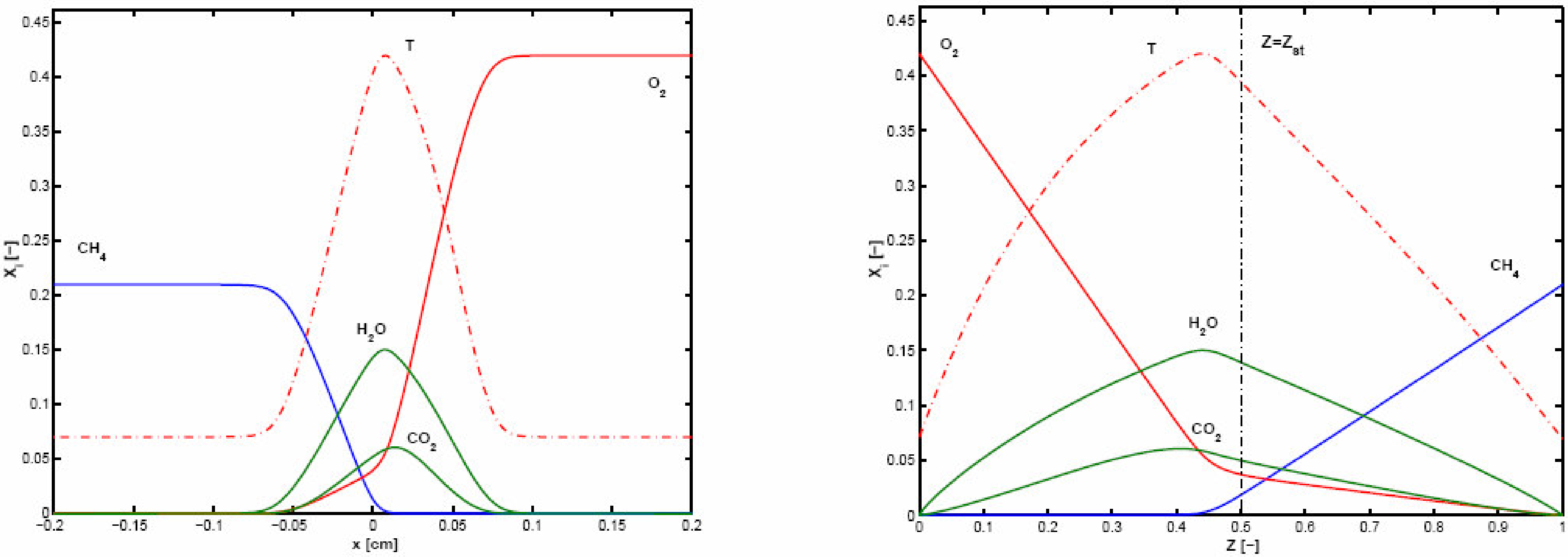
Infinitely Fast Non-premixed Reactions



$$Z = \frac{s\,Y_F - Y_{ox} + Y_{ox,2}}{s\,Y_{F,1} + Y_{ox,2}},$$

- The mixture fraction **Z** does not change due to chemical reaction, because if Y_F decreases by an amount **x** due to the chemical reaction, Y_{OX} decreases by an amount **s x** (where **s** is the stoichiometric coefficient)
- The surface where $Y_F = s\, Y_{OX}$ identifies where the reaction is faster and the temperature is higher

Finite Time Non-premixed Reactions



Internal structure of a methane-air diffusion flame in a stagnation flow (a) as a function of distance x and (b) as a function of mixture fraction Z.

- The finite reaction speed implies finite thickness of the flame front (diffusion time) → moreover the reactant species concentrations are non zero in the stoichiometric surface

Modeling Laminar Combustion

$$\frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v}\mathbf{v}) + \nabla \cdot (\boldsymbol{\tau}) = -\nabla p,$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0,$$

$$\frac{\partial(\rho Y_i)}{\partial t} + \nabla \cdot (\rho \mathbf{v} Y_i) + \nabla \cdot (\rho \mathbf{V}_i Y_i) = \boxed{r_i} \quad (i = 1, ..., N).$$

- The previous system of equations constitutes a well-posed problem if the constitutive relations are specified → In addition to stress tensor and thermal flux, the diffusion velocity must be specified in terms of the local species concentrations (for example, by Maxwell–Stefan model)
- What about the source terms r_i ?

Chemical Aspects of Combustion

- The oxidation of fuel is composed of many elementary reactions → these elementary reactions have a physical relation with microscopic processes, in contrast with overall chemical reactions where the reaction equations merely states overall conversion ratios → for example, the combustion of methane involves 36 species and 210 chain reactions

$$\nu_1' A_1 + \nu_2' A_2 + \ldots \nu_N' A_N \rightarrow \nu_1'' A_1 + \nu_2'' A_2 + \ldots \nu_N'' A_N$$

- A_i represents one of the species involved in the reaction, and $\nu_i' - \nu_i''$ the number of molecules converted in the elementary reaction

Law of Mass Action

$$\frac{q_i}{(\nu'_i - \nu''_i)} = \frac{q_j}{(\nu'_j - \nu''_j)}$$

q_i is defined as the net rate of increase of species i (in moles per volume^8 per second).
It's now common practice to define **the reaction rate** q, as being equal to the q_i for a species when $(\nu'_i - \nu''_i)$ is equal to one

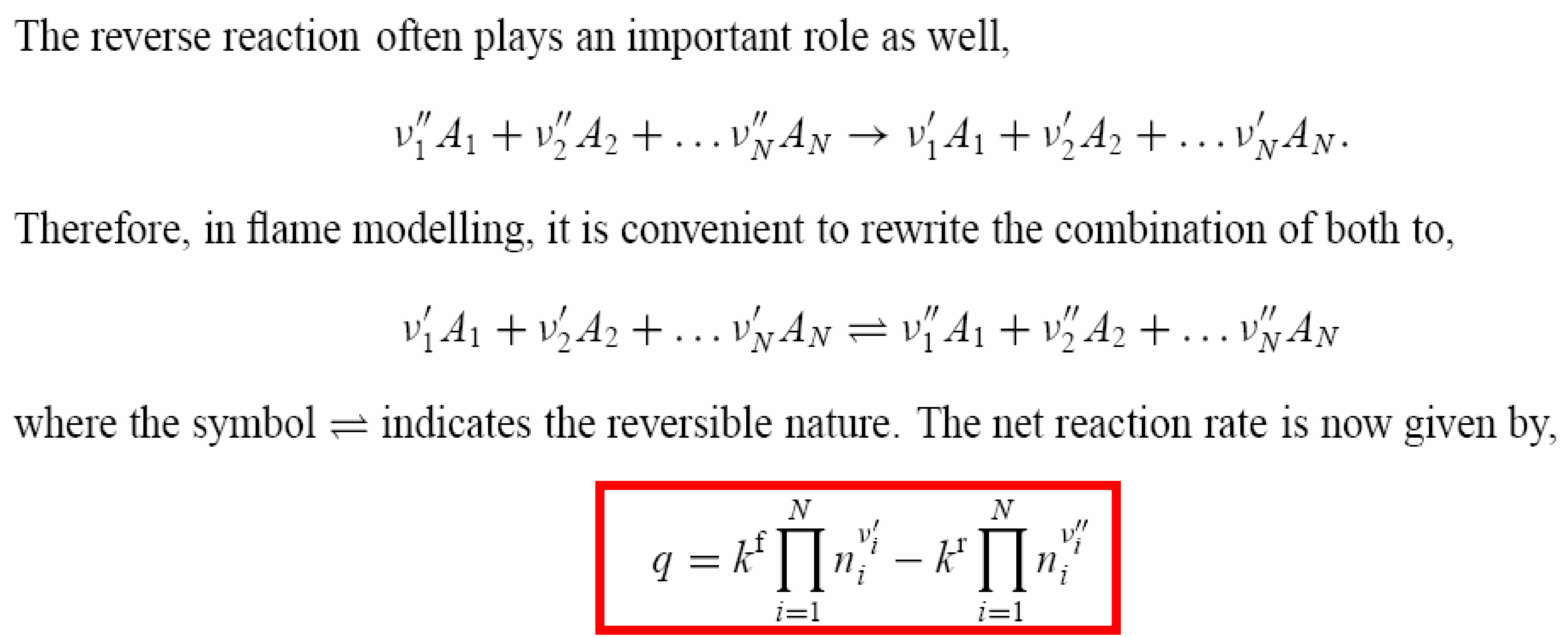
$$q_j = (\nu'_j - \nu''_j)q.$$

The phenomenological **law of mass action** now states that a reaction rate is proportional to the product of the concentrations, n_i, which leads for the formal reaction

$$\boxed{q = k \prod_{i=1}^{N} n_i^{\nu'_i}}$$

where the proportionality parameter k, sometimes is referred to as the **specific reaction rate constant**.

Reversed and Effective Reaction



The reverse reaction often plays an important role as well,

$$\nu_1'' A_1 + \nu_2'' A_2 + \ldots \nu_N'' A_N \rightarrow \nu_1' A_1 + \nu_2' A_2 + \ldots \nu_N' A_N .$$

Therefore, in flame modelling, it is convenient to rewrite the combination of both to,

$$\nu_1' A_1 + \nu_2' A_2 + \ldots \nu_N' A_N \rightleftharpoons \nu_1'' A_1 + \nu_2'' A_2 + \ldots \nu_N'' A_N$$

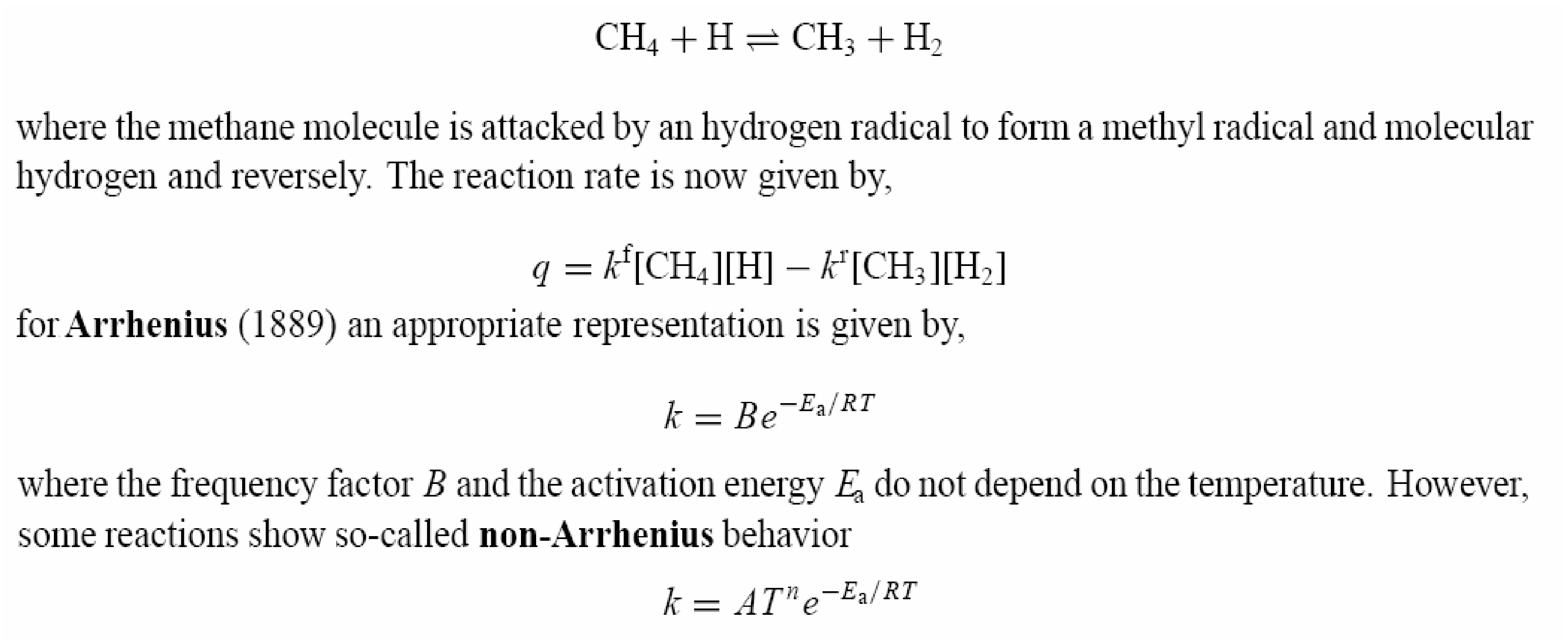
where the symbol $\rightleftharpoons$ indicates the reversible nature. The net reaction rate is now given by,

$$\boxed{q = k^{\mathrm{f}} \prod_{i=1}^{N} n_i^{\nu_i'} - k^{\mathrm{r}} \prod_{i=1}^{N} n_i^{\nu_i''}}$$

- In the last expression, the specific reaction rate constants for forward and reversed reactions appear → the equilibrium point can change due to temperature fluctuations

(2) Bimolecular Reactions

- The chemical reactions are classified according to the reaction order RO (sum of the reaction coefficients of the reactants) → for most of the combustion reactions in the chain mechanism it will not exceed 3 → e.g. RO = 2



$$CH_4 + H \rightleftharpoons CH_3 + H_2$$

where the methane molecule is attacked by an hydrogen radical to form a methyl radical and molecular hydrogen and reversely. The reaction rate is now given by,

$$q = k^{\mathrm{f}}[CH_4][H] - k^{\mathrm{r}}[CH_3][H_2]$$

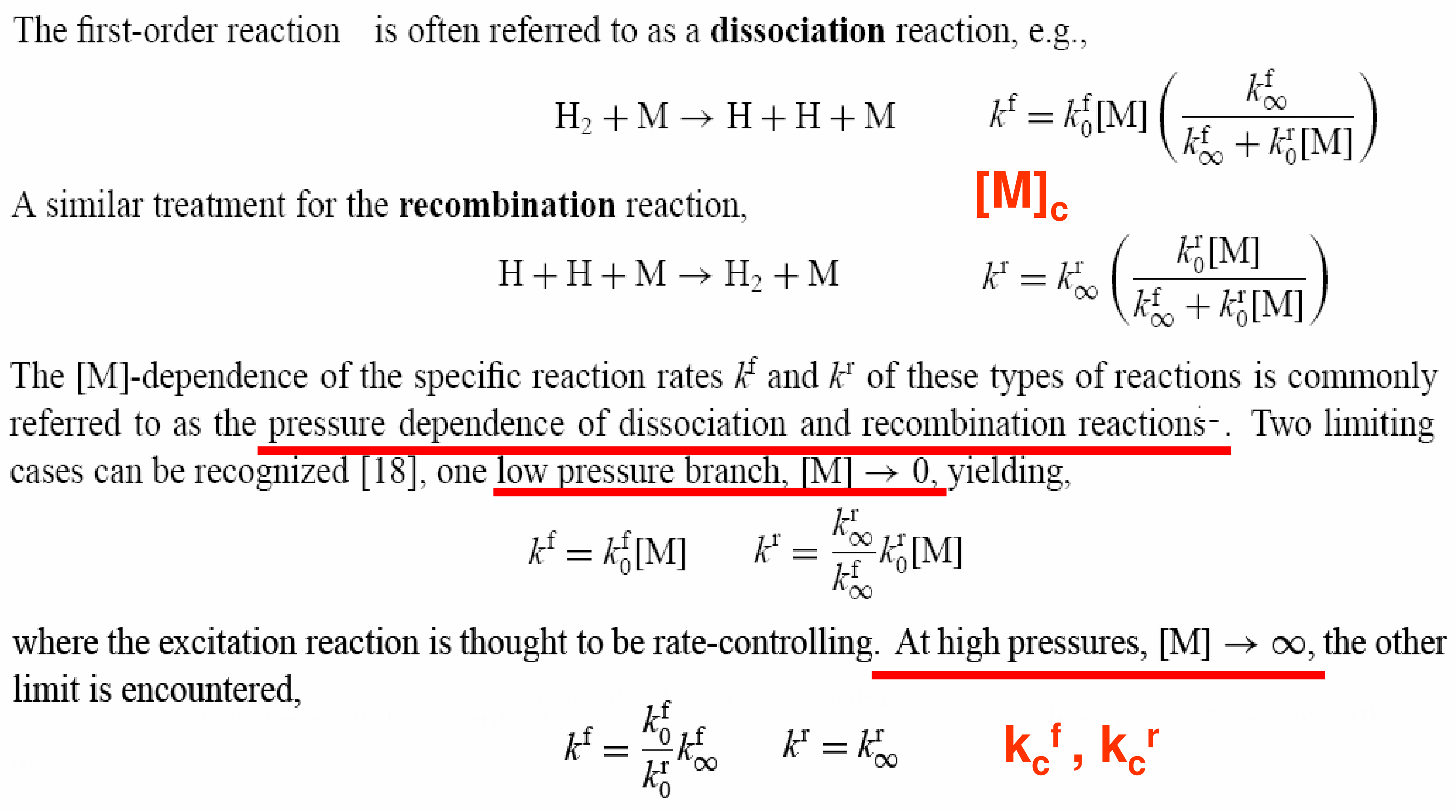
for **Arrhenius** (1889) an appropriate representation is given by,

$$k = Be^{-E_{\mathrm{a}}/RT}$$

where the frequency factor B and the activation energy E_{a} do not depend on the temperature. However, some reactions show so-called **non-Arrhenius** behavior

$$k = AT^{n}e^{-E_{\mathrm{a}}/RT}$$

(1) Dissociations and (3) Recombinations



The first-order reaction is often referred to as a **dissociation** reaction, e.g.,

$$\mathrm{H_2 + M \rightarrow H + H + M} \qquad k^{\mathrm{f}} = k_0^{\mathrm{f}}[\mathrm{M}]\left(\frac{k_\infty^{\mathrm{f}}}{k_\infty^{\mathrm{f}} + k_0^{\mathrm{r}}[\mathrm{M}]}\right)$$

$[\mathrm{M}]_c$

A similar treatment for the **recombination** reaction,

$$\mathrm{H + H + M \rightarrow H_2 + M} \qquad k^{\mathrm{r}} = k_\infty^{\mathrm{r}}\left(\frac{k_0^{\mathrm{r}}[\mathrm{M}]}{k_\infty^{\mathrm{f}} + k_0^{\mathrm{r}}[\mathrm{M}]}\right)$$

The [M]-dependence of the specific reaction rates k^{f} and k^{r} of these types of reactions is commonly referred to as the pressure dependence of dissociation and recombination reactions. Two limiting cases can be recognized [18], one low pressure branch, [M] → 0, yielding,

$$k^{\mathrm{f}} = k_0^{\mathrm{f}}[\mathrm{M}] \qquad k^{\mathrm{r}} = \frac{k_\infty^{\mathrm{r}}}{k_\infty^{\mathrm{f}}}k_0^{\mathrm{r}}[\mathrm{M}]$$

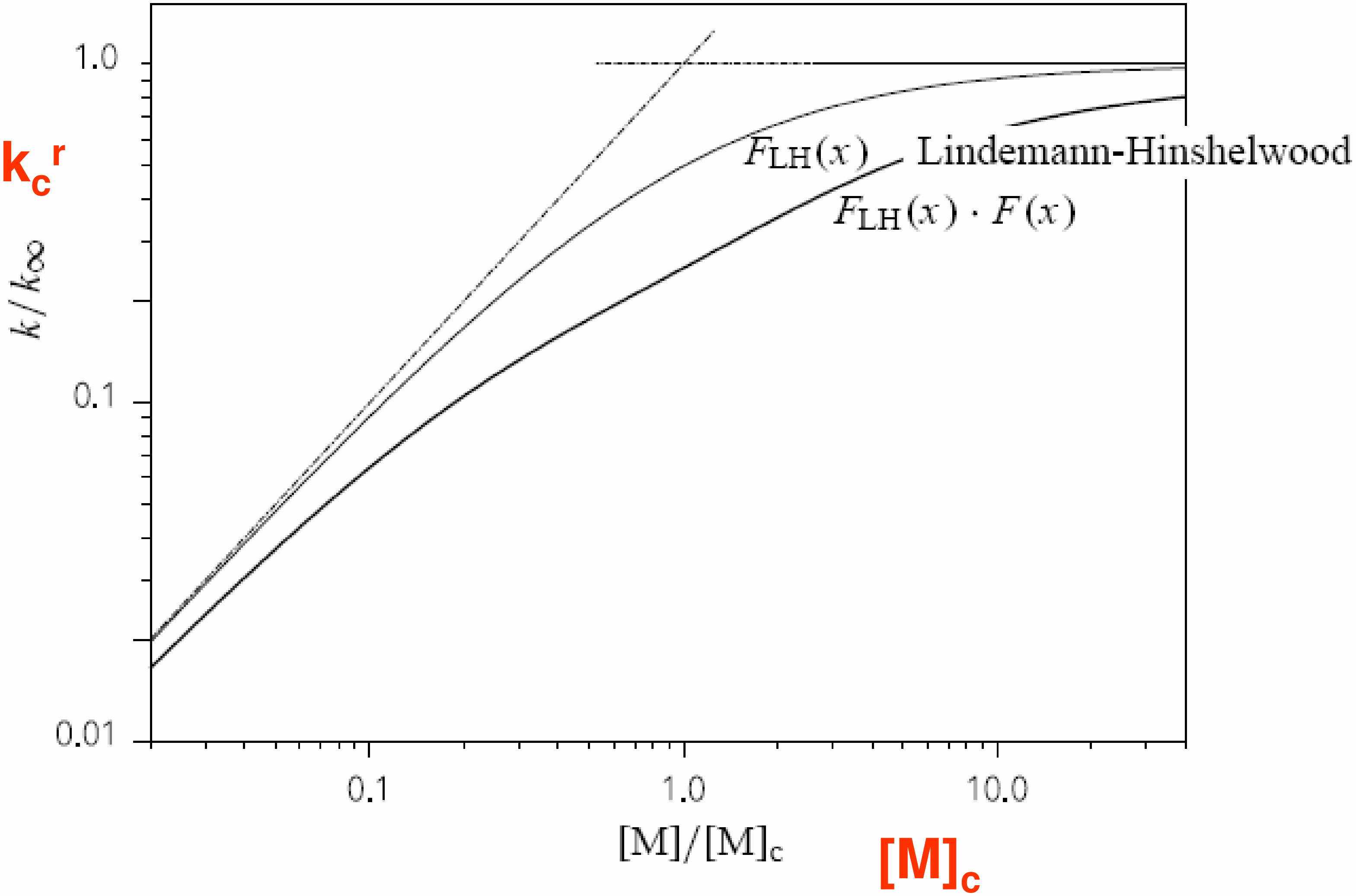
where the excitation reaction is thought to be rate-controlling. At high pressures, [M] → ∞, the other limit is encountered,

$$k^{\mathrm{f}} = \frac{k_0^{\mathrm{f}}}{k_0^{\mathrm{r}}}k_\infty^{\mathrm{f}} \qquad k^{\mathrm{r}} = k_\infty^{\mathrm{r}}$$

k_c^{f} , k_c^{r}

Fall – off Curve in Reduced Quantities

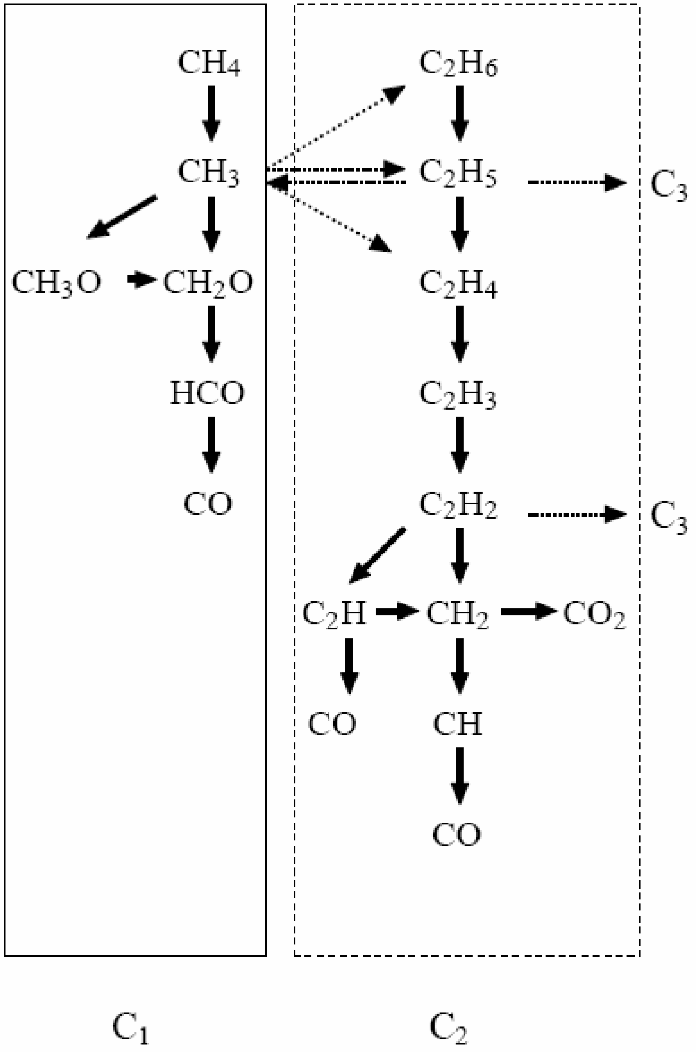
k_c^f , k_c^r



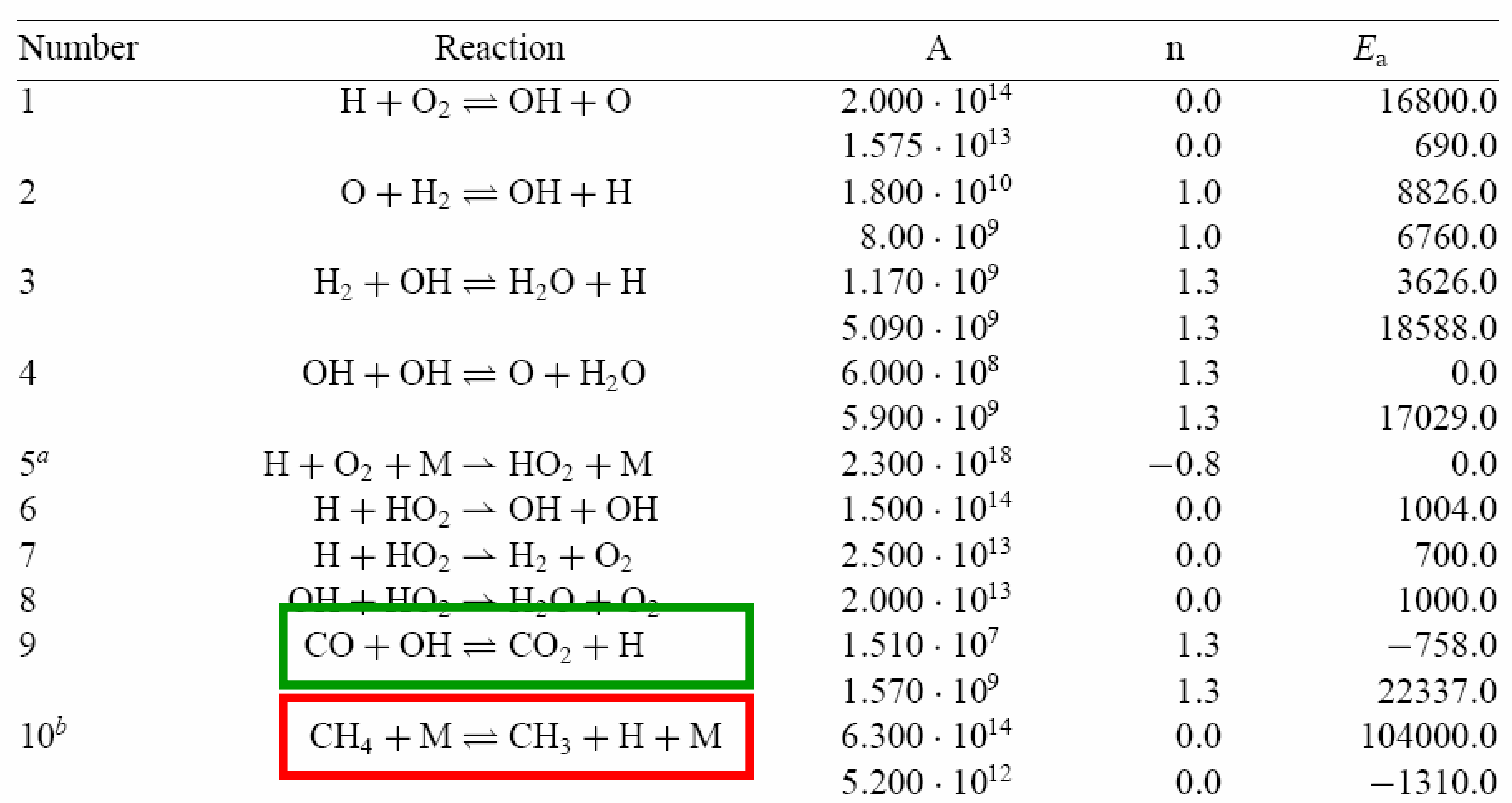
$[M]_c$

Example: Methane – Air Combustion

- The combustion reactions can be grouped in proper chain reactions, identified by progressive numbers: C_1, C_2,…
- However if initial concentration of fuel is not too high, then it is possible to consider only the skeleton chain C_1, involving 25 reactions and 15 species
- Considering both chain C_1 and C_2 involves 210 reactions and 36 species, allowing to consider wider initial conditions



Methane – Air Combustion: r_1 – r_{10} of C_1

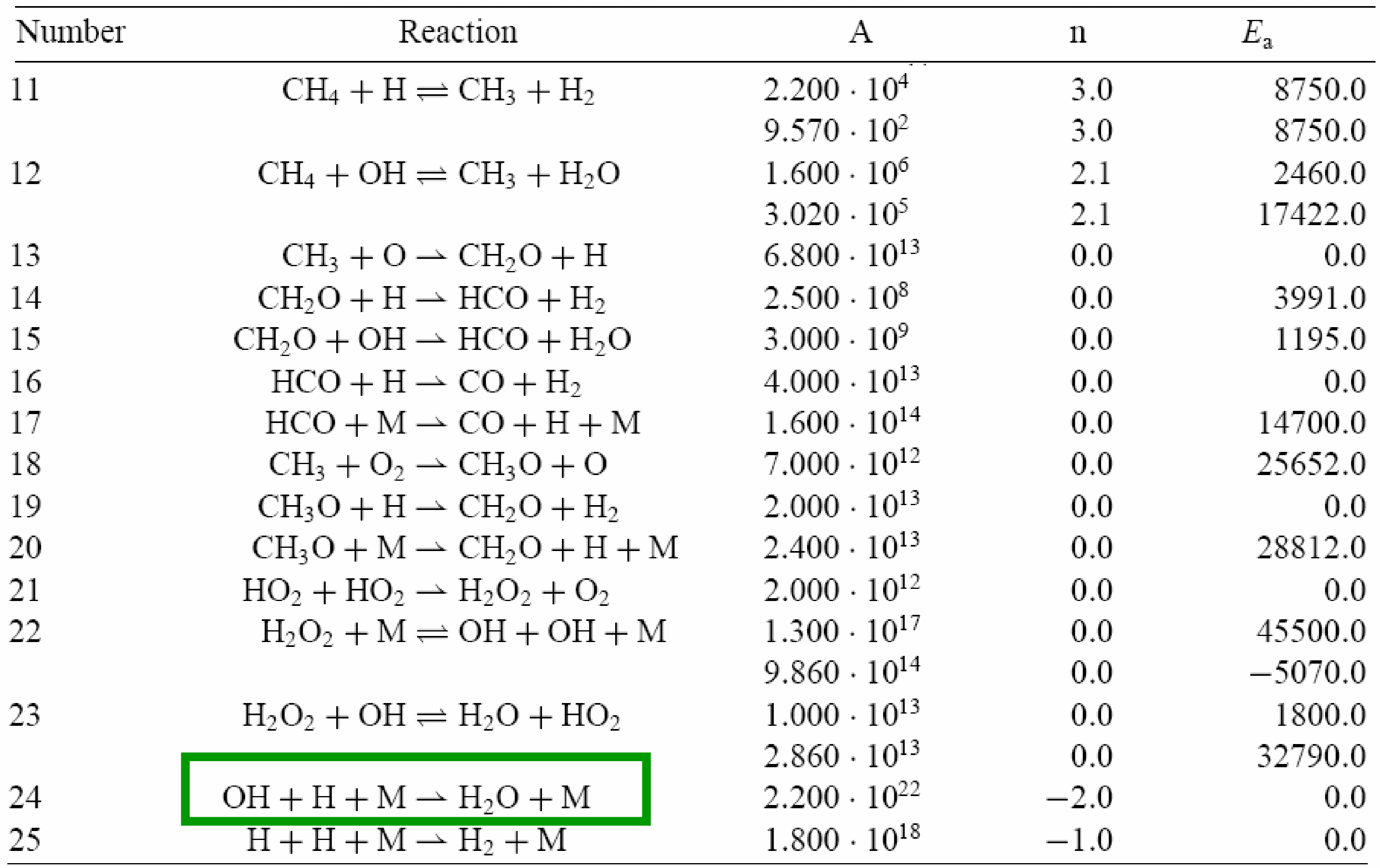


Number	Reaction	A	n	E_a
1	$H + O_2 \rightleftharpoons OH + O$	$2.000 \cdot 10^{14}$	0.0	16800.0
		$1.575 \cdot 10^{13}$	0.0	690.0
2	$O + H_2 \rightleftharpoons OH + H$	$1.800 \cdot 10^{10}$	1.0	8826.0
		$8.00 \cdot 10^{9}$	1.0	6760.0
3	$H_2 + OH \rightleftharpoons H_2O + H$	$1.170 \cdot 10^{9}$	1.3	3626.0
		$5.090 \cdot 10^{9}$	1.3	18588.0
4	$OH + OH \rightleftharpoons O + H_2O$	$6.000 \cdot 10^{8}$	1.3	0.0
		$5.900 \cdot 10^{9}$	1.3	17029.0
5[a]	$H + O_2 + M \rightharpoonup HO_2 + M$	$2.300 \cdot 10^{18}$	−0.8	0.0
6	$H + HO_2 \rightharpoonup OH + OH$	$1.500 \cdot 10^{14}$	0.0	1004.0
7	$H + HO_2 \rightharpoonup H_2 + O_2$	$2.500 \cdot 10^{13}$	0.0	700.0
8	$OH + HO_2 \rightharpoonup H_2O + O_2$	$2.000 \cdot 10^{13}$	0.0	1000.0
9	$CO + OH \rightleftharpoons CO_2 + H$	$1.510 \cdot 10^{7}$	1.3	−758.0
		$1.570 \cdot 10^{9}$	1.3	22337.0
10[b]	$CH_4 + M \rightleftharpoons CH_3 + H + M$	$6.300 \cdot 10^{14}$	0.0	104000.0
		$5.200 \cdot 10^{12}$	0.0	−1310.0

Methane – Air Combustion: Ignition

- The reaction set $\mathbf{r_1} - \mathbf{r_8}$ is the main reaction chain in H_2–O_2 sub-system which is embedded in any hydrocarbon reaction mechanisms
- The reaction $\mathbf{r_{10}}$ is a thermal (T) decomposition reaction and it is the only initiation reaction of the skeletal mechanism → this initiation reaction is of minor importance for concentration profiles, burning velocity and flame temperature in a steady flame → however, it is important to analyze ignition (spark–ignition engines, engine knock, …) → it is a decomposition reaction and this means that is driven by the inert partial pressure (**p**)
- The reaction $\mathbf{r_9}$ is the oxidation of CO in CO_2 and it is quite slow

Methane – Air Combustion: r_{11} – r_{25} of C_1



Number	Reaction	A	n	E_a
11	$CH_4 + H \rightleftharpoons CH_3 + H_2$	$2.200 \cdot 10^{4}$	3.0	8750.0
		$9.570 \cdot 10^{2}$	3.0	8750.0
12	$CH_4 + OH \rightleftharpoons CH_3 + H_2O$	$1.600 \cdot 10^{6}$	2.1	2460.0
		$3.020 \cdot 10^{5}$	2.1	17422.0
13	$CH_3 + O \rightharpoonup CH_2O + H$	$6.800 \cdot 10^{13}$	0.0	0.0
14	$CH_2O + H \rightharpoonup HCO + H_2$	$2.500 \cdot 10^{8}$	0.0	3991.0
15	$CH_2O + OH \rightharpoonup HCO + H_2O$	$3.000 \cdot 10^{9}$	0.0	1195.0
16	$HCO + H \rightharpoonup CO + H_2$	$4.000 \cdot 10^{13}$	0.0	0.0
17	$HCO + M \rightharpoonup CO + H + M$	$1.600 \cdot 10^{14}$	0.0	14700.0
18	$CH_3 + O_2 \rightharpoonup CH_3O + O$	$7.000 \cdot 10^{12}$	0.0	25652.0
19	$CH_3O + H \rightharpoonup CH_2O + H_2$	$2.000 \cdot 10^{13}$	0.0	0.0
20	$CH_3O + M \rightharpoonup CH_2O + H + M$	$2.400 \cdot 10^{13}$	0.0	28812.0
21	$HO_2 + HO_2 \rightharpoonup H_2O_2 + O_2$	$2.000 \cdot 10^{12}$	0.0	0.0
22	$H_2O_2 + M \rightleftharpoons OH + OH + M$	$1.300 \cdot 10^{17}$	0.0	45500.0
		$9.860 \cdot 10^{14}$	0.0	−5070.0
23	$H_2O_2 + OH \rightleftharpoons H_2O + HO_2$	$1.000 \cdot 10^{13}$	0.0	1800.0
		$2.860 \cdot 10^{13}$	0.0	32790.0
24	$OH + H + M \rightharpoonup H_2O + M$	$2.200 \cdot 10^{22}$	−2.0	0.0
25	$H + H + M \rightharpoonup H_2 + M$	$1.800 \cdot 10^{18}$	−1.0	0.0

Methane – Air Combustion: Breakup

- Once initialized, the fuel breakup to carbon – monoxide proceeds via a chain of reactions $\mathbf{r_{11} – r_{20}}$ → this mechanism is claimed to be very fast, which means that every intermediate product is rapidly consumed even at very low concentrations (the final oxidation of CO has been already discussed)
- The total fuel breakup chain in CH_4 flames consumes radicals → the following classification of elementary reactions holds, namely
  - chain – branching reactions: these accounts for a fast increase of the concentration of the radicals O, OH, H;
  - shuffle – or chain – propagating reactions;
  - finally, chain – breaking reactions.

Balance of the Radical Pool

- Chain – branching reactions (the most important is reaction $\mathbf{r_1}$) → they are referred as the radical pool, because, out of the initially present stable species (O_2) and a H radical, it produces two new radicals
- Chain – propagating reactions (overall effect of reactions $\mathbf{r_2} – \mathbf{r_4}$) → the overall effect of these latter three reactions does not lead to an increase in the radical pool but it is merely a conversion of radicals into another
- Chain – breaking reactions ($\mathbf{r_5}$, $\mathbf{r_{24}}$, $\mathbf{r_{25}}$) → the net effect of this reaction set reduces the radical pool because it converts the radicals into stable products and is responsible for the formation of the final products

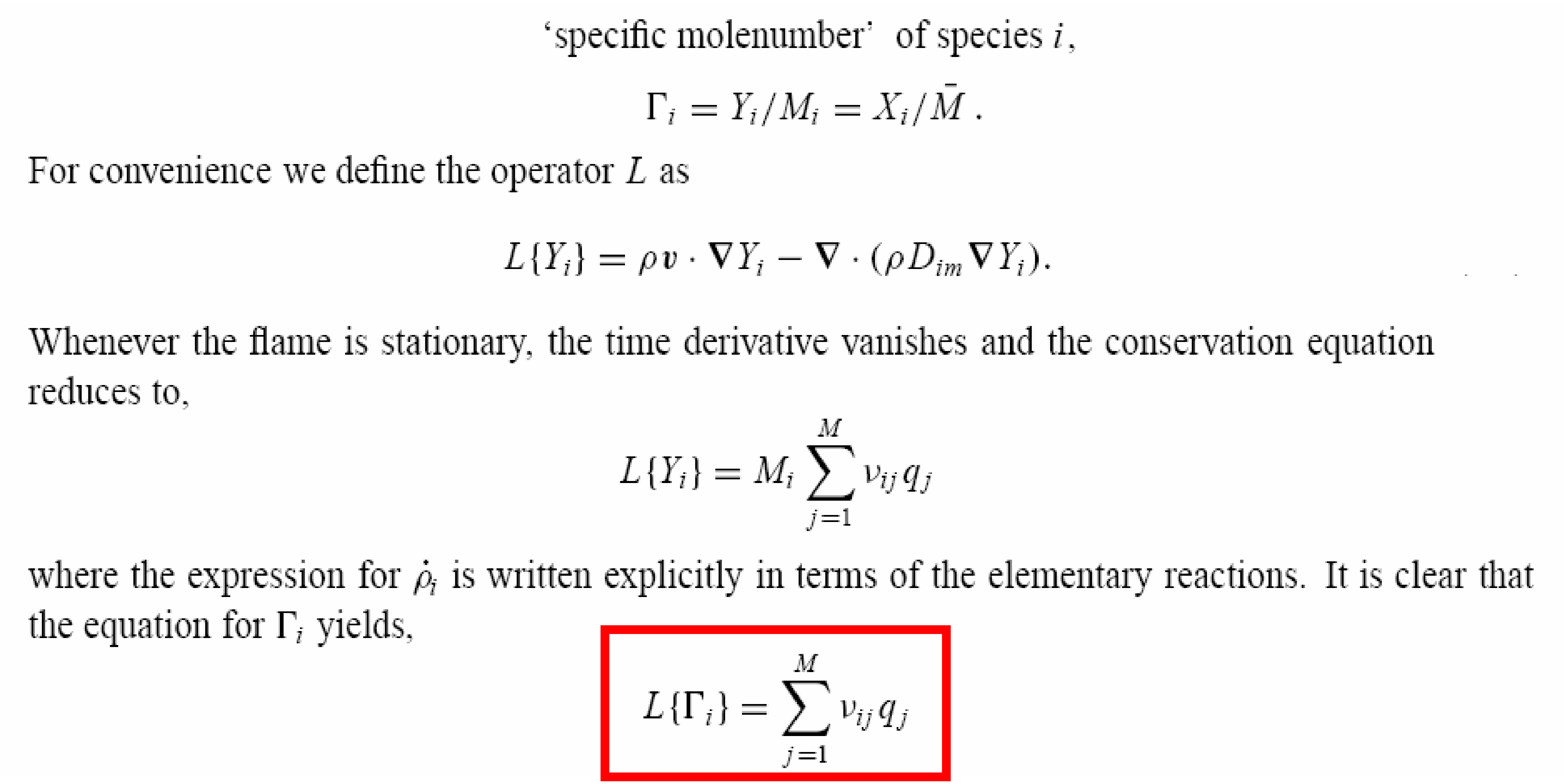
Reduced Chemical Models

- Detailed chemical models are very demanding from the computational point of view → the stiffness present in the governing equations (even in a simple diffusion model like that of Maxwell – Stefan) forces one to consider implicit formulations, solved by means of iterative (Newton–type) methods
- For this reason, two modeling practices are popular in the engineering field:
  - reduction of the problem size;
  - removing the stiffness in the governing equations.
- In order to achieve the previous goals, the systematic reduction techniques are considered, which improve the performance of the old global reaction models

Systematic Reduction Techniques

- Techniques based on global reaction models (GRM) → these models replace the complex chain reactions with an overall reaction, ruled by a generalized Arrhenius–like reaction rate with tunable parameters used for best–fitting the experimental data
- Traditional Systematic Reduction Technique → the idea is to apply the quasi steady–state approximation (QSSA) and/or the partial equilibrium approximation (PEA) to eliminate a number of species in the model and to replace the corresponding PDE equations by algebraic relations
- Mathematical Systematic Reduction Technique → the idea similar to the previous one, but the mathematical algorithm automatically "decides" what species to be eliminated

Compact Notation (Stationary Flame)



'specific molenumber' of species i,

$$\Gamma_i = Y_i/M_i = X_i/\bar{M}\,.$$

For convenience we define the operator L as

$$L\{Y_i\} = \rho \boldsymbol{v} \cdot \nabla Y_i - \nabla \cdot (\rho D_{im} \nabla Y_i).$$

Whenever the flame is stationary, the time derivative vanishes and the conservation equation reduces to,

$$L\{Y_i\} = M_i \sum_{j=1}^{M} \nu_{ij} q_j$$

where the expression for $\dot{\rho}_i$ is written explicitly in terms of the elementary reactions. It is clear that the equation for Γ_i yields,

$$\boxed{L\{\Gamma_i\} = \sum_{j=1}^{M} \nu_{ij} q_j}$$

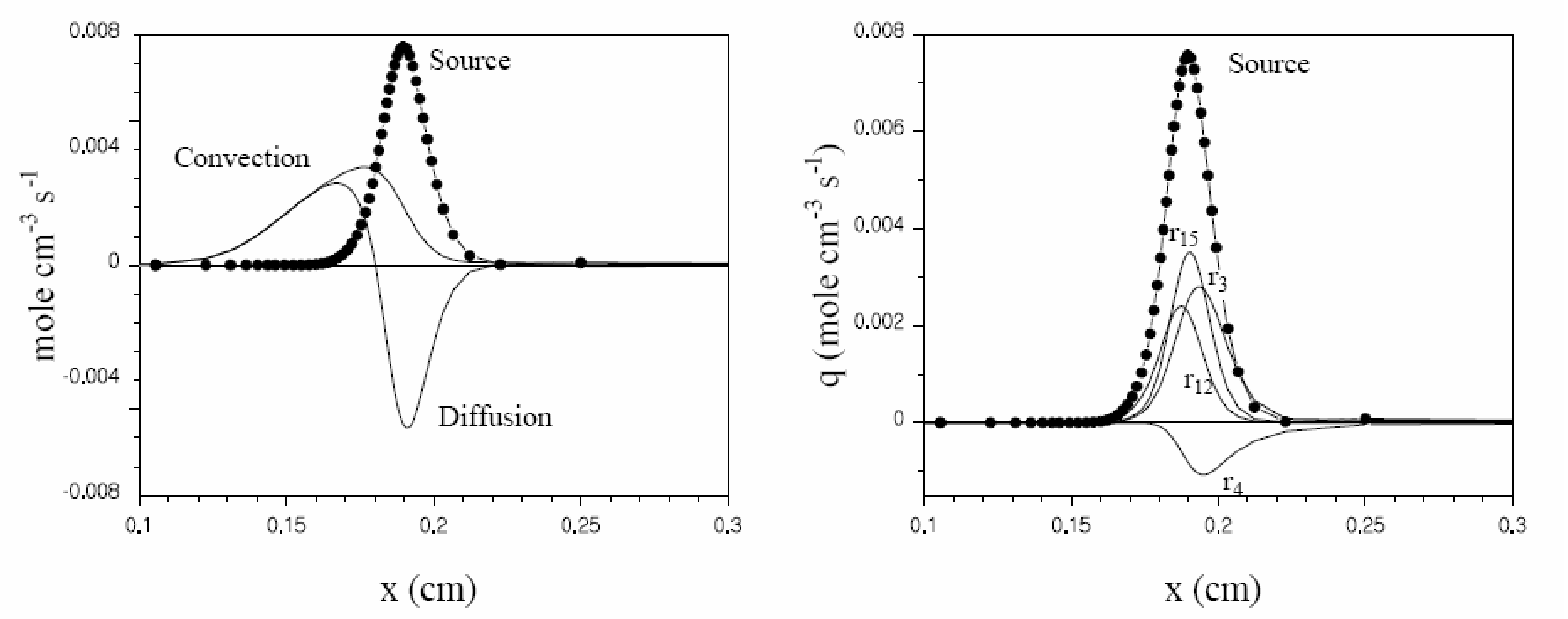
QSS and Partial Equilibrium Approximation

- Quasi steady–state approximation (QSSA) → it simply states that the chemical source for some species is zero, i.e. **$L(\Gamma_i) = 0$**, and it provides an algebraic equation for each species considered to be in steady state (involving many reactions in general)
- Partial equilibrium approximation (PEA) → in contrast with the QSSA, this is an approximation applied to a specific reaction, i.e. **$q_j = 0$**: for this reason, the species involved in such a reaction relate to each through

$$A_1 + A_2 \rightleftharpoons B_1 + B_2$$

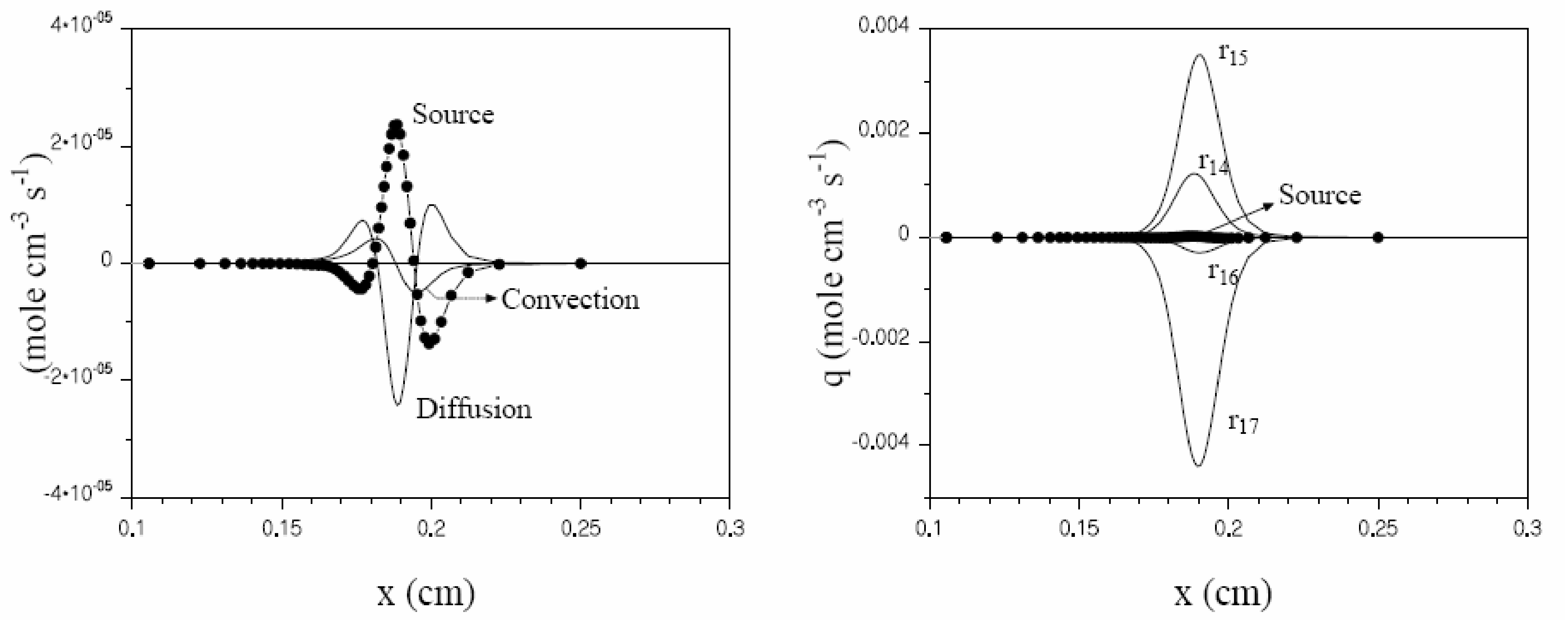
$$q_j = 0 \qquad \frac{[B_1][B_2]}{[A_1][A_2]} = K = \frac{k^{\mathrm{f}}}{k^{\mathrm{r}}}.$$

Non Steady–state Species: H_2O



- It is clear that the contribution of the elementary reactions is comparable to the magnitude of the net reaction rate as well as the magnitude of the convective and diffusive parts

Steady–state Species: HCO



- It is clear that the magnitude of the reaction terms is almost negligible compared to that of the elementary reactions of which it is composed

Selection of Steady–state Species

- It is possible to look at the mole fraction of each species in the flame, in order to decide to which species is possible to apply the steady–state approximation → if the elementary reactions are fast, then every reaction creating a particle is effectively balanced with a reaction consuming it
- In the skeleton chain C_1 model, one has 15 species and 15 PDE equations describing the species dynamics → Considering (for example) 8 species for which the steady–state approximation is acceptable, then the reduced model involves only 15 – 8 = 7 elementary species and (taking into account that 3 conservation conditions hold for single atoms H, C, O) 15 – 8 – 3 = 4 (reduced) elementary reactions

Simplification of the Original Model 1/2

$$\begin{aligned}
L\{\Gamma_{CH_4}\} &= -q_{10} - q_{11} - q_{12} \\
\boxed{0 =} L\{\Gamma_{CH_3}\} &= q_{10} + q_{11} + q_{12} + q_{13} - q_{18} \\
\boxed{0 =} L\{\Gamma_{CH_3O}\} &= q_{18} - q_{19} - q_{20} \\
\boxed{0 =} L\{\Gamma_{CH_2O}\} &= q_{13} - q_{14} - q_{15} + q_{19} + q_{20} \\
\boxed{0 =} L\{\Gamma_{HCO}\} &= q_{14} + q_{15} - q_{16} - q_{17} \\
L\{\Gamma_{CO}\} &= -q_9 + q_{16} + q_{17} \\
L\{\Gamma_{CO_2}\} &= q_9 \\
L\{\Gamma_{H_2}\} &= -q_2 - q_3 + q_7 + q_{11} + q_{14} + q_{16} + q_{19} + q_{25}
\end{aligned}$$

- Which reactions are to be eliminated is arbitrary and does not affect the results of the computation as long as the expressions for the steady–state species are not truncated

Simplification of the Original Model 2/2

$$\begin{aligned}
L\{\Gamma_{\mathrm{H}}\} &= -q_1 + q_2 + q_3 - q_5 - q_6 - q_7 + q_9 + q_{10} - q_{11} + \\
&\quad q_{13} - q_{14} - q_{16} + q_{17} - q_{19} + q_{20} - q_{24} - 2q_{25} \\
L\{\Gamma_{\mathrm{O_2}}\} &= -q_1 - q_5 + q_7 + q_8 - q_{18} + q_{21} \\
\boxed{0 =} L\{\Gamma_{\mathrm{O}}\} &= q_1 - q_2 + q_4 - q_{13} + q_{18} \\
\boxed{0 =} L\{\Gamma_{\mathrm{OH}}\} &= q_1 + q_2 - q_3 - 2q_4 + 2q_6 - q_8 - q_9 - q_{12} - q_{15} + 2q_{22} - q_{23} - q_{24} \\
\boxed{0 =} L\{\Gamma_{\mathrm{HO_2}}\} &= q_5 - q_6 - q_7 - q_8 - 2q_{21} + q_{23} \\
L\{\Gamma_{\mathrm{H_2O}}\} &= q_3 + q_4 + q_8 + q_{12} + q_{15} + q_{23} + q_{24} \\
\boxed{0 =} L\{\Gamma_{\mathrm{H_2O_2}}\} &= q_{21} - q_{22} - q_{23} \\
L\{\Gamma_{\mathrm{N_2}}\} &= 0
\end{aligned}$$

- Once the simplified system of equations is deduced, it is possible to express it in terms of the residual non steady–state species

Reduced Model → 4 Reactions

$$
\begin{aligned}
L\{\Gamma_{CH_4}\} &= -q_{I} \\
L\{\Gamma_{CO}\} &= -q_{II} + q_{I} \\
L\{\Gamma_{CO_2}\} &= q_{II} \\
L\{\Gamma_{H_2}\} &= 4q_{I} + q_{II} + q_{III} - q_{IV} \\
L\{\Gamma_{H}\} &= -2q_{I} - 2q_{III} + 2q_{IV} \\
L\{\Gamma_{O_2}\} &= -q_{IV} \\
L\{\Gamma_{H_2O}\} &= -q_{I} - q_{II} + 2q_{IV}
\end{aligned}
$$

$$
\begin{aligned}
CH_4 + 2H + H_2O &\rightleftharpoons CO + 4H_2 & (r_{I}) \\
CO + H_2O &\rightleftharpoons CO_2 + H_2 & (r_{II}) \\
H + H + M &\rightleftharpoons H_2 + M & (r_{III}) \\
O_2 + 3H_2 &\rightleftharpoons 2H + 2H_2O. & (r_{IV})
\end{aligned}
$$

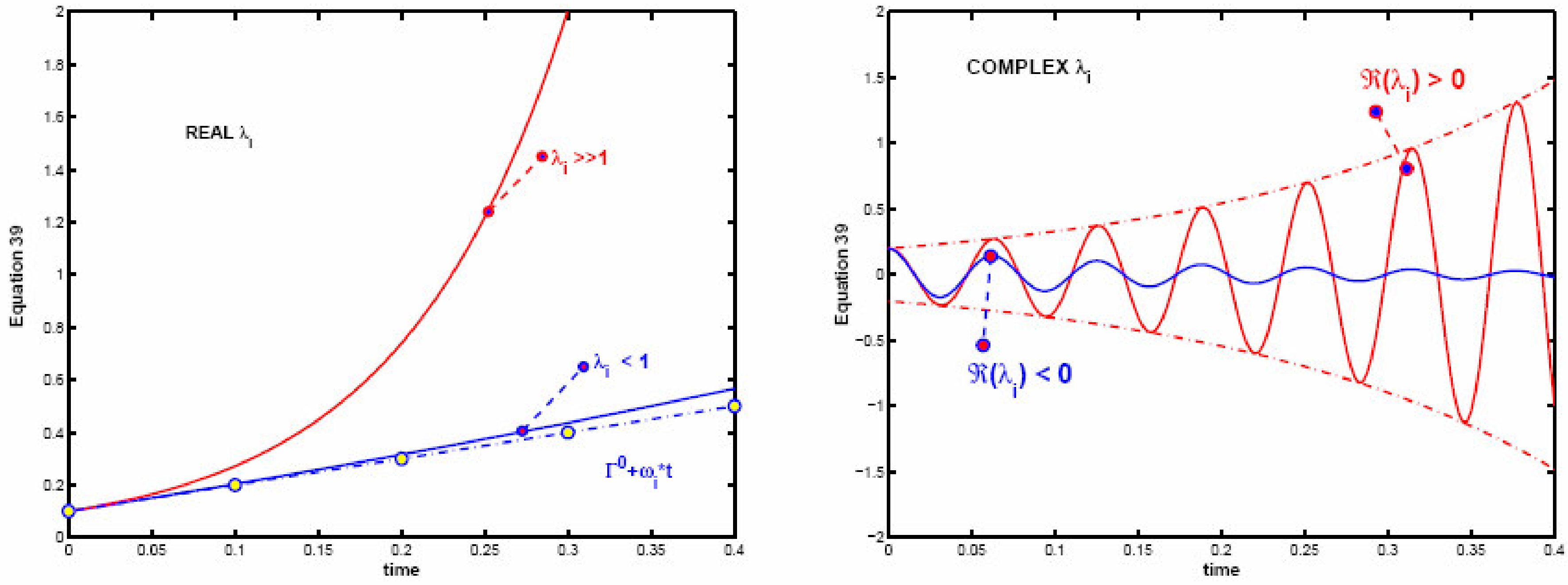
- The global reactions allows one to get some insight in the actual (leading) combustion physics → however, from the computational point of view, the previous set is not closed: in fact, **q_{I}**, **q_{II}**, **q_{III}**, **q_{IV}** depend on both steady–state and non steady–state species → non–linear system must be solved

Truncation of Steady–State Relations

- The simplified expressions for the steady–state species are derived by means of the following assumptions
  - Only the leading reactions are considered;
  - The partial equilibrium approximation (PEA) is applied wherever is possible, in order to get explicit expressions of steady–state species which are functions of non steady–state species.
- The previous simplifications lead to explicit expressions, which are called truncated in order to highlight that the original coupling among all the species has been somehow violated

Mathematical Systematic Reduction

$$\frac{\partial \boldsymbol{\Gamma}}{\partial t} \approx \boldsymbol{w}(\boldsymbol{\Gamma}^0) + \boldsymbol{J}(\boldsymbol{\Gamma} - \boldsymbol{\Gamma}^0).$$



Mathematical Systematic Reduction

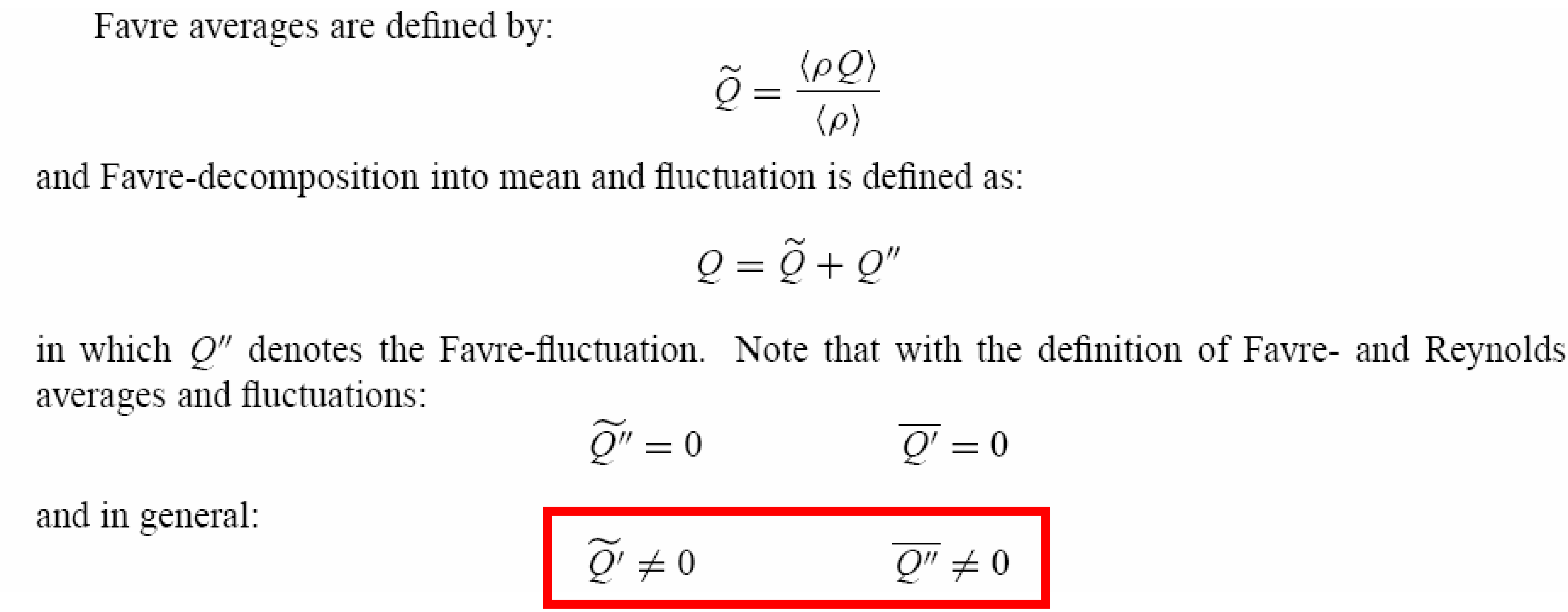
- The larger the eigenvalue the faster the process will be → a process with negative real part of the eigenvalue will extinguish and reach a steady–state: if the imaginary part is large, then this relaxation will be oscillatory → On the other hand, if the real part is positive, then the associated process will not relax to a steady–state
- Hence the fastest time scales pose the best candidates to be reduced, i.e. to be excluded from a detailed analysis which involves the differential operators → in this case, the simplifications is done directly by means of the orthogonal basis in terms of eigenvalues and eigenvectors: this is quite general and it can be adaptively tuned according to the solved reactive flow

Turbulent Combustion

- The combination of non–linear fluid dynamics with complex non–linear kinetics causes very complex phenomena
- Combustion in laminar flames is already complex due to combination of complex diffusion properties and complex kinetics with a wide range of chemical time and length scales → turbulence adds to this the complexity of a wide range of time and length scales in flow phenomena
- Essentially the simplified models distinguish between
  - turbulent premixed flames
  - turbulent non–premixed flames (also celled diffusion flames);
  - spray flames

Reynolds vs. Favre Averaging

- In turbulent flames, density fluctuations can have large effects on the turbulence flow field → to simplify the equations describing variable density flow it is common to use density–averaged (Favre) averaging



Favre averages are defined by:

$$\widetilde{Q} = \frac{\langle \rho Q \rangle}{\langle \rho \rangle}$$

and Favre-decomposition into mean and fluctuation is defined as:

$$Q = \widetilde{Q} + Q''$$

in which Q'' denotes the Favre-fluctuation. Note that with the definition of Favre- and Reynolds averages and fluctuations:

$$\widetilde{Q''} = 0 \qquad \overline{Q'} = 0$$

and in general:

$$\boxed{\widetilde{Q'} \neq 0 \qquad \overline{Q''} \neq 0}$$

Closure Problem

$$\langle\rho\rangle \frac{\mathrm{D}}{\mathrm{D}t}\widetilde{\phi}_\alpha = -\frac{\partial}{\partial x_j}\langle J_j^\alpha\rangle \boxed{+ \langle\rho\rangle\widetilde{S}_\alpha - \frac{\partial}{\partial x_j}\langle\rho\rangle\widetilde{u_j''\phi_\alpha''}}$$

- Because of the highly non–linear behavior of the chemical source term, the average value can not be expressed accurately as a function of the scalar mean and variance → the development of better models for closing the means chemical reaction rate has proceed along different lines for the cases with
  - **premixed reactants**: propagation is essential and a model for chemical conversion at the flame front is needed (or at least a correlation for the flame speed)
  - and **non–premixed reactants**: mixing is essential and to describe a non–reacting scalar (mixture fraction Z) is sufficient

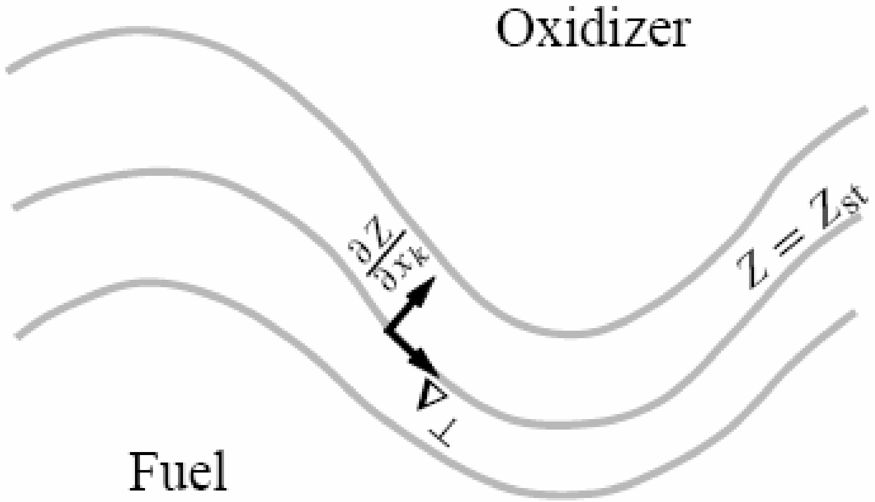
Premixed Reactants

- Turbulence increases the area of the flame front (wrinkling) and also modifies the flame front (both stretch and curvature) → correlations have been developed for the relation between turbulence intensity and conversion enhancement factor → the model categories exist
  - flamelet models: they relay on the presence of a clearly defined and relatively thin flame front; at first the substructure of the flame front is disregarded or estimated by a separate laminar flame calculation (Bray–Moss–Libby model, flame surface model, G–equation model)
  - (Probability Density Function) PDF models: they compute the mean source term exactly as function of the PDF of concentrations; usually a form of the PDF is assumed and it is expressed as function of the lower moments (mean, variance, co–variance)

Non–premixed Reactants

- More variety exists in non–premixed combustion → the mixture fraction **Z** satisfies a transport equation without chemical source term →in the limit of fast reactions, the mixture fraction together with a fast chemistry model completely defines the state of the system
  - mixed–is–burnt model: infinitely fast irreversible global reaction of fuel and oxidizer to products; intermediate species not included
  - chemical equilibrium model: considers the intermediate species, but assumes that the reactions are always fast enough to reach full chemical equilibrium
  - laminar flamelet model: the local state of the mixture in the flame front is assumed to be the same as that in a laminar diffusion flame; the deviation from chemical equilibrium is taken into account by the balance between diffusion processes and finite reaction rate

Modeling Mixture Fraction

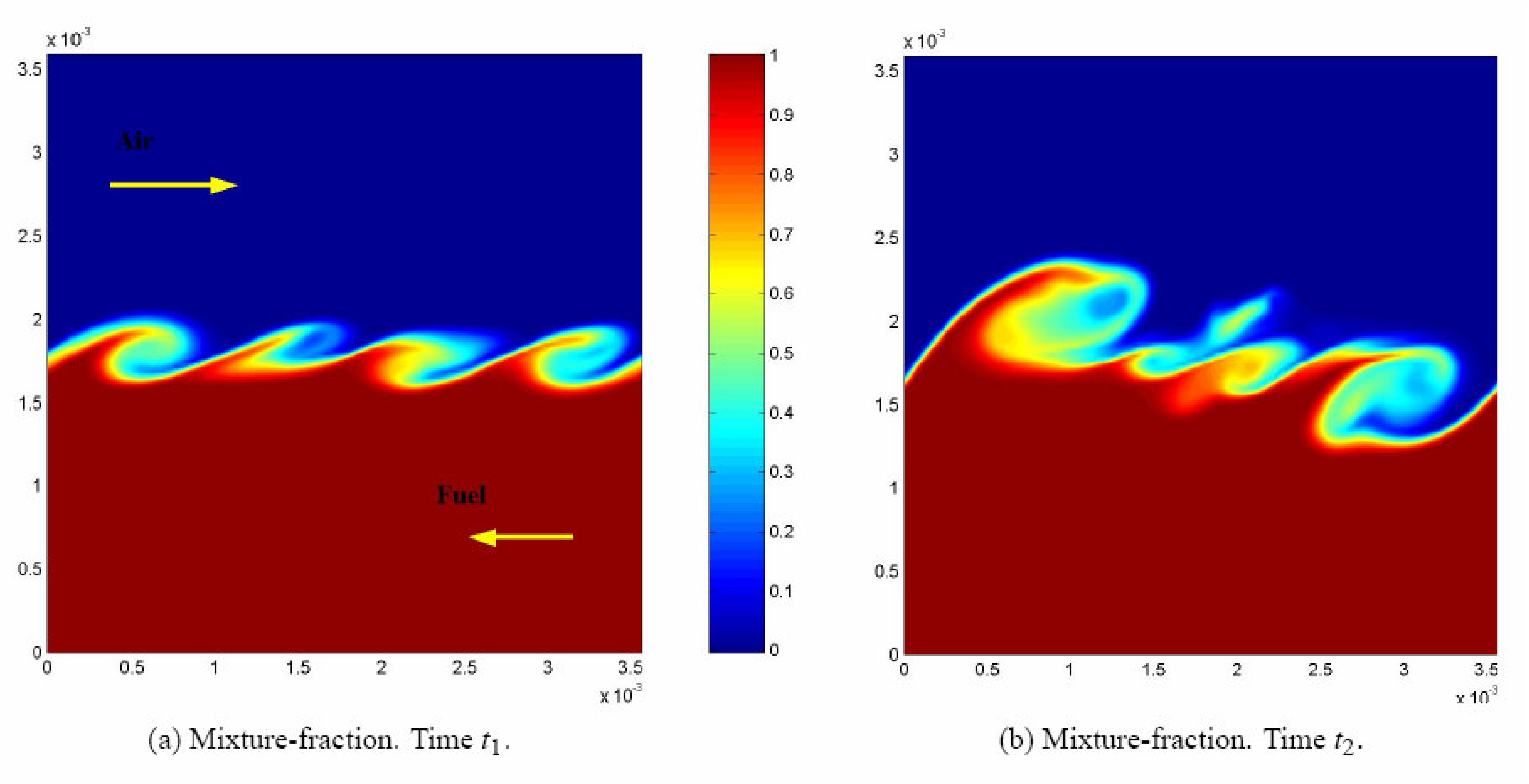


$$Z = \frac{\nu Y_{\mathrm{fu}} - Y_{\mathrm{ox}} + Y_{\mathrm{ox},2}}{\nu Y_{\mathrm{fu},1} + Y_{\mathrm{ox},2}}$$

$$\frac{\partial \rho Z}{\partial t} + \nabla \cdot (\rho \vec{v} Z) = \nabla \cdot \left(\frac{1}{\boxed{Le}} \frac{\lambda}{c_p} \nabla Z \right)$$

Lewis Number

Flamelet Modeling in Non–premixed Flows



(a) Mixture-fraction. Time t_1.

(b) Mixture-fraction. Time t_2.

Summary

- Multicomponent modeling may involve large computational demand but nowadays it relies on well–developed models (Maxwell–Stefan model), which allow one to take into account even non–conventional mass transport phenomena
- Combustion modeling is still a challenging task (at least in most of the practical engineering applications): in particular, the problem for turbulent reacting flows is that different time and length scales exist due to both complex fluid flow and complex chemistry, which interact each other according to the considered combustion regime

Further Readings

- R. Taylor, R. Krishna, Multicomponent Mass Transfer, John Wiley & Sons, 1993.
- C. K. Law, Combustion Physics, Cambridge University Press, 2006.
- Course on Combustion (including notes) by Eindhoven University of Technology: http://www.combustion.tue.nl/course

Acknowledgements

Prof. M. C. Annesini – Dipartimento di Ingegneria Chimica, Università degli Studi di Roma “La Sapienza”, Italy.

Prof. L. P. H. de Goey, Prof. L. M. T. Somers – Department of Mechanical Engineering, Eindhoven University of Technology, NL.