Turbulent Combustion Modeling

Combustion Summer School

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Course Overview

Part II: Turbulent Combustion

- Turbulence
- Turbulent Premixed Combustion
- Turbulent Non-Premixed Combustion
- Turbulent Combustion Modeling
- Applications

- Moment Methods for reactive scalars
- Simple Models in Fluent: EBU,EDM, FRCM, EDM/FRCM
- Introduction in Statistical Methods: PDF, CDF,…
- Transported PDF Model
- Modeling Turbulent Premixed Combustion
  - BML-Model
  - Level Set Approach/G-equation
- Modeling Turbulent Non-Premixed Combustion
  - Conserved Scalar Based Models for Non-Premixed Turbulent Combustion
  - Flamelet-Model
  - Application: RIF, steady flamelet model

Balance Equation for Reactive Scalars

- The term „reactive scalar“
  - Mass fraction Y_α of all components $\alpha = 1, \ldots N$
  - Temperature T

$$\psi_i = (Y_1, Y_2, \ldots Y_N, T)^{\mathrm{T}}$$

- Balance equation for $\psi_i,\ i = 1, \ldots N+1$

[redacted]

  - D_i: mass diffusivity, thermal diffusivity
  - S_i: mass/temperature source term

Balance Equation for Reactive Scalars

- Neglecting the molecular transport (assumption: *Re*↑)
- Gradient transport assumption for the turbulent transport

$$-\widetilde{u_j''\psi_i''} = D_\mathrm{t}\frac{\partial\widetilde{\psi}_i}{\partial x_j}, \quad \text{mit} \quad D_\mathrm{t} = \frac{\nu_\mathrm{t}}{Sc_\mathrm{t}}$$

→ Averaged transport equation

not closed

[redacted]

→ Simplest possible approach:

Express unclosed terms as a function of mean values

Moment Methods for Reactive Scalars: Error Estimation

- Assumption: heat release expressed by

$$\omega_T = \rho S_T(T) = \rho B(T_\mathrm{b} - T)\exp\left(-\frac{E}{\mathcal{R}T}\right)$$

  - B: includes frequency factor und heat of reaction
  - T_b: adiabatic flame temperature
  - E: activation energy

- Approach for modeling the chemical source term

[redacted]

- Proven method → Decomposition into mean and fluctuation

$$T = \widetilde{T} + T''$$

Moment Methods for Reactive Scalars: Error Estimation

- Taylor expansion at $T \approx \widetilde{T}$ (for [redacted]) of terms

$$\widetilde{S}_T(T) = B(T_\mathrm{b} - T)\,\exp\left(-\frac{E}{\mathcal{R}T}\right)$$

  - Pre-exponential term

$$(T_\mathrm{b} - T)\Big|_{T\approx\widetilde{T}} \approx T_\mathrm{b} - \widetilde{T} - T''$$

  - Exponential term

$$-\frac{E}{\mathcal{R}T}\bigg|_{T\approx\widetilde{T}} \approx -\frac{E}{\mathcal{R}}\left[\frac{1}{\widetilde{T}} - \frac{1}{\widetilde{T}^2}\left(T - \widetilde{T}\right)\right]\bigg|_{\widetilde{T}+T''} = -\frac{E}{\mathcal{R}\widetilde{T}} + \frac{ET''}{\mathcal{R}\widetilde{T}^2}$$

- Leads to

$$\widetilde{S}_T(T)\Big|_{T\approx\widetilde{T}} \approx B\left(T_\mathrm{b} - \widetilde{T} - T''\right)\exp\left(-\frac{E}{\mathcal{R}\widetilde{T}}\right)\exp\left(\frac{ET''}{\mathcal{R}\widetilde{T}^2}\right)$$

Moment Methods for Reactive Scalars: Error Estimation

- As a function of Favre-mean at $\widetilde{T}$

$$\widetilde{S}_T\left(\widetilde{T}\right) = B\left(T_\mathrm{b} - \widetilde{T}\right) \exp\left(-\frac{E}{\mathcal{R}\widetilde{T}}\right)$$

yields

$$\boxed{\widetilde{S}_T(T) = \widetilde{S}_T(\widetilde{T}) \left(1 - \frac{T''}{T_\mathrm{b} - \widetilde{T}}\right) \exp\left(\frac{ET''}{\mathcal{R}\widetilde{T}^2}\right)}$$

- Typical values in the reaction zone of a flame

$$\frac{E}{\mathcal{R}\widetilde{T}} = \mathcal{O}(10) \quad \text{und} \quad 0{,}1 \leq \left|\frac{T''}{\widetilde{T}}\right| \leq 0{,}3$$

- Error around a factor of 10!
- Moment method for reactive scalars inappropriate due to strong non-linear effect of the chemical source term

Example: Non-Premixed Combustion in Isotropic Turbulence

- Favre averaged transport equation

[redacted]

- Gradient transport model

$$\left(\widetilde{u_j Y_\alpha} - \tilde{u}_j \tilde{Y}_\alpha\right) = -D_\mathrm{t} \frac{\partial \tilde{Y}_\alpha}{\partial x_j}$$

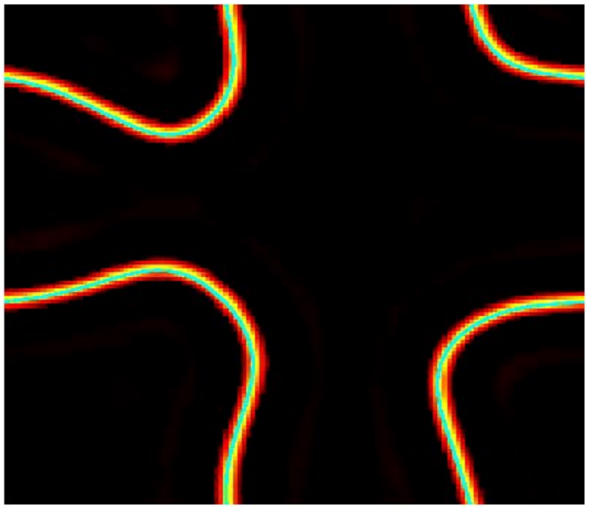
- One step global reaction

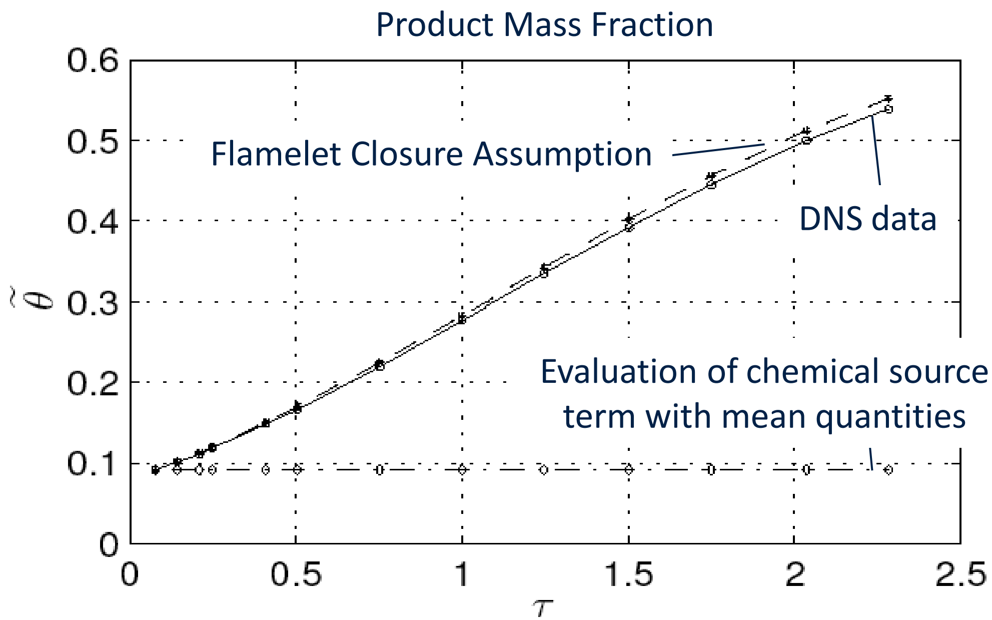
$$\widetilde{\dot{m}_\alpha'''} = M_\alpha \frac{\rho^2}{M_\mathrm{F} M_\mathrm{O}} Y_\mathrm{F} Y_\mathrm{O}\, A \,\exp\left(-\frac{E}{\mathcal{R} T}\right)$$

- Decaying isotropic turbulence

$$\frac{\partial \bar{\rho} \tilde{Y}_\alpha}{\partial t} = \widetilde{\dot{m}_\alpha'''}$$

Example: Non-Premixed Combustion in Isotropic Turbulence





→ Closure by mean values does not work!

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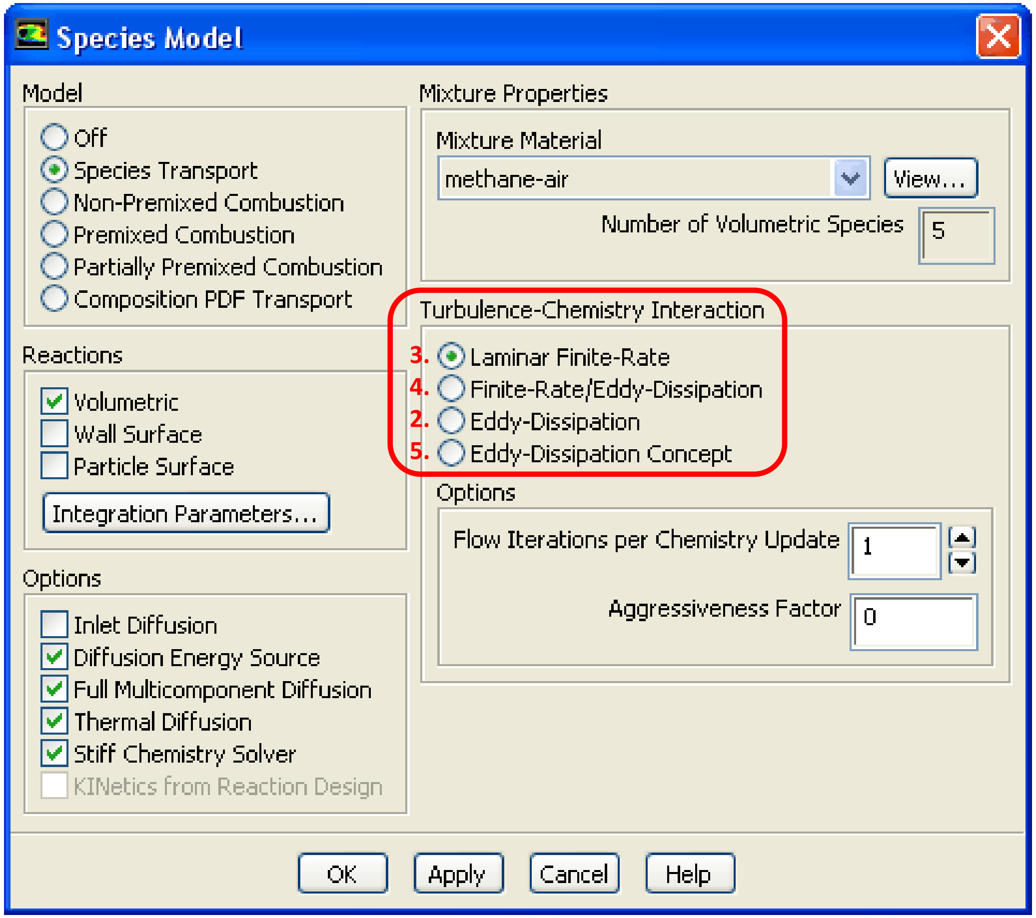
Simple Models for Turbulent Combustion

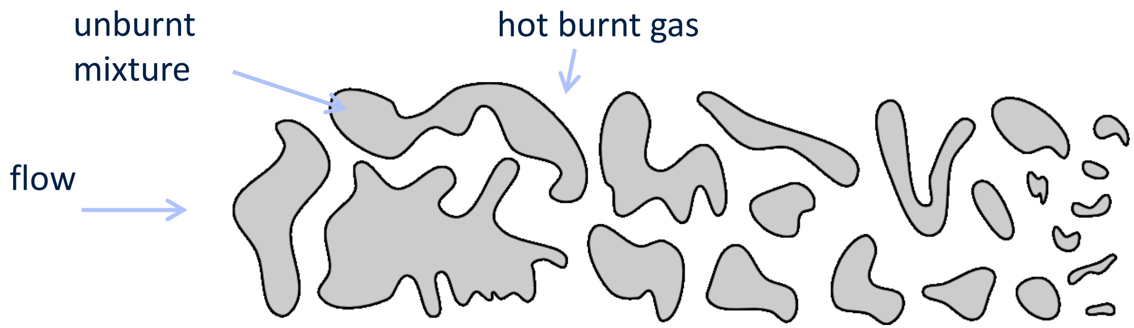
- Example: standard models in Fluent
- Very simple models, e.g. based on
  - very fast chemistry
  - no consideration of turbulence



Quelle: Fluent 12 user's guide

1. Eddy-Break-Up-Model

First approach for closing the chemical source term was made by Spalding (1971) in premixed combustion



- Assumption: very fast chemistry (after pre-heating)
- Combustion process
  - Breakup of eddies from the unburnt mixture → smaller eddies

  → Large surface area (with hot burnt gas)

  → Duration of this breakup determines the pace

→ Eddy-Break-Up-Model (EBU)

1. Eddy-Break-Up-Modell

- Averaged turbulent reaction rate for the products

$$\overline{\omega}_{\mathrm{P}} = \rho C_{\mathrm{EBU}} \frac{\varepsilon}{k} \left(\overline{Y_{\mathrm{P}}''^2} \right)^{1/2}$$

  - $\overline{Y_{\mathrm{P}}''^2}$: variance of mass fraction of the product
  - C_{EBU}: Eddy-Break-Up constant
- EBU-modell
  - turbulent mixing sufficiently describes the combustion process
  - chemical reaction rate is negligible
- Problems with EGR, lean/rich combustion

→ Further development by Magnussen & Hjertager (1977): Eddy-Dissipation-Model (EDM)…

2. Eddy-Dissipation-Model

- EDM: typical model for eddy breakup
  - Assumption: very fast chemistry
  - Turbulent mixing time is the dominant time scale

$$\widetilde{S}_i \sim \tau^{-1} = \frac{\widetilde{\varepsilon}}{\widetilde{k}}$$

- Chemical source term

$$\widetilde{S}_i = A\,\nu_i' M_i\,\frac{\widetilde{\varepsilon}}{\widetilde{k}}\,\mathrm{min}\left(\frac{\widetilde{Y}_E}{\nu_E' M_E}, B\frac{\sum \widetilde{Y}_P}{\sum \nu_P'' M_P}\right)$$

  - Y_E, Y_P: mass fraction of reactant/product
  - A, B: Model parameter (determined by experiment)

2. Eddy-Dissipation-Model

Example: diffusion flame, one step reaction

$$\boxed{\nu'_F \mathrm{F} + \nu'_O \mathrm{O} \rightarrow \nu''_P \mathrm{P}}$$

- $Y_F > Y_{F,st}$, therefore $Y_O < Y_F \rightarrow Y_E = Y_O$

$$\widetilde{S}_F = A\, \nu'_F M_F \frac{\widetilde{\varepsilon}}{\widetilde{k}} \frac{\widetilde{Y}_O}{\nu'_O M_O} = A \frac{\widetilde{\varepsilon}}{\widetilde{k}} \widetilde{Y}_{F,st}$$

- $Y_F < Y_{F,st} \rightarrow Y_E = Y_F$

$$\widetilde{S}_F = A\, \nu'_F M_F \frac{\widetilde{\varepsilon}}{\widetilde{k}} \frac{\widetilde{Y}_F}{\nu'_F M_F} = A \frac{\widetilde{\varepsilon}}{\widetilde{k}} \widetilde{Y}_F$$

Summary EDM

- Controlled by mixing
- Very fast chemistry
- Application: turbulent premixed and nonpremixed combustion
- Connects turbulent mixing with chemical reaction
  - rich or lean?

  → full or partial conversion
- Advantage: simple and robust model
- Disadvantage
  - No effects of chemical non-equilibrium (formation of NO, local extinction)
  - Areas of finite-rate chemistry:
    - Fuel consumption is overestimated
    - Locally too high temperatures

3. Finite-Rate-Chemistry-Model (FRCM)

- Chemical conversion with finite-rate
- Capable of reverse reactions
- Chemical source term for species *i* in a reaction *α*

$$\widetilde{S}_{i,\alpha} = \widetilde{\Gamma} M_i (\nu''_{i,\alpha} - \nu'_{i,\alpha}) \left(k_{f,\alpha} \prod_i \left[\frac{\overline{\rho}\widetilde{Y}_i}{M_i} \right]^{\nu'_{i,\alpha}} - k_{b,\alpha} \prod_i \left[\frac{\overline{\rho}\widetilde{Y}_i}{M_i} \right]^{\nu''_{i,\alpha}} \right)$$

  - $k_{f,\alpha}$, $k_{b,\alpha}$: reaction rates(determined by Arrhenius kinetic expressions → $f(\widetilde{T})$)
  - $\widetilde{\Gamma}$ models the influence of third bodies

$$\widetilde{\Gamma} = \sum \gamma_{i,\alpha} \frac{\overline{\rho}\widetilde{Y}_i}{M_i}$$

- Linearization of the source term centered on the operating point
  → Integration into equations for species, larger Δt realizable
- Typical approach for detailed computation of homogeneous systems

Summary FRCM

- Chemistry-controlled
- Appropriate for $t_{\text{chemistry}} > t_{\text{mixng}}$ (laminar/laminar-turbulent)
- Application
  - Laminar-turbulent
  - Non-premixed
- Source term: Arrhenius ansatz
  - Mean values for temperature in Arrhenius expression
  - → Effects of turbulent fluctuations are ignored
  - → Temperature locally too low
- Consideration of non-equilibrium effects

4. Combination EDM/FRCM

- Turbulent flow
  - Areas with high turbulence and intense mixing
  - Laminar structures
- Concept: Combination of EDM and FRCM
  - For each cell: computation of both reaction rates r_i^{EDM} and r_i^{FRCM}
  - The smaller one is picked (determines the reaction rate)

$$r_i = \min\left(r_i^{\text{EDM}}, r_i^{\text{FRCM}}\right)$$

→ Chooses locally between chemistry- and mixing-controlled

- Advantage: Meant for large range of applicability
- Disadvantage: no turbulence/chemistry interaction

5. Eddy-Dissipation-Concept (EDC)

- Extension of EDM → Considers detailed reaction kinetics
- Assumption: Reactions on small scales („*“: fine scale)

$$\xi^* = C_\xi \left(\frac{\nu\widetilde{\varepsilon}}{\widetilde{k}^2}\right)^{1/4}$$

Fluent: C_ξ = 2,1377

- Volume of small scales: ${\xi^*}^3$
- Reaction rates are determined by Arrhenius expression (cf. FRCM)
- Time scale of the reactions

$$\tau^* = C_\tau \left(\frac{\nu}{\widetilde{\varepsilon}}\right)^{1/2}$$

Fluent: C_τ = 0,4082

5. Eddy-Dissipation-Concept (EDC)

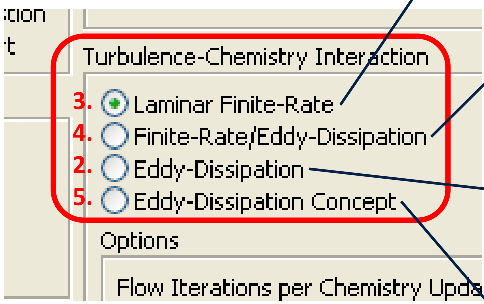
- Boundary/initial conditions for reactions (on small scales)
  - Assumption: pressure p = const.
  - Initial condition: temperature and species concentration in a cell
  - Reactions on time scale τ^*
  - Numerical integration (e.g. ISAT-Algorithm) → $\widetilde{Y_i^*}$
- Model for source term

$$\widetilde{S}_i = \frac{{\xi^*}^2}{\tau^*[1 - {\xi^*}^3]}(\widetilde{Y_i^*} - \widetilde{Y}_i)$$

Mass fraction on small scales of species *i* after reaction time τ^*

- Problem:
  - Requires a lot of processing power
  - Stiff differential equation

Summary: Simple Combustion Models



Quelle: Fluent 12 user's guide

Solely calculation by Arrhenius equation
→ turbulence is not considered

Calculation of Arrhenius reaction rate and mixing rate; selection of the smaller one
→ local choice: laminar/turbulent

Solely calculation of mixing rate
→ Chemical kinetic is not considered

Modeling of turbulence/chemistry interaction; detailed chemistry

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Introduction to Statistical Methods

- Introduction to statistical methods
  - Sample space
  - Probability
  - Cumulative distribution function(CDF)
  - Probability density function(PDF)
  - Examples for CDFs/PDFs
  - Moments of a PDF
  - Joint statistics
  - Conditional statistics

Pope, „Turbulent Flows“

Sample Space

- Probability of events in sample space

- Sample space: set of all possible events
  - Random variable U
  - Sample space variable V (independent variable)
- Event A

$$A = \{U < V_a\}$$

- Event B

$$B = \{V_a \leq U < V_b\}$$

Probability

- Probability of the event $A = \{U < V_a\}$

$$p = P(\mathrm{A}) = P\{U < V_a\}$$

- Probability p

[redacted]

impossible event

sure event

Cumulative Distribution Function (CDF)

- Probability of any event can be determined from cumulative distribution function (CDF)

$$F(V) = P\{U < V\}$$

- Event A

$$A = \{U < V_a\}$$

$$P(A) = P\{U < V_a\} = F(V_a)$$

- Event B

$$B = \{V_a \le U < V_b\}$$

$$\begin{aligned} P(B) &= P\{V_a \le U < V_b\} \\ &= P\{U < V_b\} - P\{U < V_a\} \\ &= F(V_b) - F(V_a) \end{aligned}$$

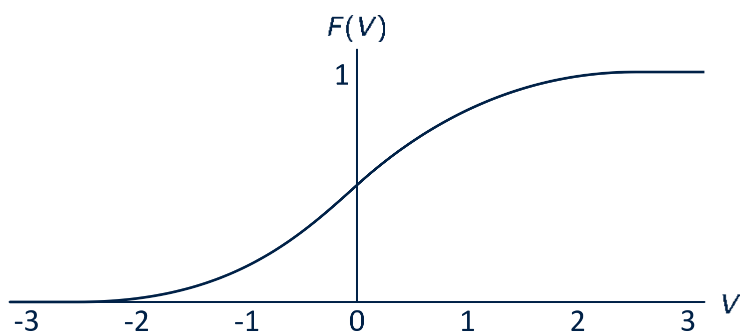
Cumulative Distribution Function (CDF)

- Three basic properties of a CDF
  1. Occuring of event $\{U < -\infty\}$ is impossible → $F(-\infty) = 0$
  2. Occuring of event $\{U < +\infty\}$ is sure → $F(+\infty) = 1$
  3. *F* is a non-decreasing function

$$F(V_b) \geq F(V_a) \quad \text{für} \quad V_b > V_a$$

as

$$F(V_b) - F(V_a) = P\{V_a \leq U < V_b\} \geq 0$$

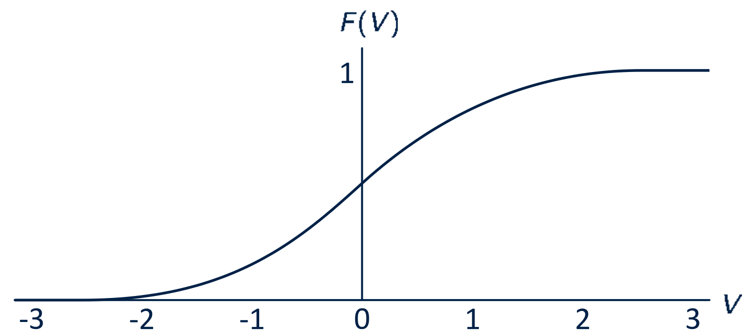


CDF of Gaussian distributed random variable

Probability Density Function (PDF)

- Derivative of the CDF → probability density function

$$f(V) = \frac{\mathrm{d}F(V)}{\mathrm{d}V}$$

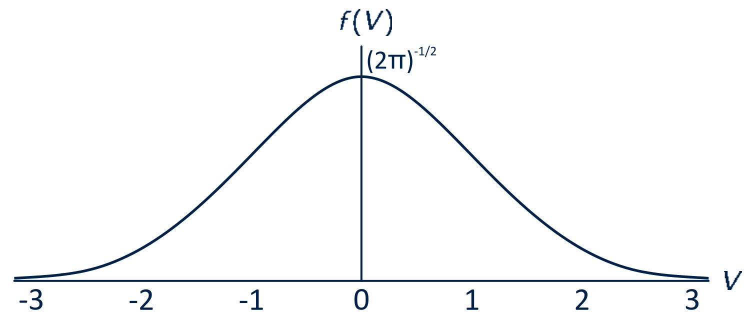


- Three basic properties of a PDF
  1. CDF non-decreasing
     → PDF $f(V) \geq 0$
  2. Satisfies the normalization condition

$$\int_{-\infty}^{\infty} f(V)\mathrm{d}V = 1$$

  3. For infinite sample space variable

[redacted]

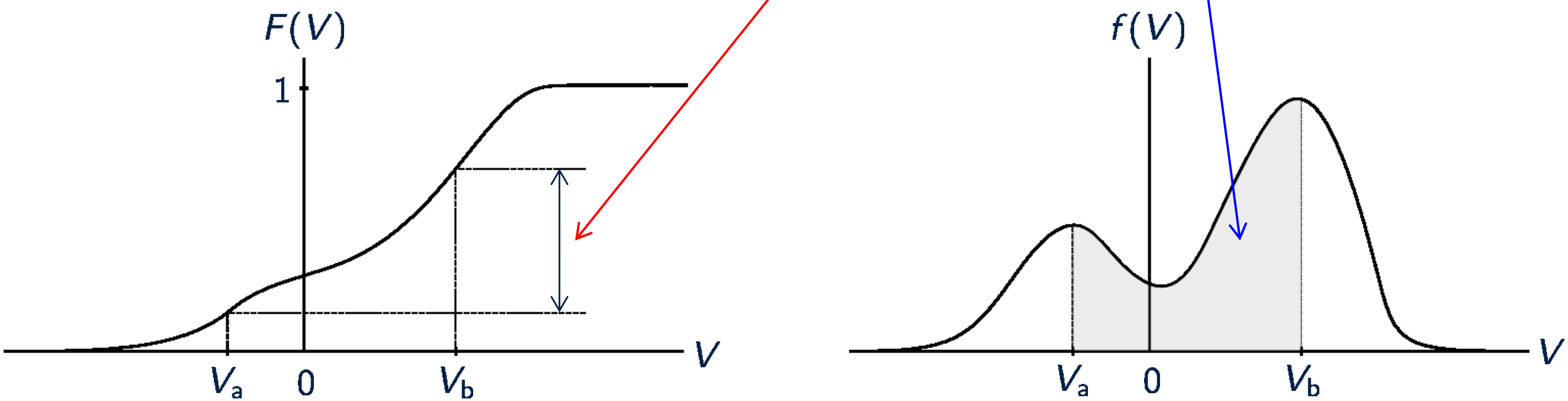


PDF of Gaussian distributed random variable

Probability Density Function (PDF)

- Examining the particular interval $V_a \leq U < V_b$

$$P\{V_a \leq U < V_b\} = \boxed{F(V_b) - F(V_a)} = \boxed{\int_{V_a}^{V_b} f(V)\,\mathrm{d}V}$$



- Interval V_b - $V_a \to 0$: [redacted]

Uniform distribution

$$f(V) = \begin{cases} \dfrac{1}{b-a}, & \text{for } a \leq V < b, \\ 0, & \text{for } V < a \text{ and } V \geq b. \end{cases}$$

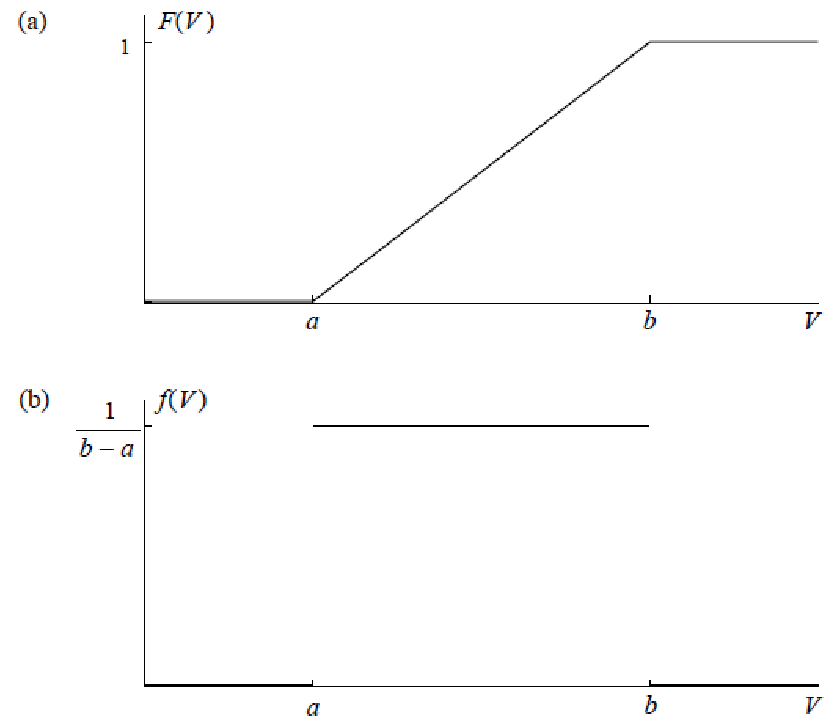


Figure 3.5: The CDF (a) and the PDF (b) of a uniform random variable (Eq. (3.39)).

Source:
Pope, „Turbulent Flows“

Example for CDF/PDF

Exponential distribution

$$f(V) = \begin{cases} \dfrac{1}{\lambda}\exp(-V/\lambda), & \text{for } V \geq 0, \\ 0, & \text{for } V < 0. \end{cases}$$

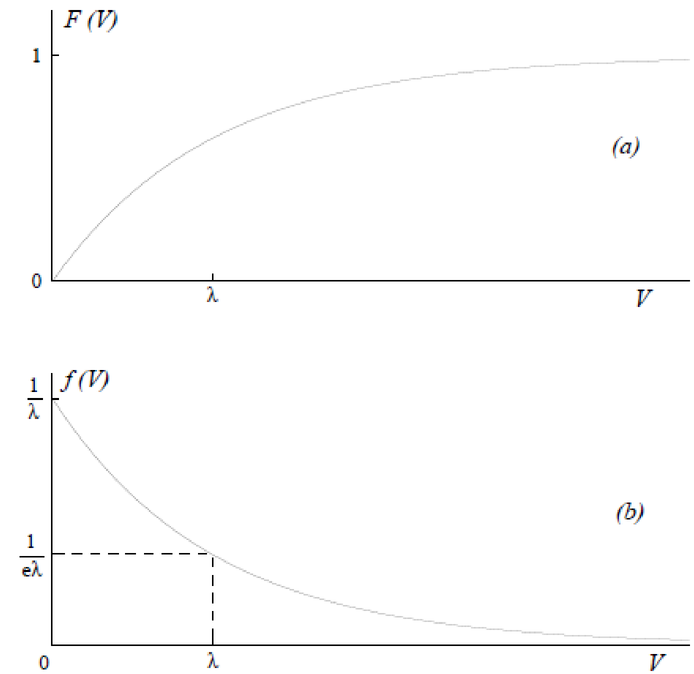
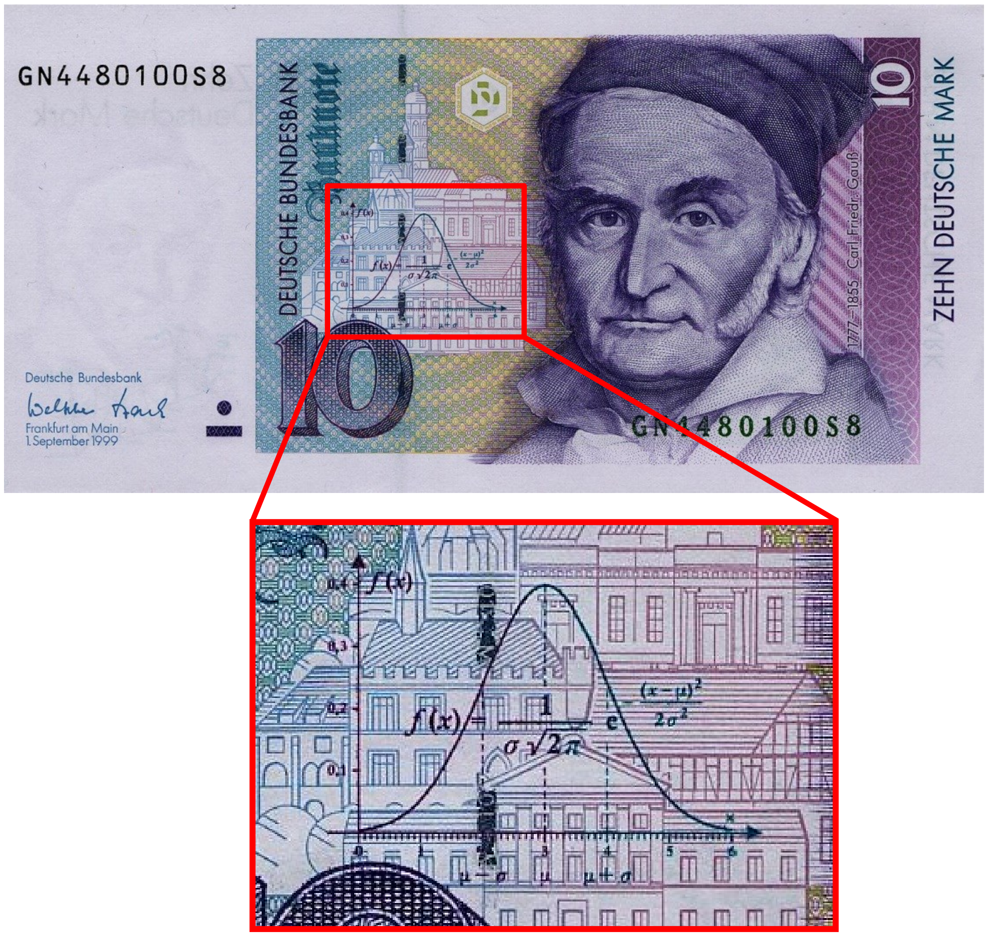


Figure 3.6: The CDF (a) and PDF (b) of an exponentially-distributed random variable (Eq. (3.40)).

Source:
Pope, „Turbulent Flows“

Example for CDF/PDF

Normal distribution



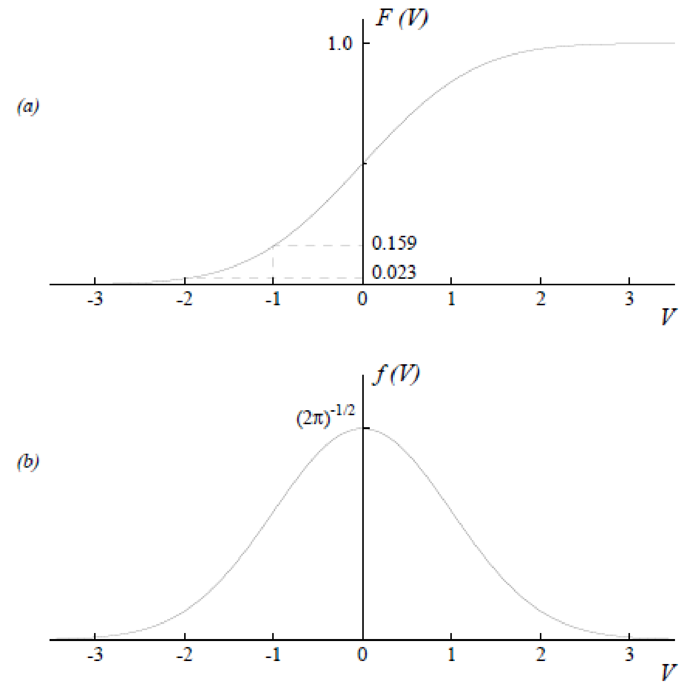


Figure 3.7: The CDF (a) and PDF (b) of a standardized Gaussian random variable.

Source:
Pope, „Turbulent Flows“

Example for CDF/PDF

Delta-function distribution

$$F(V) = P\{U < V\} = \begin{cases} 0, & \text{for } V \le a, \\ p, & \text{for } a < V \le b, \\ 1, & \text{for } V > b, \end{cases}$$

or

$$F(V) = pH(V-a) + (1-p)H(V-b).$$

$$f(V) = p\delta(V-a) + (1-p)\delta(V-b).$$

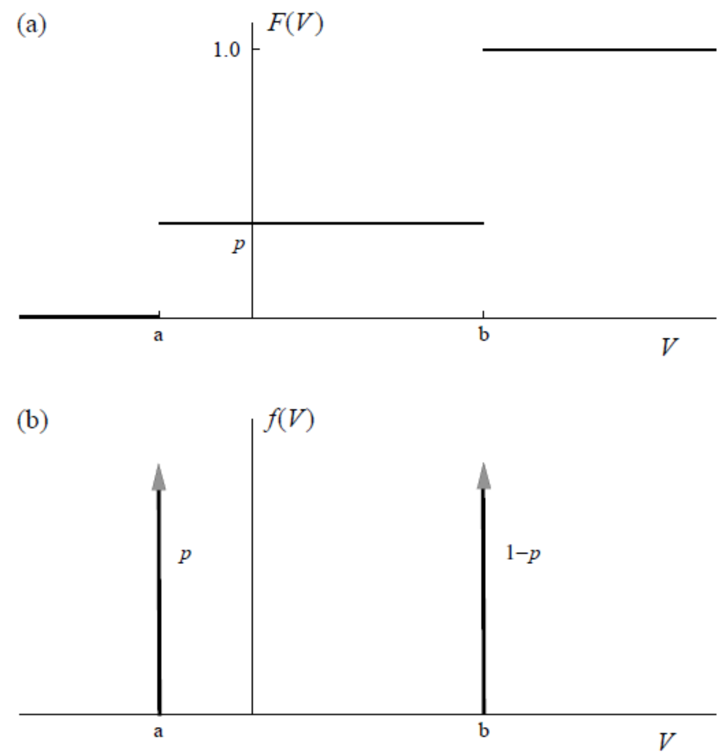


Figure 3.10: The CDF (a) and the PDF (b) of the discrete random variable U, Eq. (3.69).

Source:
Pope, „Turbulent Flows“

Moments of a PDF

- PDF of U is known → *n*-th moment

$$\overline{U^n} = \int_{-\infty}^{\infty} V^n f(V)\,\mathrm{d}V$$

- For any function of V, e.g. Q(V)

$$\boxed{\overline{Q(U)^n} = \int_{-\infty}^{\infty} Q(V)^n f(V)\,\mathrm{d}V}$$

- Example: first moment (n = 1): mean of U

$$\overline{U} = \int_{-\infty}^{\infty} V\, f(V)\,\mathrm{d}V$$

Central Moments

- *n*-th central moment

$$\mu_n = \overline{(U - \overline{U})^n} = \int_{-\infty}^{\infty} (V - \overline{U})^n f(V)\,\mathrm{d}V$$

- Example: second central moment (n = 2): variance of *U*

$$\overline{U'^2} = \overline{(U - \overline{U})^2} = \int_{-\infty}^{\infty} \left(V - \overline{U}\right)^2 f(V)\mathrm{d}V$$

Joint Cumulative Density Function

- Joint CDF (jCDF) of random variables U_1, U_2 (in general U_i, i = 1,2,…)

$$F_{1,2}(V_1, V_2) = P\{U_1 < V_1, U_2 < V_2\}$$

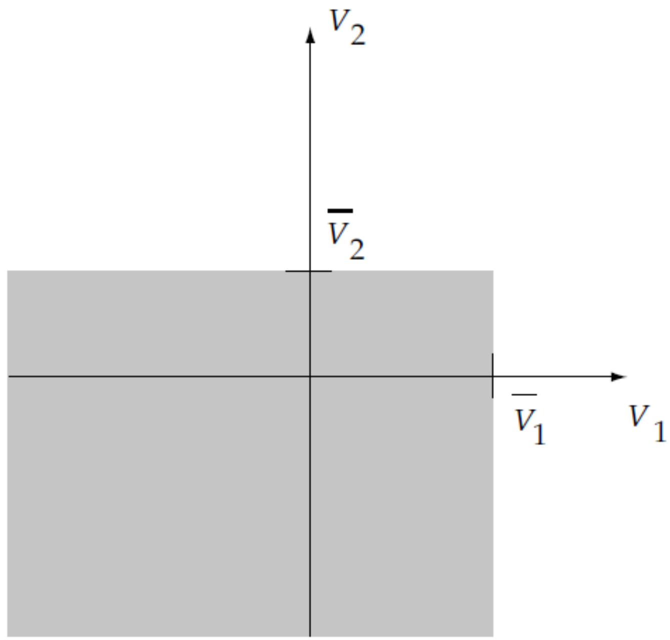


Figure 3.14: The V_1-V_2 sample space showing the region corresponding to the event $\{U_1 < \overline{V}_1,\ U_2 < \overline{V}_2\}$.

Source:
Pope, „Turbulent Flows"

Joint Cumulative Density Function

- Basic properties of a jCDF
  - Non-decreasing function

[redacted]

  - Since $\{U_1 < -\infty\}$ is impossible →

$$F_{1,2}(-\infty, V_2) = P\{U_1 < -\infty, U_2 < V_2\} = 0$$

  - Since $\{U_1 < +\infty\}$ is certain →

$$F_{1,2}(+\infty, V_2) = P\{U_1 < +\infty, U_2 < V_2\} = P\{U_2 < V_2\} = F_2(V_2)$$

equally

marginal CDF

$$F_1(V_1) = F_{1,2}(V_1, \infty)$$

Joint Probability Density Function

- Joint PDF (jPDF)

$$f_{1,2}(V_1, V_2) = \frac{\partial^2 F_{1,2}(V_1, V_2)}{\partial V_1 \partial V_2}$$

- Fundamental property:

$$P\{V_{1a} \le U_1 < V_{1b}, V_{2a} \le U_2 < V_{2b}\} = \int_{V_{1a}}^{V_{1b}} \int_{V_{2a}}^{V_{2b}} f_{1,2}(V_1, V_2)\, dV_2\, dV_1$$

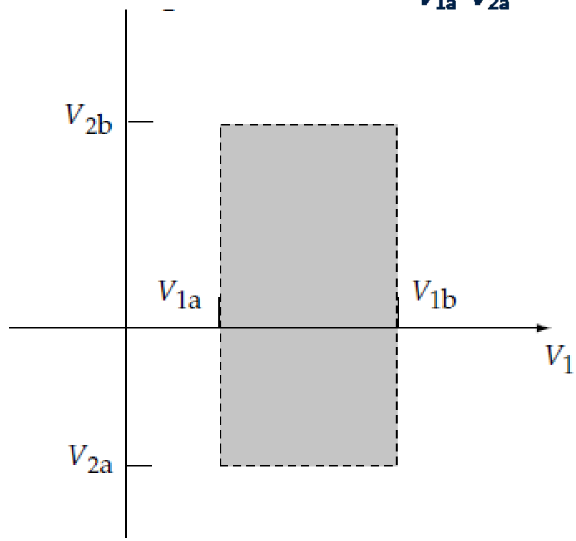


Figure 3.15: The V_1-V_2 sample space showing the region corresponding to the event $\{V_{1a} \le U_1 < V_{1b},\ V_{2a} \le U_2 < V_{2b}\}$, see Eq. (3.87).

Source:
Pope, „Turbulent Flows“

Joint Probability Density Function

- Basic properties of a jPDF
  - Non-negative:

$$f_{1,2}(V_1, V_2) \geq 0$$

  - Satisfies the normalization condition

$$\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} f_{1,2}(V_1, V_2)\,\mathrm{d}V_2\,\mathrm{d}V_1 = 1$$

  - Marginal PDF

$$f_2(V_2) = \int_{-\infty}^{+\infty} f_{1,2}(V_1, V_2)\,\mathrm{d}V_1$$

Joint Statistics

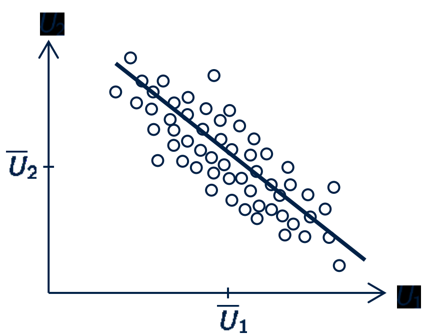
- For a function $Q(U_1,U_2,\ldots)$

$$\overline{Q(U_1, U_2, \ldots)^n} = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \ldots\; Q(V_1, V_2, \ldots)^n f_{1,2,\ldots}(V_1, V_2, \ldots) \ldots \mathrm{d}V_2 \mathrm{d}V_1$$

From joint pdf of ***V***, all moments can be obtained for all functions of ***V***

- Example: i = 1, 2; n = 1; [redacted] , covariance of U_1 and U_2

Scatterplot of two velocity-components U_1 and U_2



$$\overline{U_1' U_2'} = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} (V_1 - \overline{U_1})(V_2 - \overline{U_2}) f_{1,2}(V_1, V_2)\, \mathrm{d}V_2\, \mathrm{d}V_1$$

 – Covariance shows the correlation of two variables

Conditional PDF

- PDF of U_2 conditioned on U_1 = V_1

$$f_{2|1}(V_2|U_1 = V_1) = f_{2|1}(V_2|V_1) = \frac{f_{1,2}(V_1, V_2)}{f_1(V_1)}$$

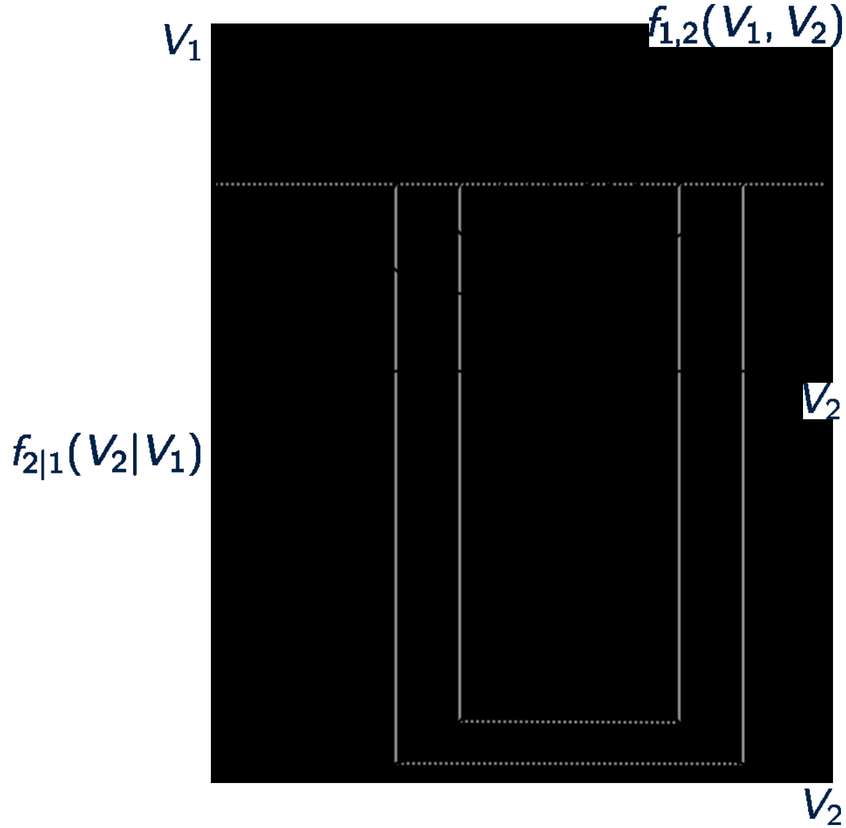
Bayes-Theorem

- jPDF $f_{1,2}(V_1,V_2)$ scaled so that
  it satisfies the normalization condition

$$\int_{-\infty}^{+\infty} f_{2|1}(V_2|V_1)\,\mathrm{d}V_2 = 1$$

- Conditional mean of a function $Q(U_1,U_2)$

$$\overline{Q(U_1, U_2)|U_1 = V_1} = \int_{-\infty}^{+\infty} Q(V_1, V_2) f_{2|1}(V_2|V_1)\,\mathrm{d}V_2$$



Statistical Independence

- If U_1 and U_2 are statistically independent, conditioning has no effect

[redacted]

- Bayes-Theorem

$$f_{2|1}(V_2|V_1) = \frac{f_{1,2}(V_1, V_2)}{f_1(V_1)} \quad \Rightarrow \quad f_1(V_1) f_{2|1}(V_2|V_1) = f_{1,2}(V_1, V_2)$$

- Therefore:

[redacted]

- Independent variables → uncorrelated
- In general the converse is not true

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The PDF Transport Equation Model

- Models based on a pdf transport equation for velocity and reactive scalars are usually formulated for one-point statistics

  → One-point/multi-variable joint statistics

- A transport equation for joint probability density function P(**v**, ***ψ*** ; **x**, t) of velocity ***v*** and all reactive scalars ***ψ*** can be derived (cf. O'Brien, 1980; Pope, 1985, 2000)

$$\frac{\partial(\rho P)}{\partial t} + \nabla \cdot (\rho \boldsymbol{v} P) + (\rho \boldsymbol{g} - \nabla \bar{p}) \cdot \nabla_v P + \sum_{i=1}^{n} \frac{\partial}{\partial \psi_i}[\omega_i \, P] =$$

$$\nabla_v \cdot [\langle -\nabla \cdot \boldsymbol{\tau} + \nabla \; p' | \boldsymbol{v}, \boldsymbol{\psi} \rangle P] - \sum_{i=1}^{n} \frac{\partial}{\partial \psi_i}[\langle \nabla \cdot (\rho D \nabla \psi_i) | \boldsymbol{v}, \boldsymbol{\psi} \rangle P]$$

where ∇_v is gradient with respect to velocity components, angular brackets are conditional means, and the same symbol is used for random and sample space variables

PDF Transport Equation: Formulation

- One-point/one-time joint velocity/scalar PDF transport equation

$$\frac{\partial(\rho P)}{\partial t} + \nabla\cdot(\rho \boldsymbol{v} P) + (\rho \boldsymbol{g} - \nabla \bar{p})\cdot\nabla_v P + \sum_{i=1}^{n} \frac{\partial}{\partial \psi_i}[\omega_i\, P] =$$

$$\nabla_v \cdot [\langle -\nabla\cdot\boldsymbol{\tau} + \nabla\;\, p' | \boldsymbol{v}, \boldsymbol{\psi}\rangle P] - \sum_{i=1}^{n} \frac{\partial}{\partial \psi_i}[\langle \nabla\cdot(\rho D \nabla \psi_i) | \boldsymbol{v}, \boldsymbol{\psi}\rangle P]$$

- First two terms on the l.h.s. are local change and convection in physical space
- Third term represents transport in velocity space by gravity and mean pressure
- Last term on l.h.s. contains chemical source terms

- All these terms are in closed form, since they are local in physical space
  - Pressure gradient does not present a closure problem, since pressure is calculated independently of pdf equation using mean velocity field
  - For chemically reacting flows, it is of particular interest that the chemical source terms can be treated exactly

PDF Transport Equation: Closure Problem

- One-point/one-time joint velocity/scalar PDF transport equation

$$\frac{\partial(\rho P)}{\partial t} + \nabla\cdot(\rho \boldsymbol{v} P) + (\rho \boldsymbol{g} - \nabla\bar{p})\cdot\nabla_v P + \sum_{i=1}^{n}\frac{\partial}{\partial\psi_i}[\omega_i\, P] =$$

$$\nabla_v\cdot[\langle -\nabla\cdot\boldsymbol{\tau} + \nabla\ p'|\boldsymbol{v},\boldsymbol{\psi}\rangle P] - \sum_{i=1}^{n}\frac{\partial}{\partial\psi_i}[\langle\nabla\cdot(\rho D\nabla\psi_i)|\boldsymbol{v},\boldsymbol{\psi}\rangle P]$$

- First unclosed term on r.h.s. describes transport of PDF in velocity space induced by viscous stresses and fluctuating pressure gradient

- Second term represents transport in reactive scalar space by molecular fluxes

→ This term represents molecular mixing and is unclosed

PDF Transport Equation: Fast chemistry

- For fast chemistry, mixing and reaction take place in thin layers where molecular transport and the chemical source term balance each other
  - Hence, closed chemical source term and unclosed molecular mixing term are closely linked to each other
  - Pope and Anand (1984) have illustrated this for the case of premixed turbulent combustion by comparing a standard pdf closure for the molecular mixing term with a formulation, where the molecular diffusion term was combined with the chemical source term to define a modified reaction rate
  - They call the former distributed combustion and the latter flamelet combustion and find considerable differences in the Damköhler number dependence of the turbulent burning velocity normalized with the turbulent intensity

PDF Transport Equation: Application

- PDF transport equation is scalar equation in many dimensions
  - Mesh-based techniques not attractive for high-dimensional equations

    $\longrightarrow$ Monte-Carlo simulation techniques (cf. Pope, 1981, 1985)

- Monte-Carlo methods represent PDF by large number of so-called notional particles
  - Particles should be considered different realizations of turbulent reactive flow
  - Statistical error decreases with $N^{1/2}$

    $\longrightarrow$ Slow convergence

- Application mostly only for joint scalar PDF coupled with Eulerian RANS flow solver
  - Coupling between Lagrangian and Eulerian solver important

- Applications often in steady RANS

  → Large particle number achieved by time averaging

PDF Transport Equation: Application in LES

- Density weighted joined scalar filtered density function F_L (FDF) defined using filter kernel G

$$F_{\mathrm{L}}(\psi;\mathbf{x},t) = \int_{-\infty}^{+\infty} \rho(\mathbf{y},t)\xi[\psi,\phi(\mathbf{y},t)]G(\mathbf{y}-\mathbf{x})\,\mathrm{d}\mathbf{y}$$

- Note: FDF does not have the statistical properties as a PDF

- Challenges:
  - LES is unsteady
    - $\longrightarrow$ Large number of notional particles required in each cell at each point in time
  - Keep number of particles per cell uniform
  - Two-way conservative interpolation between particles and mesh
  - Large number of cells makes chemistry integration even more expensive
    - $\longrightarrow$ In situ adaptive tabulation
  - Eulerian/Lagrangian coupling needs to be achieved at all times

Application TPDF Model in LES of Turbulent Jet Flames

- LES/FDF of Sandia flames D and E (Raman & Pitsch, 2007)
  - Joint scalar pdf
  - Eulerian/Lagrangian coupling
    - $\longrightarrow$ Density computed through filtered enthalpy equation for improve numerical stability
  - Detailed chemical mechanism (19 species)
  - 30-50 particles per cell
  - Simple mixing model (Interaction by exchange with the mean, IEM)

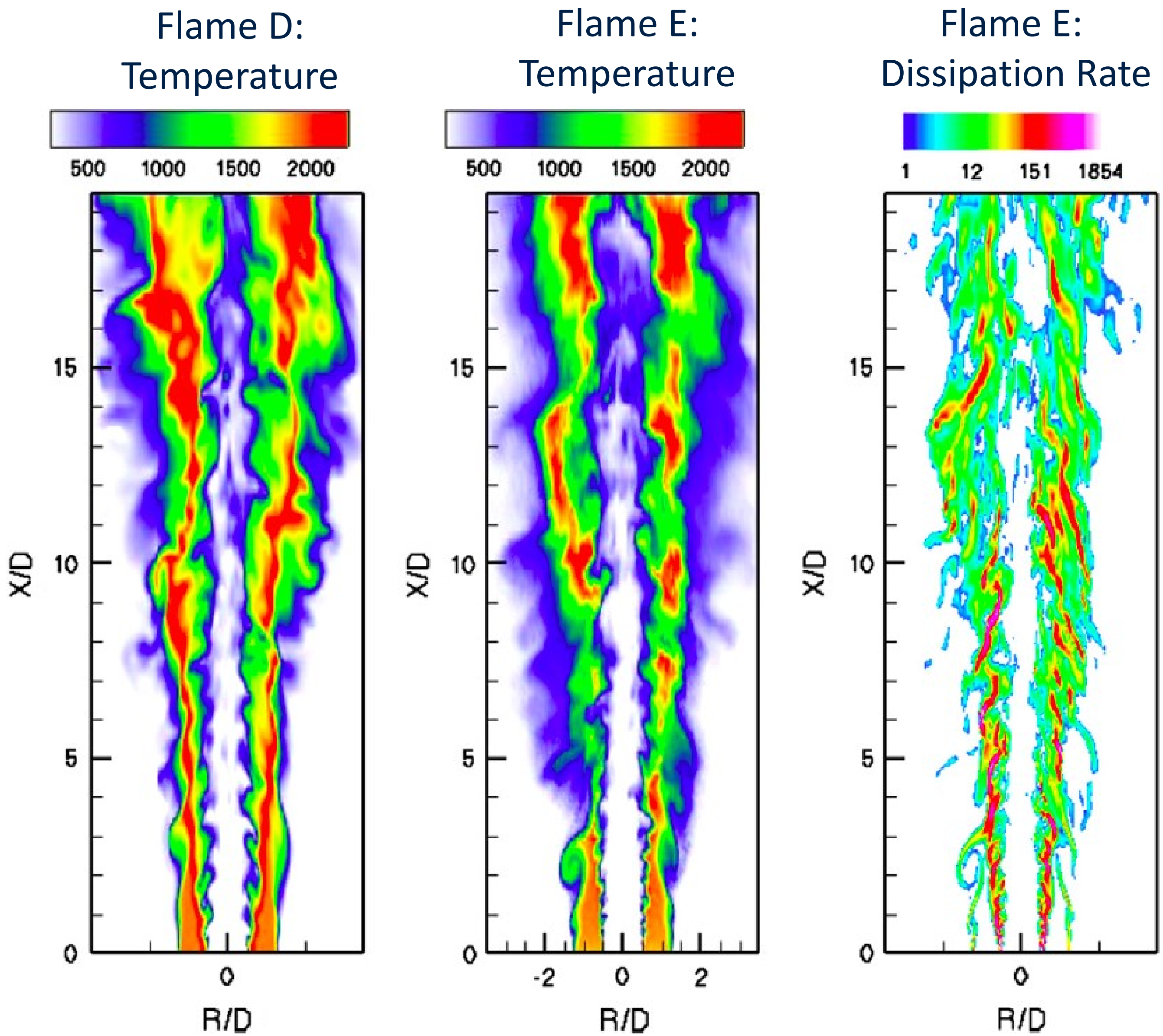
$$\mathrm{d}\boldsymbol{\psi} = -\frac{1}{\tau_\phi}\left(\boldsymbol{\psi} - \widetilde{\boldsymbol{\phi}}\right)\mathrm{d}t + \mathbf{S}(\boldsymbol{\psi})\,\mathrm{d}t$$

    - Mixing time needs to be modeled → Usually $\tau_\phi = t_t / C_\phi$ where C_ϕ = const
    - Here, new dynamic model for C_ϕ
  - Modeled stochastic differential equation for particle-position

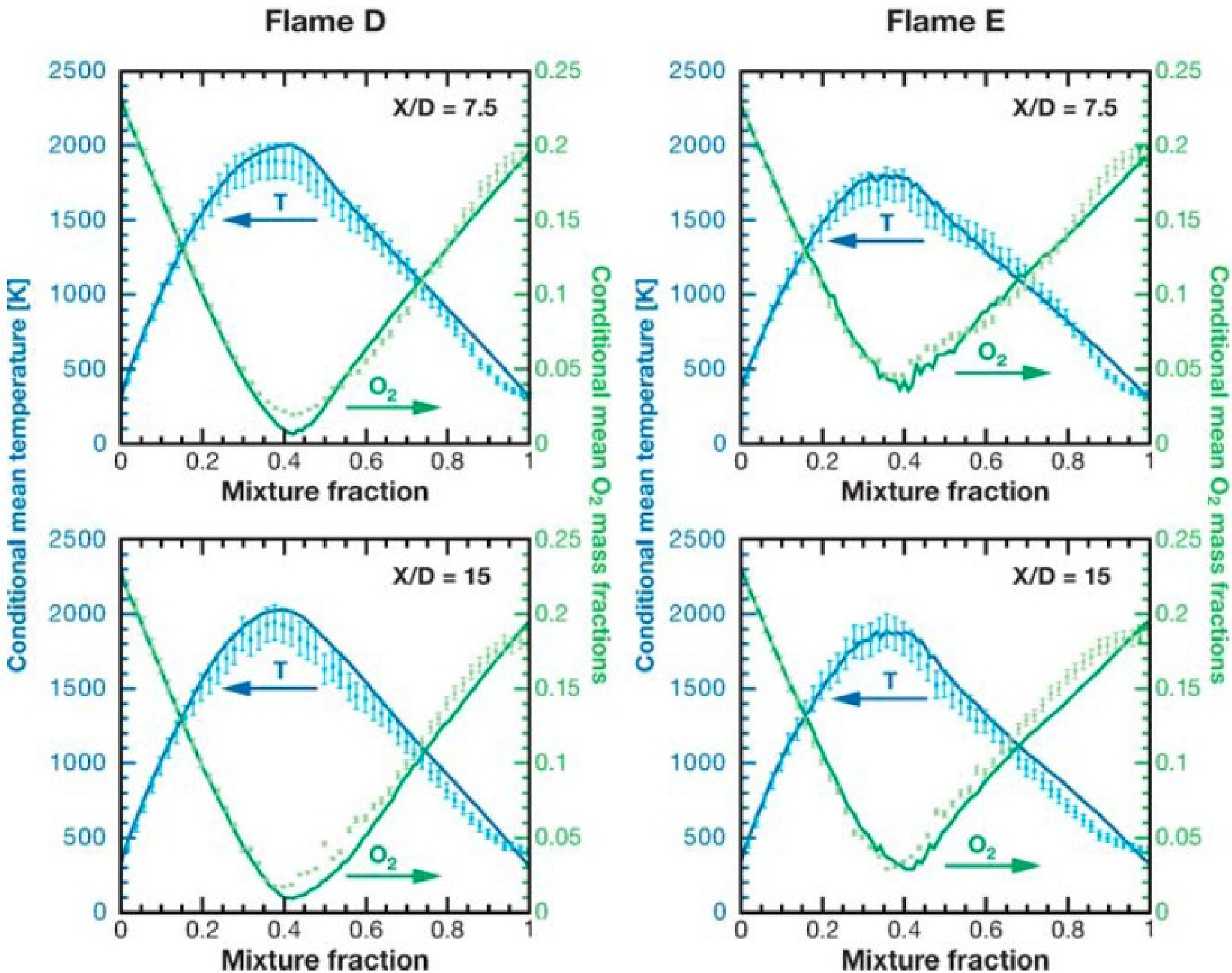
$$d\mathbf{x}^* = \left[\tilde{\mathbf{u}} + \frac{1}{\bar{\rho}}\nabla\bar{\rho}(D + D_\mathrm{T})\right]\mathrm{d}t + \sqrt{2(D + D_\mathrm{T})}\,\mathrm{d}\mathbf{W},$$

[1] V. Raman and H. Pitsch, A consistent LES/filtered-density function formulation for the simulation of turbulent flames with detailed chemistry, Proc. Comb. Inst., 31, pp. 1711–1719, 2007.

Application TPDF Model in LES of Turbulent Jet Flames



Application TPDF Model in LES of Turbulent Jet Flames



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Bray-Moss-Libby-Model

- Flamelet concept for premixed turbulent combustion: Bray-Moss-Libby-Model (BML)
- Premixed combustion: progress variable *c*, e.g.

$$c = \frac{T - T_{\mathrm{u}}}{T_{\mathrm{b}} - T_{\mathrm{u}}} \quad \text{or} \quad c = \frac{Y_{\mathrm{P}}}{Y_{\mathrm{P,b}}}$$

- Favre averaged transport equation (neglecting the molecular transport)

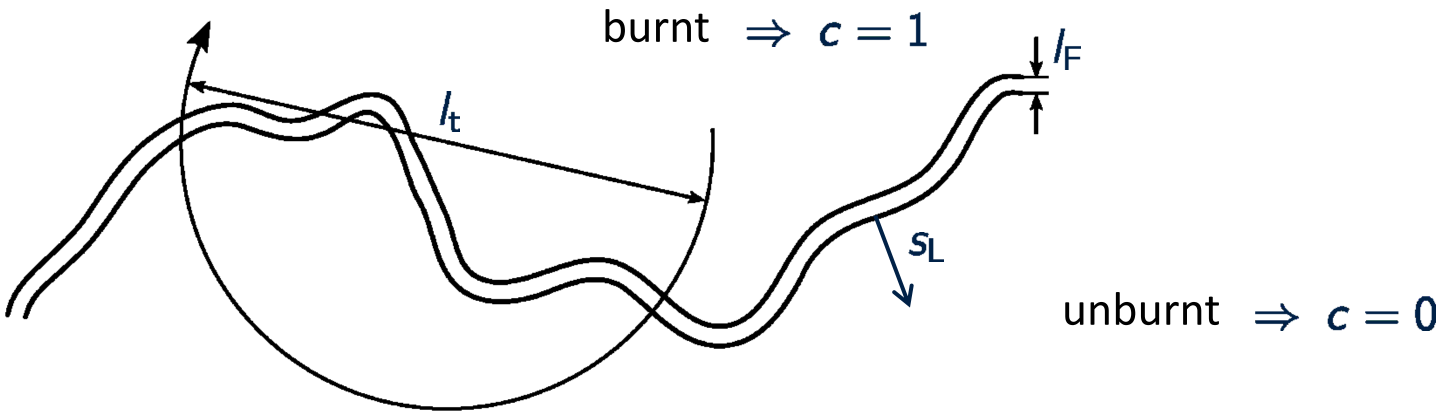
not closed

[redacted]

- Closure for turbulent transport and chemical source term by BML-Model

Bray-Moss-Libby-Model

- Assumption: very fast chemistry, flame size $l_F \ll \eta \ll l_t$



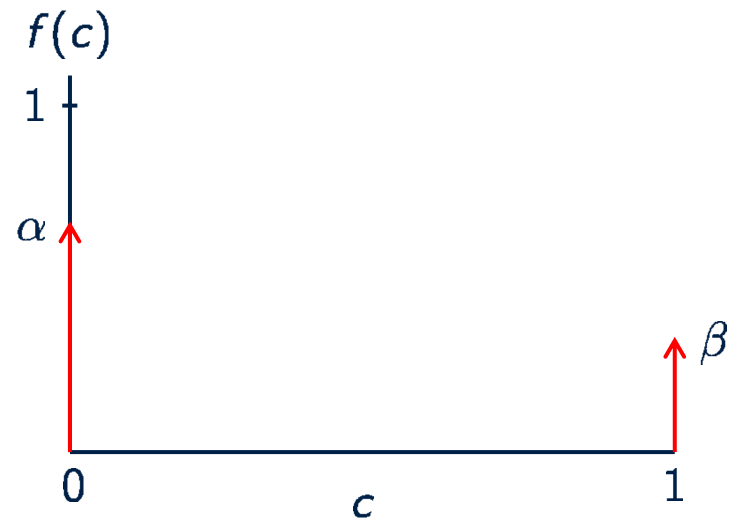
- Fuel conversion only in the area of thin flame front
  → in the flow field
  - Burnt mixture or
  - Unburnt mixture,
  - Intermediate states are very unlikely

Bray-Moss-Libby-Model

- Assumption: progress variable is expected solely to be $c = 0$ (unburnt) or $c = 1$ (burnt)
- Probability densitiy function

[redacted]

  - α, β: probabilities, to encounter burnt or unburnt mixture in the flow field
  - No intermediate states → [redacted]
  - δ: Delta function



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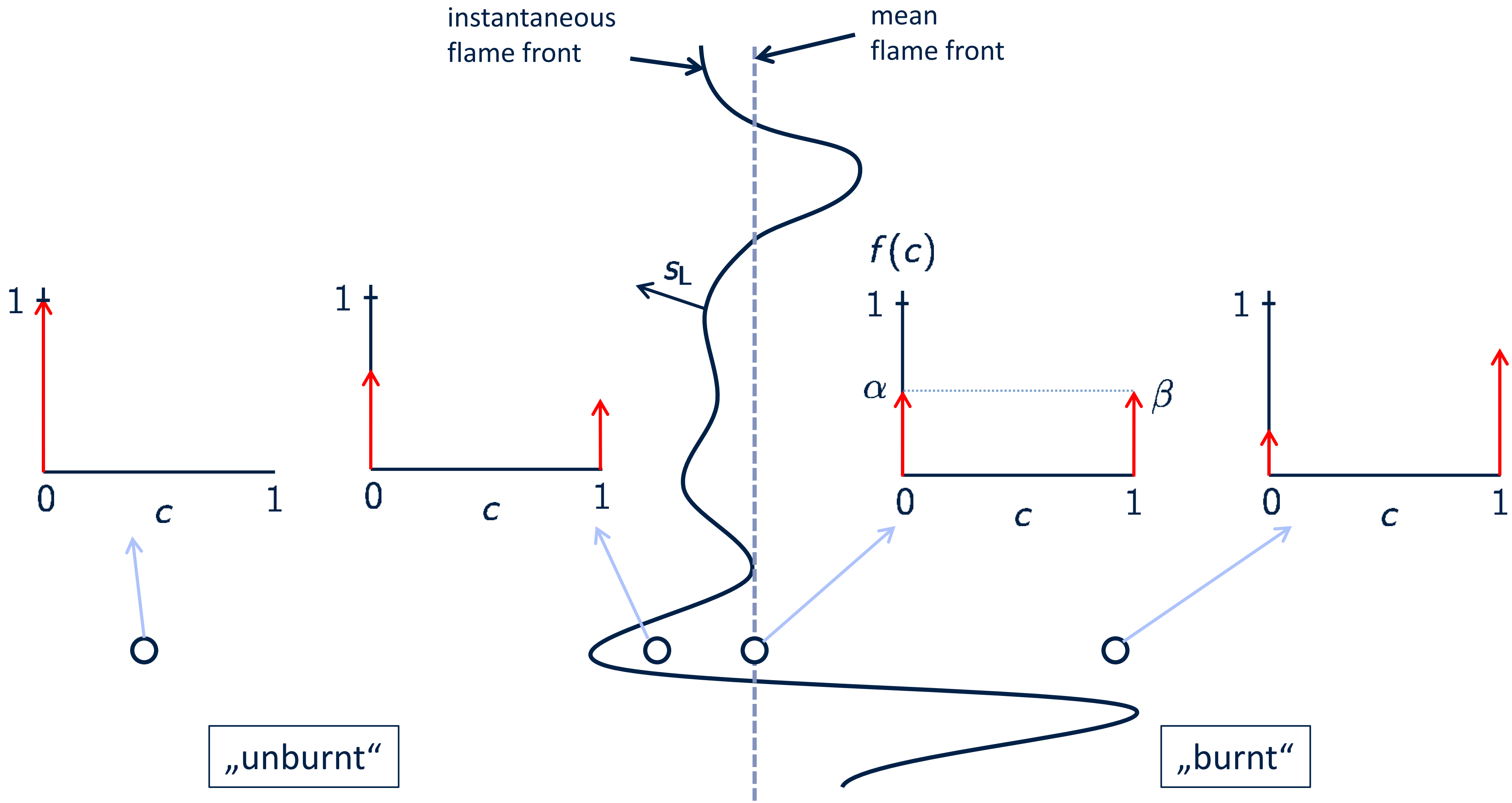
Bray-Moss-Libby-Model



BML-closure of Turbulent Transport

- For a Favre average

[redacted]

- Therefore the unclosed correlation $\widetilde{u''c''}$
  - joint PDF for u and c

[redacted] (Bayes-Theorem)

  - Introducing the BML approach for $f(c)$ leads to

$$f_{u,c}(u,c) = \alpha\delta(c)\underbrace{f_{u|c}(u|c=0)}_{\text{conditional PDF}} + \beta\underbrace{\delta(1-c)}_{\text{delta function}}f_{u|c}(u|c=1)$$

BML-closure of Turbulent Transport

- With

[redacted]

follows

[redacted]

[redacted]

Bray-Moss-Libby-Model: „countergradient diffusion“

- Because of ρu = const. → through flame front: u↑ just as much as ρ↓ →

$$(\overline{u}_\mathrm{b} - \overline{u}_\mathrm{u}) > 0$$

- Because of $c \geq 0$ →

$$\boxed{\widetilde{u''c''} = \widetilde{c}(1 - \widetilde{c})(\overline{u}_\mathrm{b} - \overline{u}_\mathrm{u}) \geq 0}$$

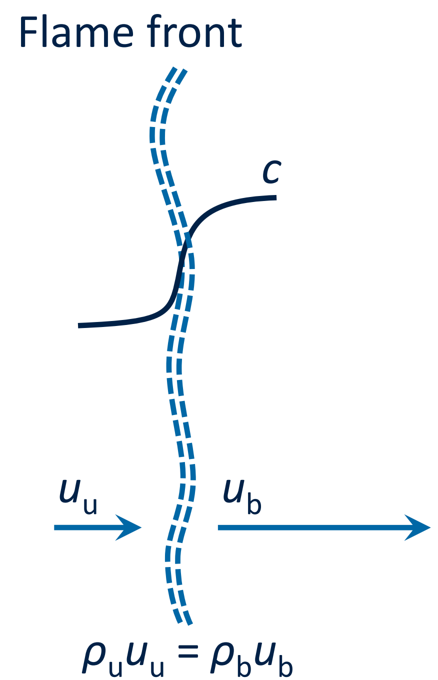
- Within the flame zone

$$\frac{\partial \widetilde{c}}{\partial x} \geq 0$$

conflict

- Gradient transport assumption would be

$$\boxed{\widetilde{u''c''} = -D_\mathrm{t} \frac{\partial \widetilde{c}}{\partial x_i} \leq 0}$$



- Conflict: „countergradient diffusion“

BML-closure of Chemical Source Term

- Closure by BML-model $f(c)$ leads to $\overline{\omega}_c = 0$
- Closure of the chemical source term, e.g. by flame-surface-density-model

$$\overline{\omega}_c = \boxed{\rho_u s_L^0 I_0}\,\boxed{\Sigma}$$

local mass conversion per area

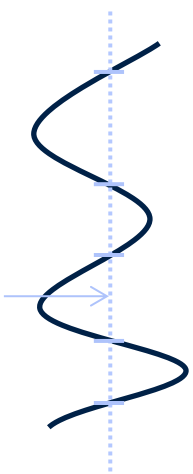
Flächen-Dichte (flamen area per volume)

  - I_0: strain factor → local increase of burning velocity by strain
- Flame-surface-density Σ
  - e.g. algebraic model:

$$\Sigma \sim \frac{\overline{c}\,(1-\overline{c})}{L_y}$$

  - Or transport equation for Σ

Flame crossing length



BML-closure of Chemical Source Term

- Transport equation for Σ

[redacted]

local change

convectiv change

turbulent transport

production due to stretching of the flame

flame-annihilation

- No chemical time scale
  - Turbulent time ($\tau = k/\varepsilon$) is the determining time scale
  - Limit of infinitely fast chemistry
  - By using transport equations
    → model for chemical source term independent of s_L

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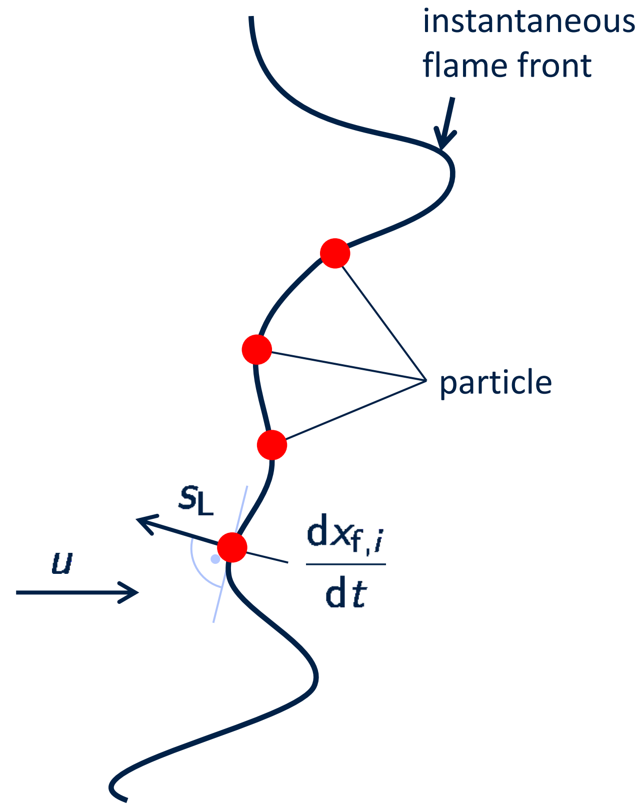
Level-Set-Approach

- Kinematics of the flame front by examining the movement of single flame front-„particles“
- Movement influenced by
  - Local flow velocity u_i, $i = 1,2,3$
  - Burning velocity s_L

$$\frac{\mathrm{d}x_{f,i}}{\mathrm{d}t} = u_i + s_L n_i$$

normal vector



G-Equation

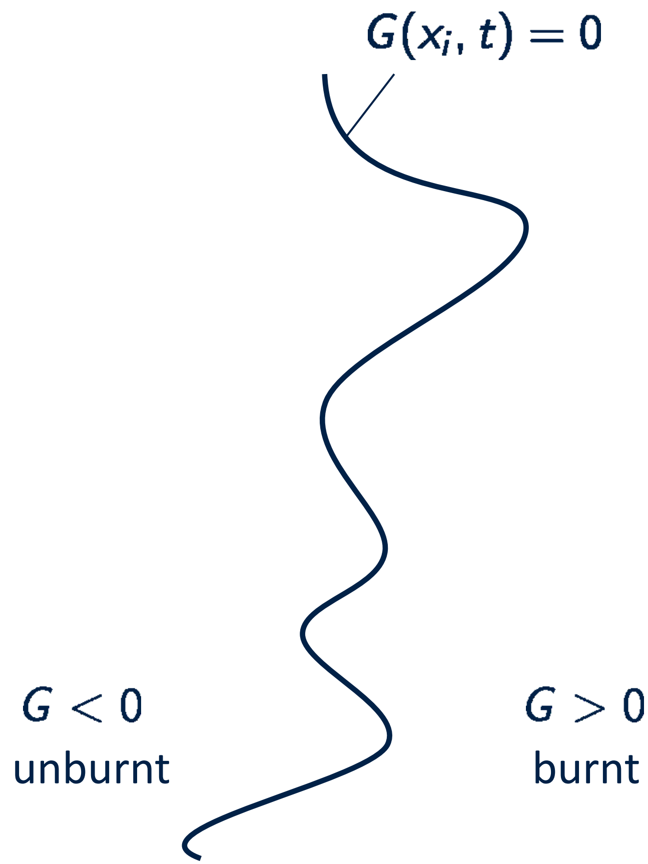
- Instead of observing a lot of particles → examination of a scalar field G

- Iso-surface G_0 is defined as the flame front

$$G(x_i, t) = G_0 = 0$$

- Substantial derivative of G (on the flame front)

$$\frac{\mathrm{D}G}{\mathrm{D}t} \equiv \boxed{\frac{\partial G}{\partial t} + \frac{\mathrm{d}x_{\mathrm{f},i}}{\mathrm{d}t}\frac{\partial G}{\partial x_i} = 0}$$



G-Equation for Premixed Combustion

- Kinematics

$$\frac{\mathrm{d}x_{f,i}}{\mathrm{d}t} = u_i + s_L\, n_i$$

normal vector

$$n_i = -\frac{\frac{\partial G}{\partial x_i}}{|\nabla G|}$$

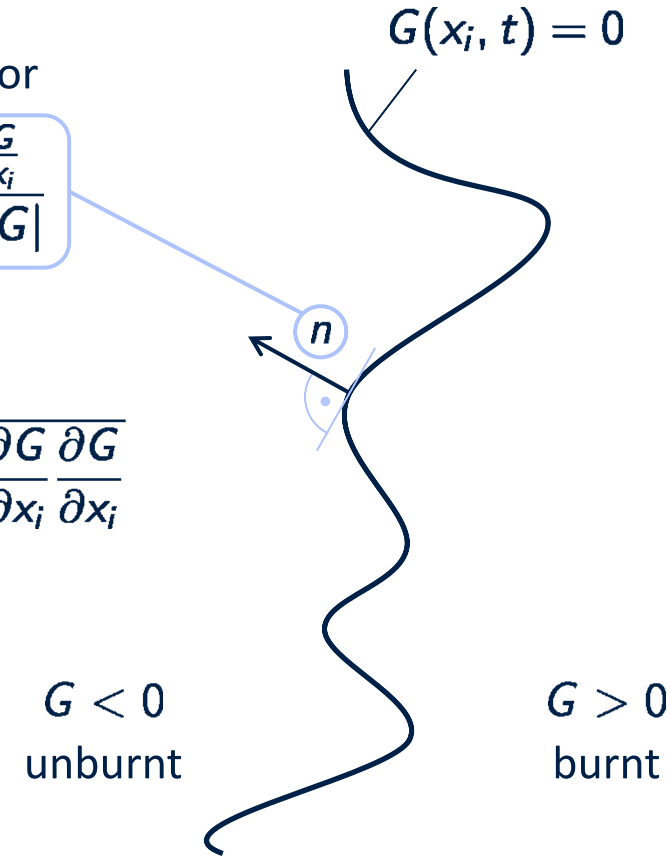
and

[redacted]

$$|\nabla G| = \sqrt{\frac{\partial G}{\partial x_i}\frac{\partial G}{\partial x_i}}$$

lead to

$$\boxed{\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = s_L\, |\nabla G|}$$



→ G-Equation for premixed combustion

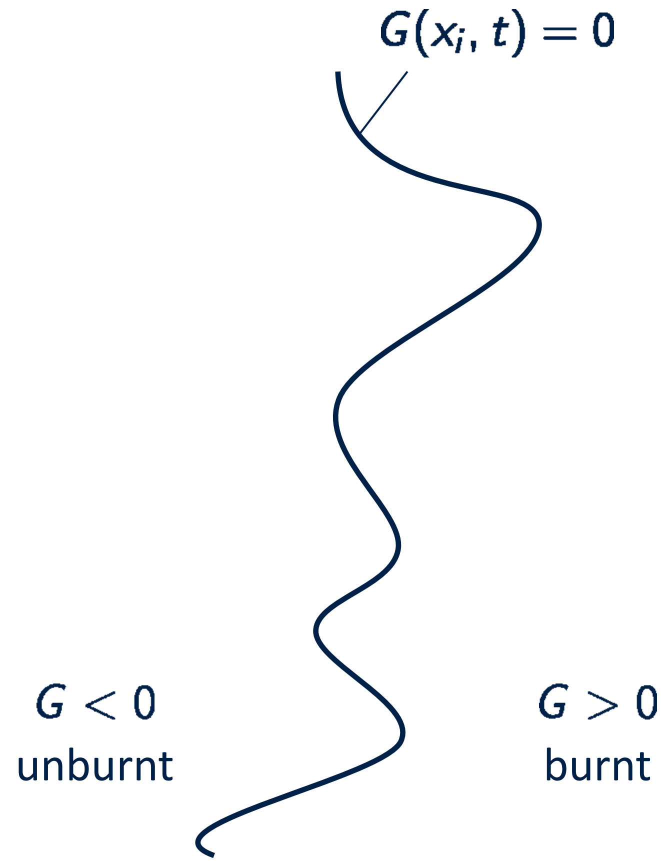
G-Equation in the Regime of Corrugated Flamelets

$$\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = s_L \, |\nabla G|$$

local change

convective change

progress of flame front by burning velocity



- No diffusive term
- Can be applied for
  - Thin flames
  - Well-defined burning velocity

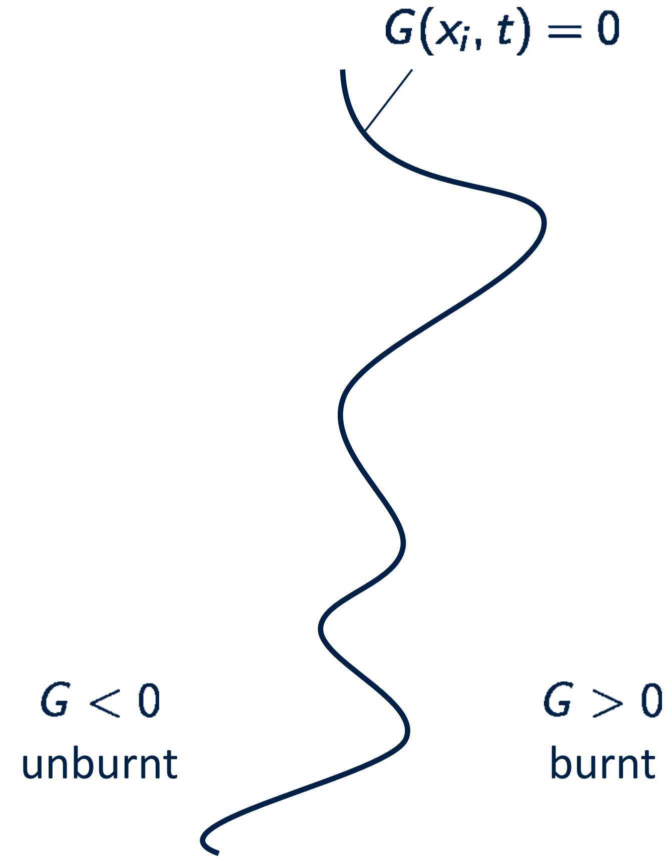
→ Regime of corrugated flamelets ($\eta >> l_F >> l_\delta$)

G-Equation in the Regime of Corrugated Flamelets

$$\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = s_L \, |\nabla G|$$

- Kinematic equation → $\neq f(\rho)$
- Valid for flame position: $G = G_0$ (= 0)
  - For solving the field equation, G needs to be defined in the entire field
  - Different possibilities to define G, e.g. signed distance function

[redacted]

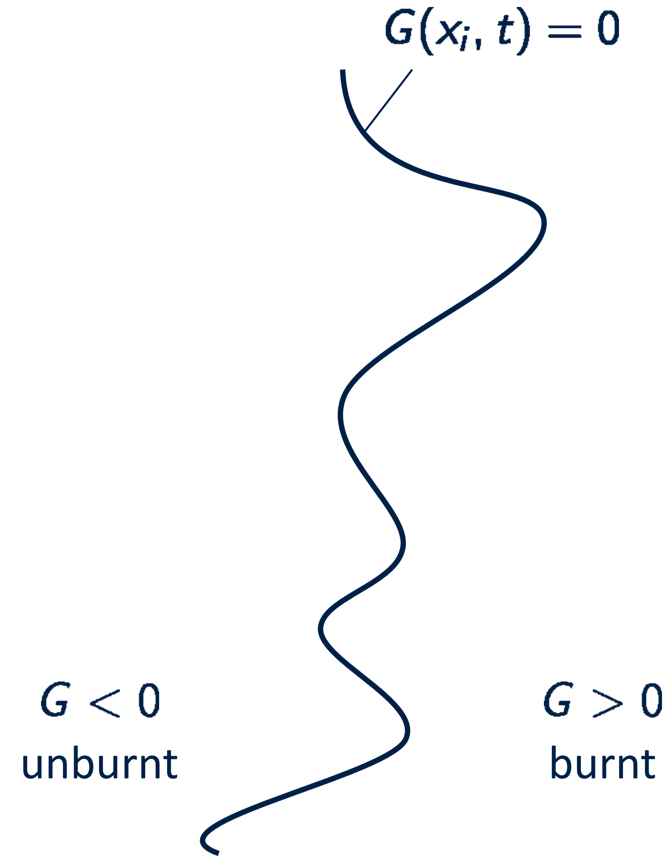


G-Equation in the Regime of Corrugated Flamelets

$$\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = s_\mathrm{L}\,|\nabla G|$$

- Influence of chemistry by s_L
- s_L not necessarily constant, influenced by
  - strain S
  - curvature κ
  - Lewis number effect
- Modified laminar burning velocity

[redacted]



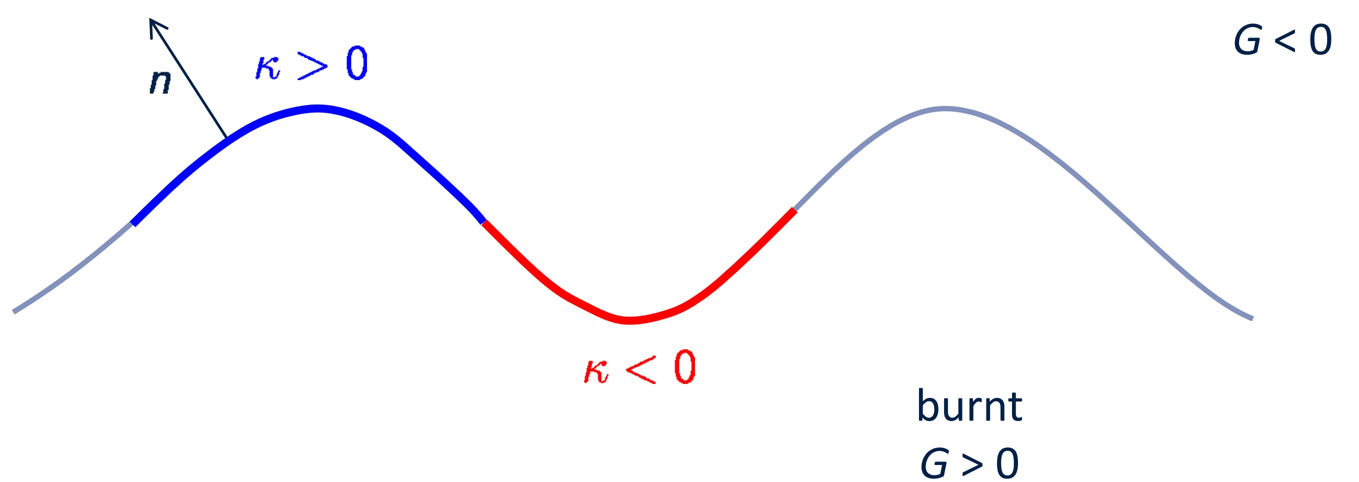
Laminar Burning Velocity: Curvature

influence of curvature

$$\kappa = \frac{\partial n_i}{\partial x_i} = \frac{\partial}{\partial x_i}\left(-\frac{\frac{\partial G}{\partial x_i}}{|\nabla G|}\right)$$

uncorrected laminar burning velocity

[redacted]



Laminar Burning Velocity: Markstein Length

uncorrected laminar
burning velocity

$$s_L = s_L^0 - s_L^0 \mathcal{L}\kappa - \mathcal{L}S$$

- Markstein length
  - Determined by experiment
  - Or by asymptotic analysis

$$\frac{\mathcal{L}_u}{l_F} = \frac{1}{\gamma} \ln\left(\frac{1}{1-\gamma}\right) + \frac{Ze\,(Le-1)}{2}\,\frac{(1-\gamma)}{\gamma} \int\limits_0^{\gamma/(1-\gamma)} \frac{\ln(1+x_i)}{x_i}\mathrm{d}x_i$$

density
ratio

Zeldovich number

$$Ze = \frac{E}{RT_b}\frac{T_b - T_u}{T_b}$$

Lewis number

$$Le = \frac{\lambda}{\rho c_p D} = \frac{Sc}{Pr}$$

Extended G-Equation

influence of curvature

$$\kappa = \frac{\partial n_i}{\partial x_i} = \frac{\partial}{\partial x_i}\left(-\frac{\frac{\partial G}{\partial x_i}}{|\nabla G|}\right)$$

uncorrected laminar burning velocity

influence of strain

$$S = -n_i \frac{\partial u_i}{\partial x_j} n_j$$

$$\boxed{s_L = s_L^0 - s_L^0 \mathcal{L}\kappa - \mathcal{L}S}$$

Markstein length

→ Extended G-Equation

$$\boxed{\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = \left(s_L^0 - s_L^0 \mathcal{L}\kappa - \mathcal{L}S\right)|\nabla G|}$$

G-Equation: Corrugated Flamelets/Thin Reaction Zones

- Previous examinations limited to the regime of corrugated flamelets
  - Thin flame structures ($\eta >> l_F >> l_\delta$)
  - Laminar burning velocity well-defined

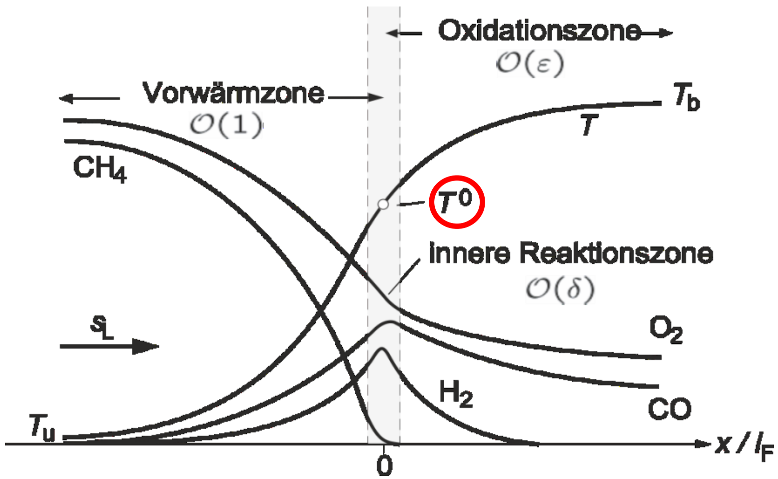
no longer valid

- Regime of thin reaction zones
  - Small scale eddies penetrate the preheating zone
  - Transient flow
  - Burning velocity not well-defined

→ Problem: Level-Set-Approach valid in the regime of thin reaction zones?

G-Equation: Regime of Thin Reaction Zones

- Assumption: „G=0“ surface is represented by inner reaction zone
- Inner reaction zone
  - Thin compared to small scale eddies, $l_\delta << \eta$
  - Described by $T(x_i,t) = T^0$
- Temperature equation



$$\rho \frac{\partial T}{\partial t} + \rho u_i \frac{\partial T}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\rho D \frac{\partial T}{\partial x_i}\right) + \omega_T$$

- Iso temperature surface $T(x_i,t) = T^0$

$$\left.\frac{\mathrm{D}T}{\mathrm{D}t}\right|_{T=T^0} \equiv \left.\frac{\partial T}{\partial t} + \frac{\partial T}{\partial x_i}\frac{\mathrm{d}x_{f,i}}{\mathrm{d}t}\right|_{T=T^0} = 0$$

$$\left(\text{cf.} \quad \frac{\partial G}{\partial t} + \frac{\partial G}{\partial x_i}\frac{\mathrm{d}x_{f,i}}{\mathrm{d}t} = 0\right)$$

G-Equation: Regime of Thin Reaction Zones

- Equation of motion of the iso temperature surface $T(x_i,t) = T^0$

$$\left.\frac{\mathrm{d}x_{\mathrm{f},i}}{\mathrm{d}t}\right|_{T=T^0} = u_{i,0} + n_i s_\mathrm{d} \qquad \left(\text{cf.} \quad \frac{\mathrm{d}x_{\mathrm{f},i}}{\mathrm{d}t} = u_i + s_\mathrm{L}\, n_i\right)$$

  – With the displacement speed s_d

$$s_\mathrm{d} = \left[\frac{\frac{\partial}{\partial x_i}\rho D \frac{\partial T}{\partial x_i} + \omega_T}{\rho\left|\nabla T\right|}\right]_{T=T_0}$$

  – Normal vector

$$n_i = -\left.\frac{\frac{\partial T}{\partial x_i}}{\left|\nabla T\right|}\right|_{T=T^0} \qquad \left(\text{cf.} \quad n_i = -\frac{\frac{\partial G}{\partial x_i}}{\left|\nabla G\right|}\right)$$

G-Equation: Regime of Thin Reaction Zones

- With $G_0 = T^0$

$$\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = \underbrace{\left[\frac{\frac{\partial}{\partial x_i}\rho D \frac{\partial T}{\partial x_i} + \omega_T}{\rho|\nabla T|}\right]_0}_{s_\mathrm{d}} |\nabla G|$$

Diffusion term → normal diffusion ($\sim s_n$) and curvature term ($\sim \kappa$)

$$\frac{\partial}{\partial x_i}\left(\rho D \frac{\partial T}{\partial x_i}\right) = \underbrace{n_j \frac{\partial}{\partial x_j}\left(\rho D n_i \frac{\partial T}{\partial x_i}\right)}_{\sim s_\mathrm{n}} - \rho D |\nabla T| \underbrace{\frac{\partial n_i}{\partial x_i}}_{\kappa}$$

→ G-equation for the regime of thin reaction zones

$$s_\mathrm{r} = \omega_\mathrm{T}/(\rho|\nabla T|)$$

$$\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = \left(\underbrace{s_\mathrm{n} + s_\mathrm{r}}_{= s_\mathrm{L,s}} - D\kappa\right)|\nabla G| \quad \Leftrightarrow \quad \boxed{\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = s_\mathrm{L,s}|\nabla G| - D\kappa|\nabla G|}$$

Common Level Set Equation for Both Regimes

- Normalize G-equation with Kolmogorov scales (η, τ_η, u_η)

[redacted] $x_i^* = x_i/\eta,$ $u_i^* = u_i/u_\eta,$

[redacted]

leads to

[redacted]

Order of Magnitude Analysis

[redacted]

$O(Ka^{-1/2})$ $O(1)$

- Non dimensional →
  - → Derivatives, u_i^*, $\kappa^* \approx O(1)$
- Typical flame
  - → $Sc = \nu/D \approx 1$ → $D/\nu = O(1)$
- Parameter: s_L/u_η
  - $Ka = u_\eta^2/s_L^2$ → $s_L/u_\eta = Ka^{-1/2}$
  - $s_{L,s} \approx s_L$

G-Equation for both Regimes

[redacted]

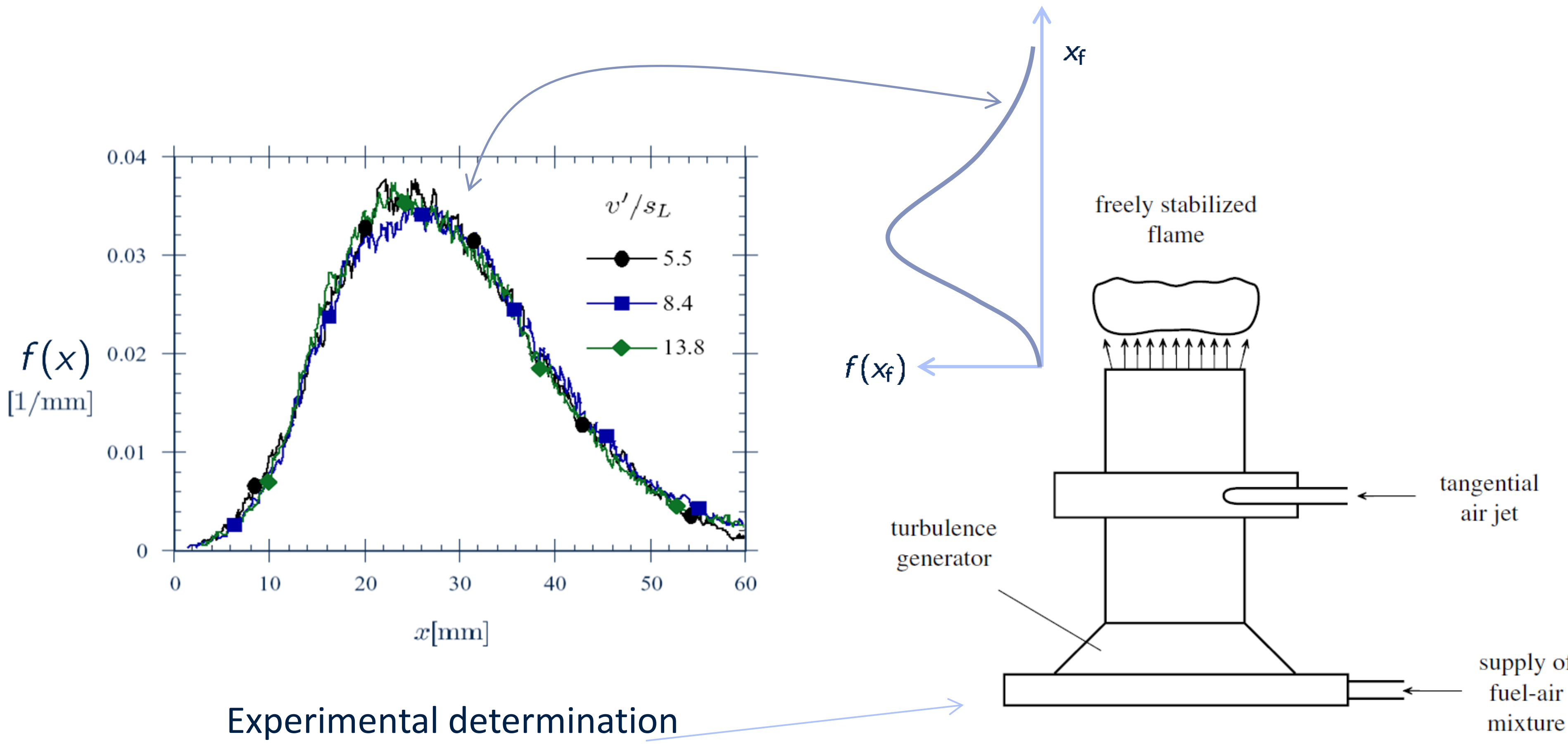
$O(Ka^{-1/2})$ $O(1)$

- Thin reaction zones: $Ka >> 1$
  → curvature term is dominant
- Corrugated flamelets: $Ka << 1$
  → s_L term is dominant
- Leading order equation in both regimes

$$\boxed{\rho\frac{\partial G}{\partial t} + \rho u_i \frac{\partial G}{\partial x_i} = (\rho s_L^0)|\nabla G| - (\rho D)\kappa|\nabla G|}$$

Assumption: $\rho_u u_u = (\rho_u s_L^0) =$ const. const.

- Probability density function of finding $G(x_i,t) = G_0 = 0$



Experimental determination
in weak swirl burner

Statistical Description of Turbulent Flame Front

- Consider steady one-dimensional premixed turbulent mean flame at position x_f

$$x_f = \int_{-\infty}^{\infty} x\, f(x)\, \mathrm{d}x$$

- Define flame brush thickness l_f from $f(x)$

[redacted]

- If G is distance function then

[redacted]

Favre-Mean- and Variance-Equation

- Equation for Favre-mean

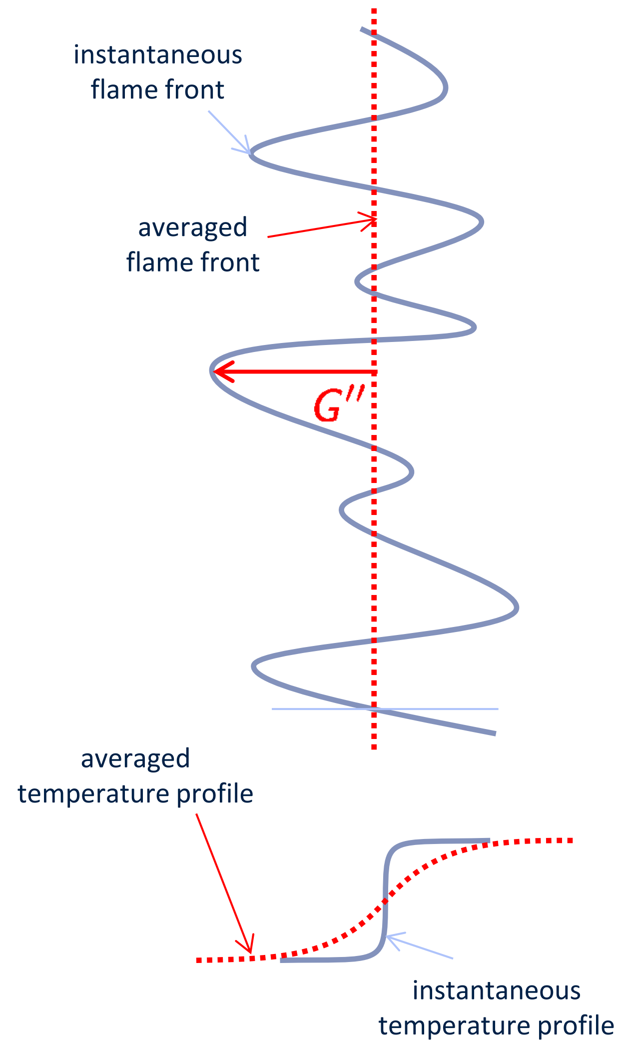
$$\bar{\rho}\frac{\partial \widetilde{G}}{\partial t} + \bar{\rho}\widetilde{u}_i\frac{\partial \widetilde{G}}{\partial x_i} + \frac{\partial}{\partial x_i}\bar{\rho}\widetilde{u''G''} = (\rho s_L^0)\overline{\sigma} - (\rho D)\overline{\kappa\sigma}$$

- Equation for variance

$$\bar{\rho}\frac{\partial \widetilde{G''^2}}{\partial t} + \bar{\rho}\widetilde{u}_i\frac{\partial \widetilde{G''^2}}{\partial x_i} + \frac{\partial}{\partial x_i}\bar{\rho}\widetilde{u_i''G''^2} =$$

$$-2\bar{\rho}\widetilde{u_i''G''}\frac{\partial \widetilde{G}}{\partial x_i} - \bar{\rho}\widetilde{\omega} - \bar{\rho}\widetilde{\chi} - (\rho D)\overline{\mathcal{K}\sigma}$$

- $\sigma = |\nabla G|$ can be interpreted as the area ratio of the flame A_T/A
- Variance describes the average size of the flame



Modeling of the Variance Equation

- Sink terms in the variance equation

[redacted]

$$-2\bar{\rho}\widetilde{u_i''G''}\frac{\partial\widetilde{G}}{\partial x_i} - \bar{\rho}\widetilde{\omega} - \bar{\rho}\widetilde{\chi} - (\rho D)\overline{\mathcal{K}\sigma}$$

  - Kinematic restoration

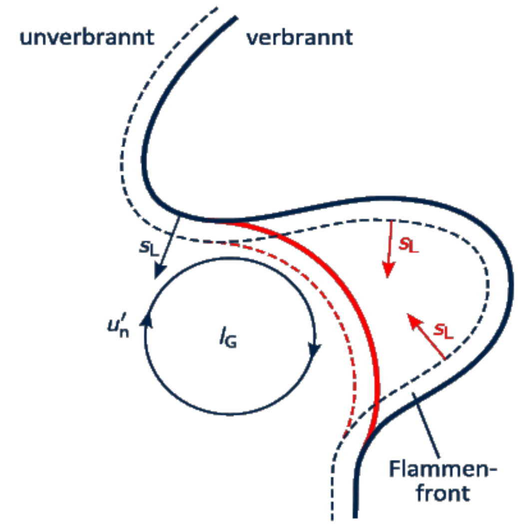
$$\widetilde{\omega} = -2(\rho s_L^0)\overline{G''\sigma}/\bar{\rho}$$

  - Scalar dissipation

$$\widetilde{\chi} = 2(\rho D)\widetilde{\left(\frac{\partial G''}{\partial x_i}\right)^2}/\bar{\rho}$$

are modeled by

$$\widetilde{\omega} + \widetilde{\chi} = c_s\frac{\widetilde{\varepsilon}}{\widetilde{k}}\widetilde{G''^2}$$



G-Equation for Turbulent Flows

- Introducing turbulent burning velocity

$$(\bar{\rho} s_{\mathrm{T}}^0)\left|\nabla \widetilde{G}\right| = (\rho s_{\mathrm{L}}^0)\bar{\sigma} \quad (\text{vgl. } s_{\mathrm{T}} A = s_{\mathrm{L}} A_{\mathrm{T}})$$

→ Equation for Favre mean

$$\bar{\rho}\frac{\partial \widetilde{G}}{\partial t} + \bar{\rho}\tilde{u}_i \frac{\partial \widetilde{G}}{\partial x_i} = (\bar{\rho} s_{\mathrm{T}}^0)\left|\nabla \widetilde{G}\right| - \bar{\rho} D_{\mathrm{t}} \tilde{\kappa}\left|\nabla \widetilde{G}\right|$$

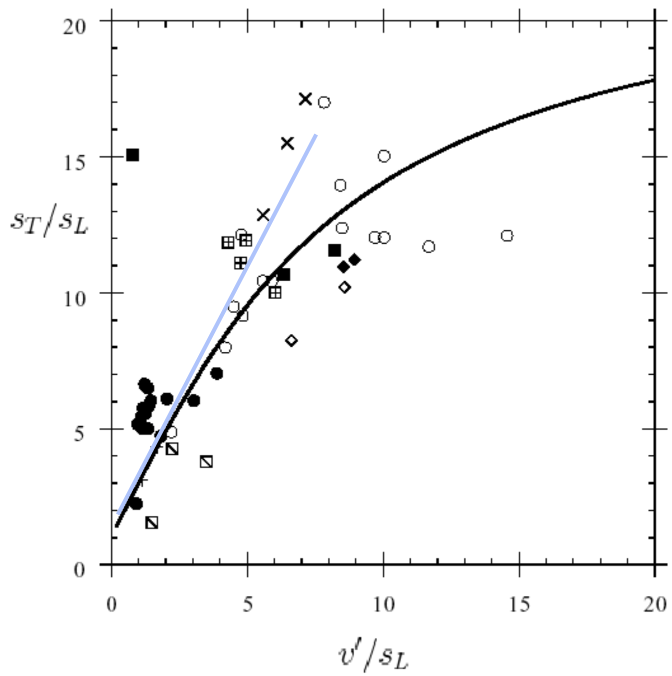
→ Equation for variance

[redacted]

G-Equation for Turbulent Flows

- Modeling of turbulent burning velocity by Damköhler theory

$$\frac{s_T}{s_L} = 1 - \alpha\frac{l_t}{l_F} + \sqrt{\left(\alpha\frac{l_t}{l_F}\right)^2 + 4\alpha\frac{u'l_t}{s_L l_F}}$$



G-Equation for Turbulent Flows

- Favre mean of G

[redacted]

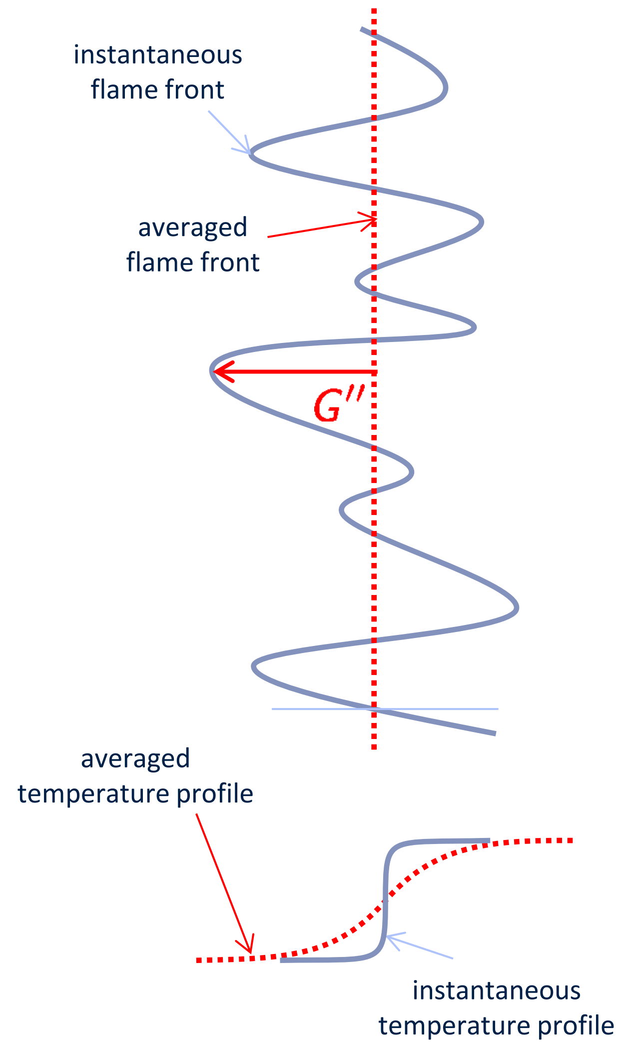
- Favre-PDF

$$\widetilde{f}(G;x,t) = \frac{1}{\sqrt{2\pi\widetilde{G''^2}\big|_0}} \exp\left(-\frac{(G-\widetilde{G})^2}{2\widetilde{G''^2}\big|_0}\right)$$

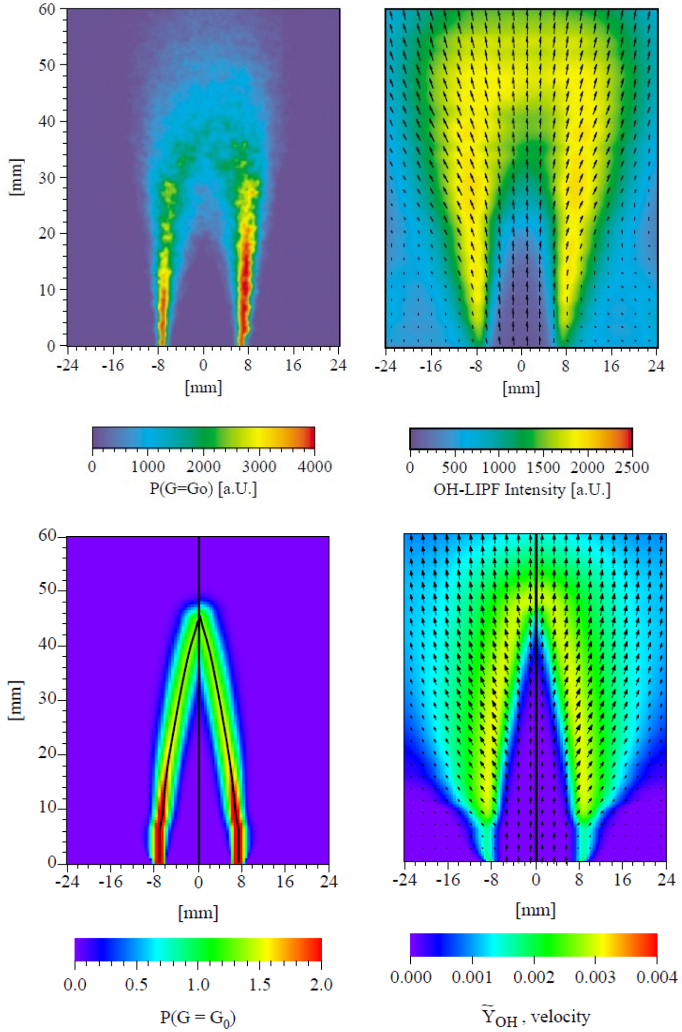
- Mean temperature (or other scalar)

$$\widetilde{T} = \int_{-\infty}^{+\infty} T(G)\,\widetilde{f}(G)\,\mathrm{d}G$$

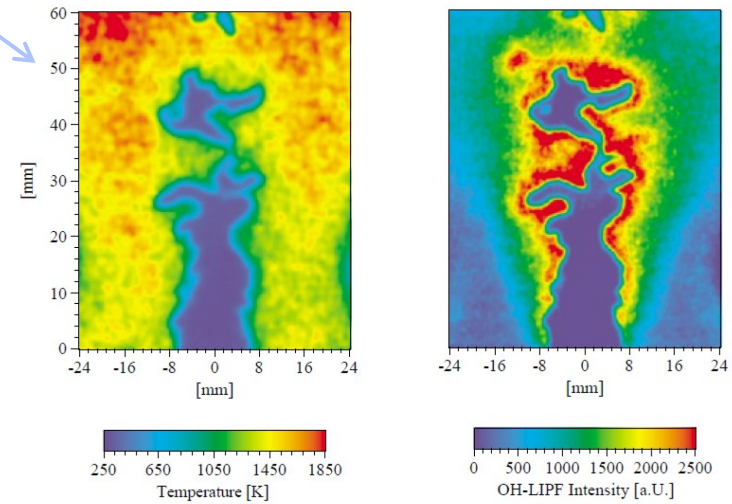
$T(G)$=$T(x)$ taken from laminar premixed flame without strain



Example: Presumed Shape PDF Approach (RANS)



experiment



computed numerically

G-Equation for LES

- Different averaging procedure[1]
- Start from progress variable C defined from temperature or reaction products
- Equation for Heaviside function centered at $C = C_0$

$$\frac{\partial}{\partial t}\left[H\left(C-C_0\right)\right]+u_j\frac{\partial}{\partial x_j}\left[H\left(C-C_0\right)\right]=$$
$$\mathcal{D}_C\kappa\left|\nabla\left[H\left(C-C_0\right)\right]\right|+\delta(C-C_0)\frac{1}{\rho}\left[n_j\frac{\partial}{\partial x_j}\left(\rho\mathcal{D}_C\left|\nabla C\right|\right)+\rho\dot{\omega}_C\right]$$

- With $\mathcal{G}\left(t,\mathbf{x}\right)=H\left(C\left(t,\mathbf{x}\right)-C_0\right)$

$$\frac{\partial}{\partial t}(\mathcal{G})+u_j\frac{\partial}{\partial x_j}(\mathcal{G})=\left(\mathcal{D}_C\kappa\right)_{C_0}\left|\nabla\mathcal{G}\right|+s_{L,C_0}\left|\nabla\mathcal{G}\right|$$

where

$$s_{L,C_0}=\left[\frac{1}{\left|\nabla C\right|\rho}\left(n_j\frac{\partial}{\partial x_j}\left(\rho\mathcal{D}_C\left|\nabla C\right|\right)+\rho\dot{\omega}_C\right)\right]_{C=C_0}$$

[1] E. Knudsen and H. Pitsch, A dynamic model for the turbulent burning velocity for large eddy simulation of premixed combustion, Combust. Flame, 154 (4), pp. 740–760, 2008.

G-Equation for LES

- Filtered Heaviside function

$$\overline{\mathcal{G}}\left(t,\mathbf{x}\right) \quad = \quad \int_V \mathcal{F}\left(\mathbf{r}\right)\mathcal{G}\left(t,\mathbf{x}+\mathbf{r}\right)d\mathbf{r}$$

- Modeled equation for filtered Heaviside function

$$\frac{\partial}{\partial t}(\overline{\mathcal{G}}) + \widetilde{u}_j \frac{\partial}{\partial x_j}(\overline{\mathcal{G}}) + \overline{\Gamma}_u = \frac{\rho_u}{\overline{\rho}}\left[\left(\overline{\mathcal{D}_C \kappa}\right)_{\overline{T},u} + s_{\overline{T},u}\right]\left|\nabla\overline{\mathcal{G}}\right|$$

describes evolution of filtered front, but cannot be adequately resolved in LES

- Introduce level set function describing filtered front evolution

$$\widehat{G}\left(\mathbf{x},t\right) = G_0 \quad \forall \quad \overline{\mathcal{G}}\left(\mathbf{x},t\right) = \mathcal{G}_0 \qquad \left|\nabla\widehat{G}\left(\mathbf{x},t\right)\right| = 1 \quad \forall \quad \overline{\mathcal{G}}\left(\mathbf{x},t\right)$$

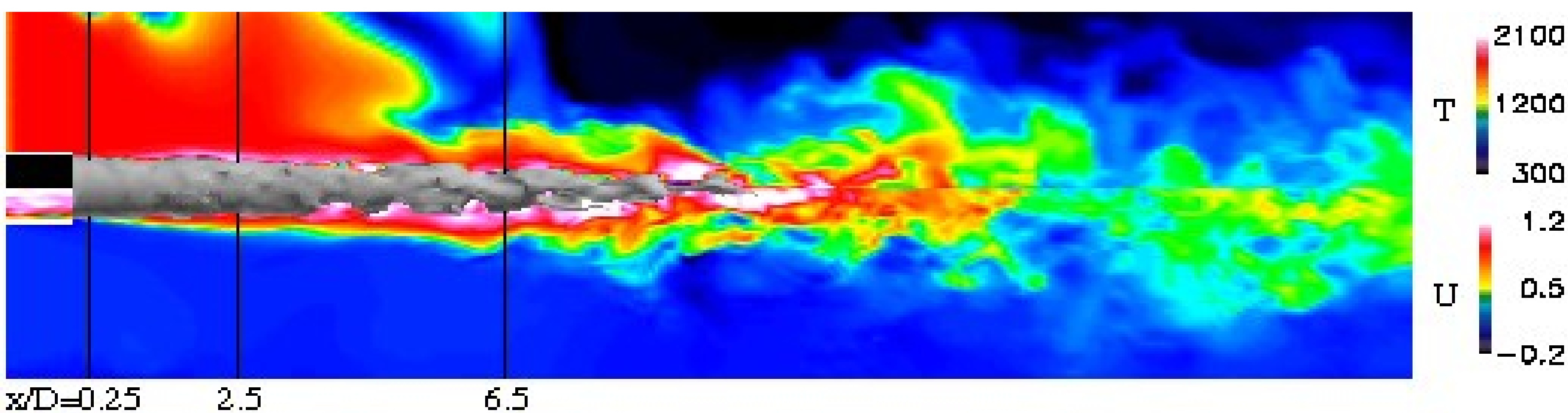
gives level set equation for filtered flame front

$$\frac{\partial}{\partial t}(\hat{G}) + \widetilde{u}_j \frac{\partial}{\partial x_j}(\hat{G}) = \frac{\rho_u}{\overline{\rho}}[\mathcal{D}_{t,u}\bar{\kappa} + s_{T,u}]|\nabla\hat{G}|$$

Example: LES of a Premixed Turbulent Bunsen Flame

- Premixed methan/air flame
- *Re* = 23486
- Broad, low velocity pilot flame → heat losses to burner
- Dilution by air co-flow

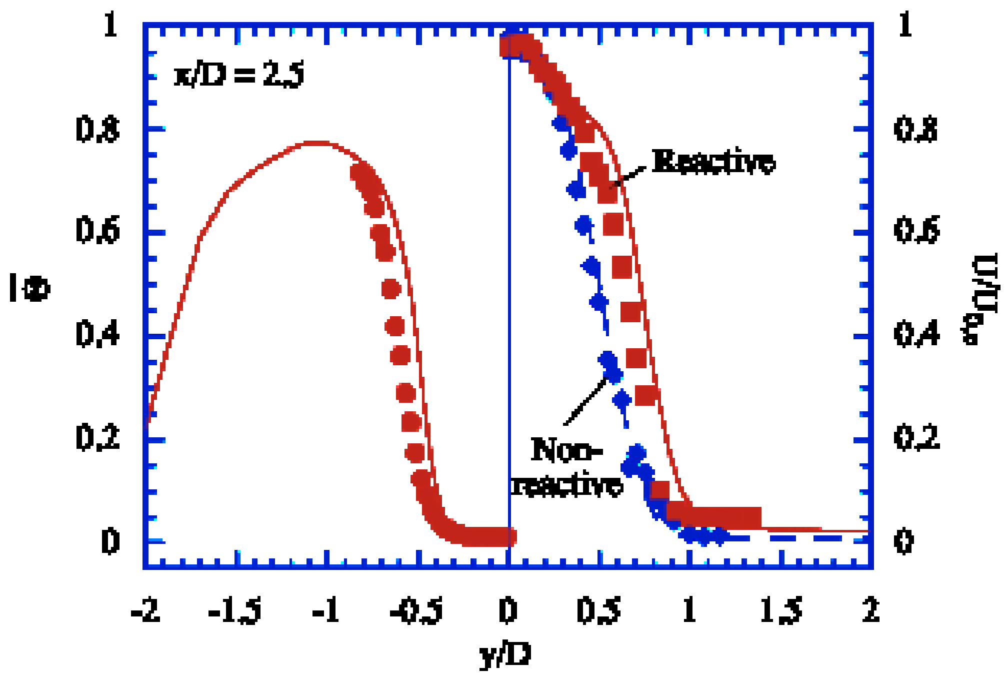
temperature



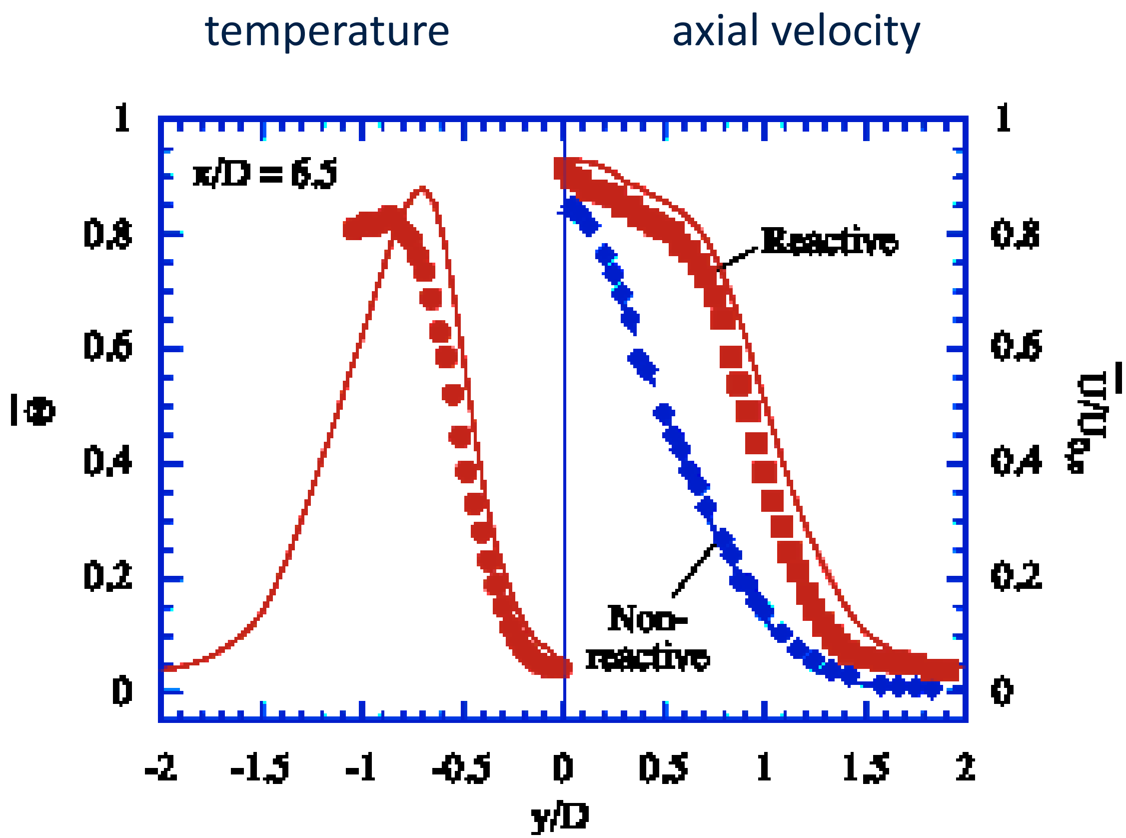
axial velocity

Time-Averaged Temperature and Axial Velocity at position x/D = 2.5

temperature axial velocity

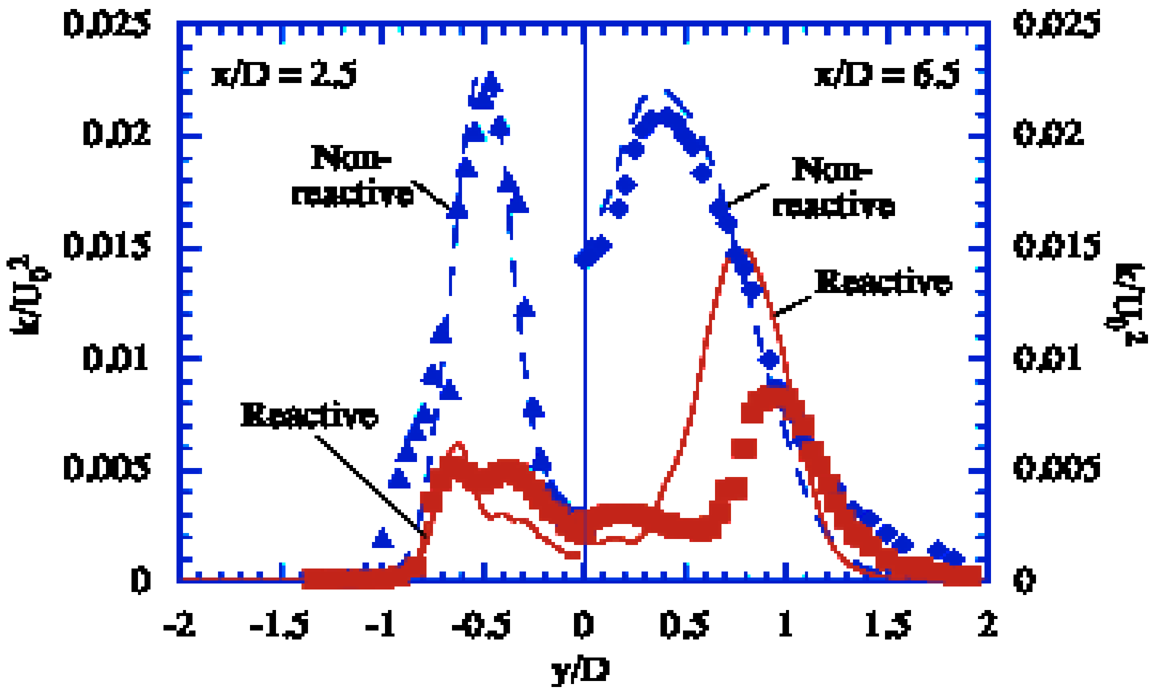


Time-Averaged Temperature and Axial Velocity at position x/D = 6.5

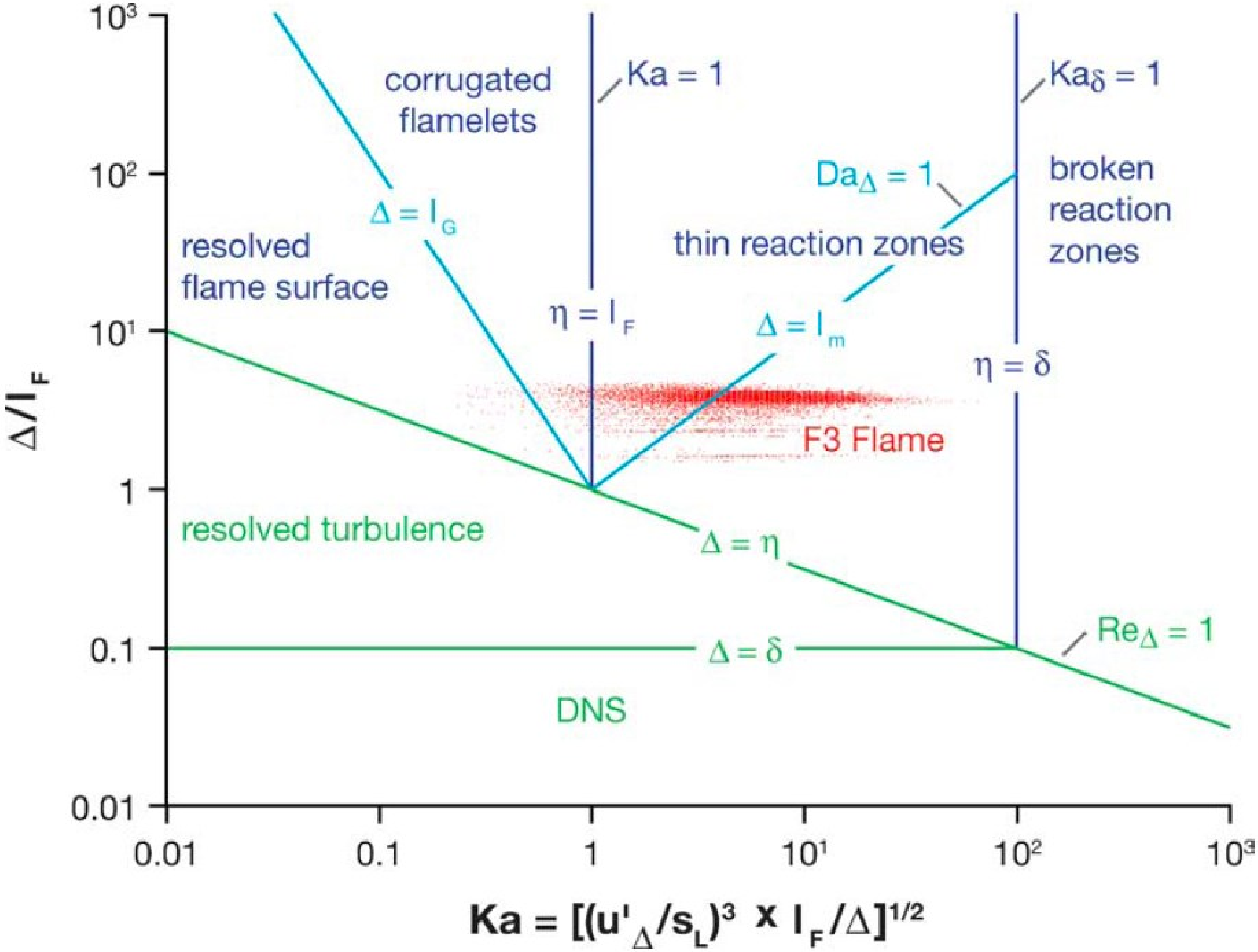


Turbulent Kinetic Energie at Position *x/D* = 2.5 and 6.5

x/D = 2,5 *x/D* = 6,5



LES Regime Diagram for Premixed Turbulent Combustion



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Mixture Fraction Z

- Assume
  - One-step global reaction: $\nu_F\, F + \nu_O\, O \rightarrow \nu_P\, P$
  - $Le_i = 1$

- Species transport and temperature equations

$$\rho \frac{\partial Y_i}{\partial t} + \rho \boldsymbol{v} \cdot \nabla Y_i = \nabla \cdot (\rho D \nabla Y_i) + W_i \nu_i w$$

$$\rho \frac{\partial T}{\partial t} + \rho \boldsymbol{v} \cdot \nabla T = \nabla \cdot (\rho D \nabla T) + \frac{Q}{c_p} w$$

- With

$$L(\phi) = \rho \frac{\partial \phi}{\partial t} + \rho \boldsymbol{v} \cdot \nabla \phi - \nabla \cdot (\rho D \nabla \phi)$$

follows

$$L(Y_i) = W_i \nu_i w$$

$$L(T) = \frac{Q}{c_p} w$$

Mixture Fraction Z

- Derive coupling function β by eliminating *w* such that

$$L(\beta) = 0$$

- With

$$\nu = \frac{W_{\mathrm{O}}\nu_{\mathrm{O}}}{W_{\mathrm{F}}\nu_{\mathrm{F}}}$$

and

$$\begin{aligned} L(\nu Y_F) &= W_{\mathrm{O}}\nu_{\mathrm{O}} w \\ L(Y_O) &= W_{\mathrm{O}}\nu_{\mathrm{O}} w \end{aligned}$$

follows

$$\beta \equiv \nu Y_{\mathrm{F}} - Y_{\mathrm{O}}$$

- Normalization between 0 and 1 gives

$$Z \equiv \frac{\beta - \beta_2}{\beta_1 - \beta_2} = \frac{\nu Y_{\mathrm{F}} - Y_{\mathrm{O}} + Y_{\mathrm{O},2}}{\nu Y_{\mathrm{F},1} + Y_{\mathrm{O},2}}$$

Transport Equation for Z

- Transport equation

$$\rho \frac{\partial Z}{\partial t} + \rho u_j \frac{\partial Z}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho D \frac{\partial Z}{\partial x_j}\right)$$

  - Advantage: $L(Z) = 0$ → No Chemical Source Term
  - BC: $Z = 0$ in Oxidator, $Z = 1$ in Fuel

- If species and temperature function of mixture fraction, then

$$\widetilde{T} = \int_{-\infty}^{+\infty} T(Z)\,\widetilde{f}(Z)\,\mathrm{d}Z \quad \text{and} \quad \widetilde{Y}_i = \int_{-\infty}^{+\infty} Y_i(Z)\,\widetilde{f}(Z)\,\mathrm{d}Z$$

- Needed:
  - Local statistics of Z (expressed by PDF)
  - Species/temperature as function of Z: $Y_i(Z)$ and $T(Z)$

Presumed PDF Approach

- Equation for the mean

[redacted]

and the variance of Z

$$-\,D_t \frac{\partial \widetilde{Z''^2}}{\partial x_i} \qquad\qquad D_t \frac{\partial \widetilde{Z}}{\partial x_i} \qquad\qquad c_\chi \frac{\widetilde{\varepsilon}}{\widetilde{k}} \widetilde{Z''^2}$$

$$\underbrace{\overline{\rho}\frac{\partial \widetilde{Z''^2}}{\partial t}}_{\text{L}} + \underbrace{\overline{\rho}\widetilde{u}_i \frac{\partial \widetilde{Z''^2}}{\partial x_i}}_{\text{C}} = \underbrace{-\frac{\partial}{\partial x_i}\left(\overline{\rho}\, \widetilde{u_i'' Z''^2}\right)}_{\text{turb. DF}} \underbrace{+ 2\overline{\rho}\left(-\widetilde{u_i'' Z''}\right)\frac{\partial \widetilde{Z}}{\partial x_i}}_{\text{P}} \underbrace{- \overline{\rho}\ \widetilde{\chi}}_{\text{DS}}$$

are known and closed

Presumed PDF Approach

- β-function pdf for mixture fraction Z

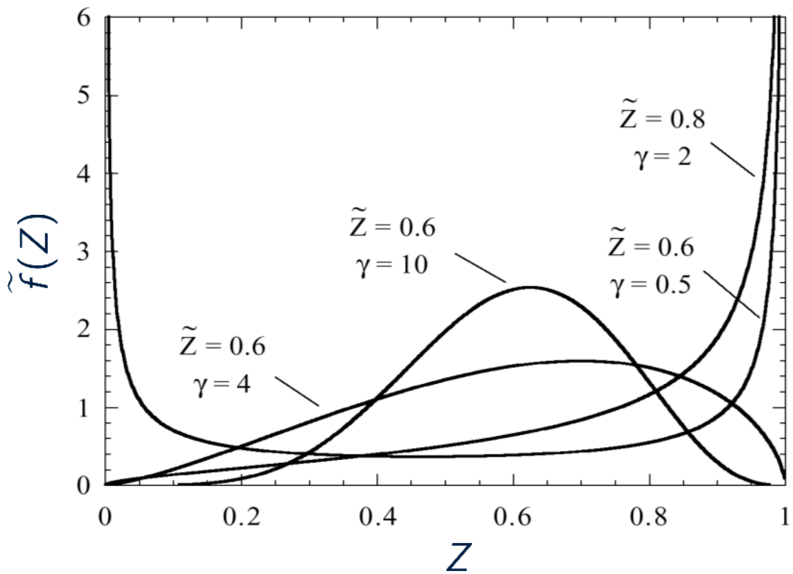
$$\widetilde{f}(Z;x_i,t)=\frac{Z^{\alpha-1}(1-Z)^{\beta-1}\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}$$

- With

$$\alpha=\widetilde{Z}\gamma,\quad \beta=(1-\widetilde{Z})\gamma \quad \text{and}$$

$$\gamma=\frac{\widetilde{Z}(1-\widetilde{Z})}{\widetilde{Z''^2}}-1\geq 0$$

$$\widetilde{T}=\int_{-\infty}^{+\infty}T(Z)\widetilde{f}(Z)\,\mathrm{d}Z,\quad \widetilde{Y}_i=\int_{-\infty}^{+\infty}Y_i(Z)\widetilde{f}(Z)\,\mathrm{d}Z$$



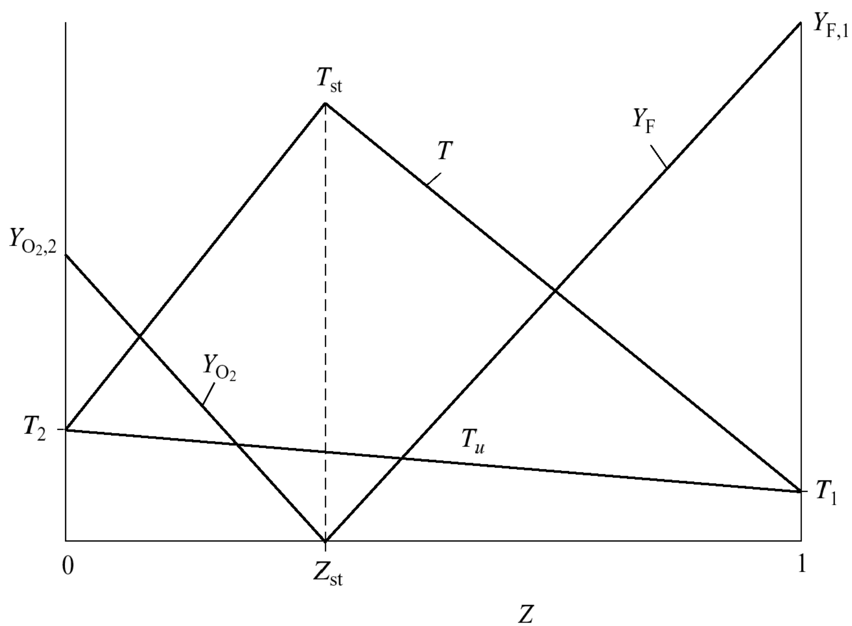
- Infinitely fast irreversible chemistry
  - Burke-Schumann solution
  - Solution = $f(Z)$
- Infinitely fast reversible chemistry
  - Chemical equilibrium
  - Solution = $f(Z)$

$$\tilde{T} = \int_{-\infty}^{+\infty} T(Z)\tilde{f}(Z)\,\mathrm{d}Z, \quad \tilde{Y}_i = \int_{-\infty}^{+\infty} Y_i(Z)\tilde{f}(Z)\,\mathrm{d}Z$$

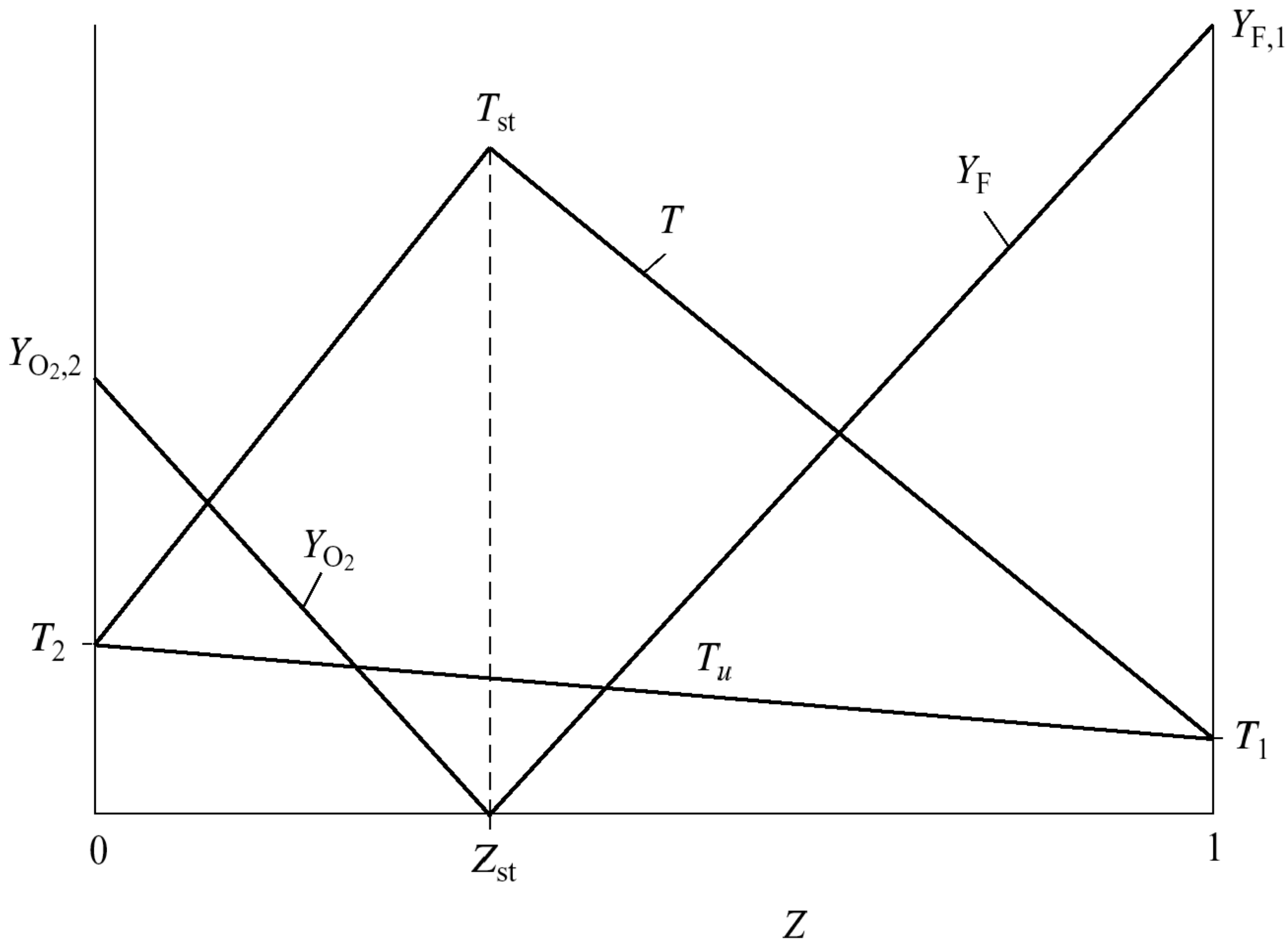
- Flamelet model for non-premixed combustion
  - Chemistry fast, but not infinitely fast
  - Solution = f(Z, χ)
- Conditional Moment Closure (CMC)
  - Similar to flamelet model
  - Solution = $f(Z, \langle \chi | Z \rangle)$

- Infinitely fast irreversible chemistry
  - Burke-Schumann solution
  - Solution = $f(Z)$
- Infinitely fast reversible chemistry
  - Chemical equilibrium
  - Solution = $f(Z)$

$$\widetilde{T} = \int_{-\infty}^{+\infty} T(Z)\widetilde{f}(Z)\,\mathrm{d}Z, \quad \widetilde{Y}_i = \int_{-\infty}^{+\infty} Y_i(Z)\widetilde{f}(Z)\,\mathrm{d}Z$$



Burke-Schumann Solution



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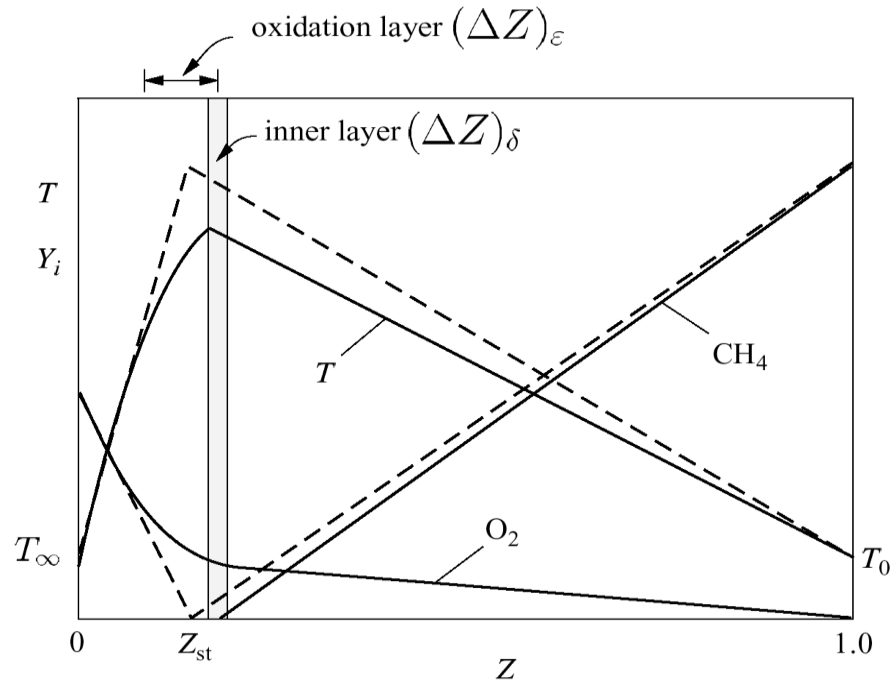
Flamelet Model for Non-Premixed Turbulent Combustion

- Basic idea: Scale separation
- Assume fast, but not infinitely fast chemistry: $1 \ll Da \ll \infty$
- Reaction zone is thin compared to small scales of turbulence and hence retains laminar structure
- Transformation and asymptotic approximation leads to flamelet equations



Flamelet Model for Non-Premixed Turbulent Combustion

- Balance equations for temperature, species and mixture fraction

$$\rho\frac{\partial T}{\partial t}+\rho u_i\frac{\partial T}{\partial x_i}-\frac{\partial}{\partial x_i}\left(\rho D\frac{\partial T}{\partial x_i}\right)=-\sum_{\alpha=1}^{n}\frac{h_\alpha}{c_p}\dot{m}_\alpha'''+\frac{\dot{q}_R'''}{c_p}+\frac{1}{c_p}\frac{\partial p}{\partial t}$$

$$\rho\frac{\partial Y_\alpha}{\partial t}+\rho u_i\frac{\partial Y_\alpha}{\partial x_i}-\frac{\partial}{\partial x_i}\left(\rho D\frac{\partial Y_\alpha}{\partial x_i}\right)=\dot{m}_\alpha'''$$

$$\rho\frac{\partial Z}{\partial t}+\rho u_i\frac{\partial Z}{\partial x_i}-\frac{\partial}{\partial x_i}\left(\rho D\frac{\partial Z}{\partial x_i}\right)=0$$

- With

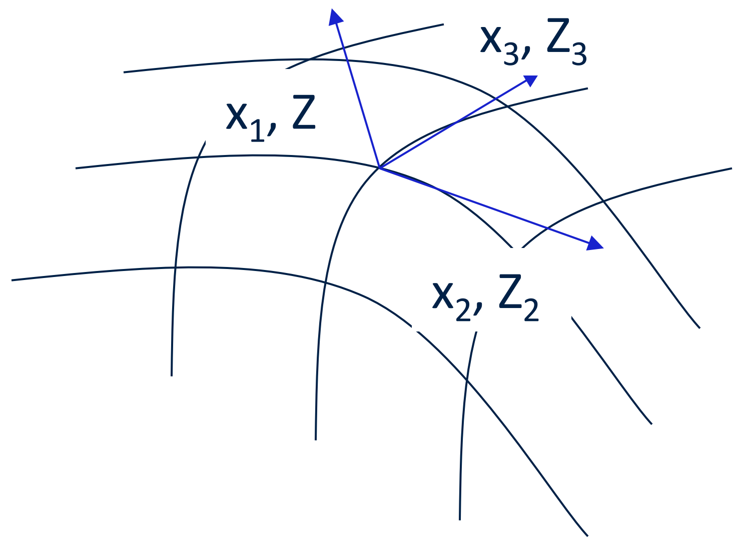
$$\mathcal{L}\equiv\rho\frac{\partial}{\partial t}+\rho u_i\frac{\partial}{\partial x_i}-\frac{\partial}{\partial x_i}\left(\rho D\frac{\partial}{\partial x_i}\right)$$

it follows

$$\mathcal{L}(T)=-\sum_{\alpha=1}^{n}\frac{h_\alpha}{c_p}\dot{m}_\alpha'''+\frac{\dot{q}_R'''}{c_p}+\frac{1}{c_p}\frac{\partial p}{\partial t},\qquad \mathcal{L}(Y_\alpha)=\dot{m}_\alpha'''\qquad \text{and}\qquad \mathcal{L}(Z)=0$$

Flamelet Equations

- Consider surface of stoichiometric mixture
- Reaction zone confined to thin layer around this surface
- Transformation to surface attached coordinate system
- $x_1, x_2, x_3, t \rightarrow Z(x_1, x_2, x_3, t), Z_2, Z_3, \tau$



Transformation rules

- Transformation: $x_1, x_2, x_3, t \rightarrow Z(x_1, x_2, x_3, t), Z_2, Z_3, \tau$ (where $Z_2 = x_2$, $Z_3 = x_3$, $\tau = t$)

[redacted]

- Example: Temperature T

0 0 1

[redacted] $\longrightarrow$ [redacted]

0 0 0

[redacted] $\longrightarrow$ [redacted]

1 0 0

[redacted] $\longrightarrow$ [redacted]

Analogous for x_3

Flamelet Equations

- Temperature equation

$$\mathcal{L}(T) = -\sum_{\alpha=1}^{n} \frac{h_\alpha}{c_p} \dot{m}_\alpha''' + \frac{\dot{q}_R'''}{c_p} + \frac{1}{c_p}\frac{\partial p}{\partial t} = \dot{\omega}_T$$

→ Transformed temperature equation:

$$\rho \frac{\partial T}{\partial \tau} + \rho u_j \frac{\partial T}{\partial Z_j} - \rho D \left[2 \frac{\partial Z}{\partial x_j} \frac{\partial^2 T}{\partial Z \partial Z_j} + \frac{\partial^2 T}{\partial Z_j^2} \right] - \frac{\partial}{\partial x_j} \left(\rho D \frac{\partial T}{\partial Z_j} \right) - \rho D \left(\frac{\partial Z}{\partial x_i} \right)^2 \frac{\partial^2 T}{\partial Z^2} = \dot{\omega}_T, \quad j = 2, 3$$

Flamelet Equations

$$\boxed{\rho\frac{\partial T}{\partial \tau}} + \rho u_j\frac{\partial T}{\partial Z_j} - \rho D\left[2\frac{\partial Z}{\partial x_j}\frac{\partial^2 T}{\partial Z\partial Z_j} + \frac{\partial^2 T}{\partial Z_j^2}\right] - \frac{\partial}{\partial x_j}\left(\rho D\frac{\partial T}{\partial Z_j}\right)$$

small

$$\boxed{-\rho D\left(\frac{\partial Z}{\partial x_i}\right)^2\frac{\partial^2 T}{\partial Z^2} = \dot{\omega}_{\mathrm{T}},} \quad j = 2, 3$$

Local change

Describes mixing

Source term

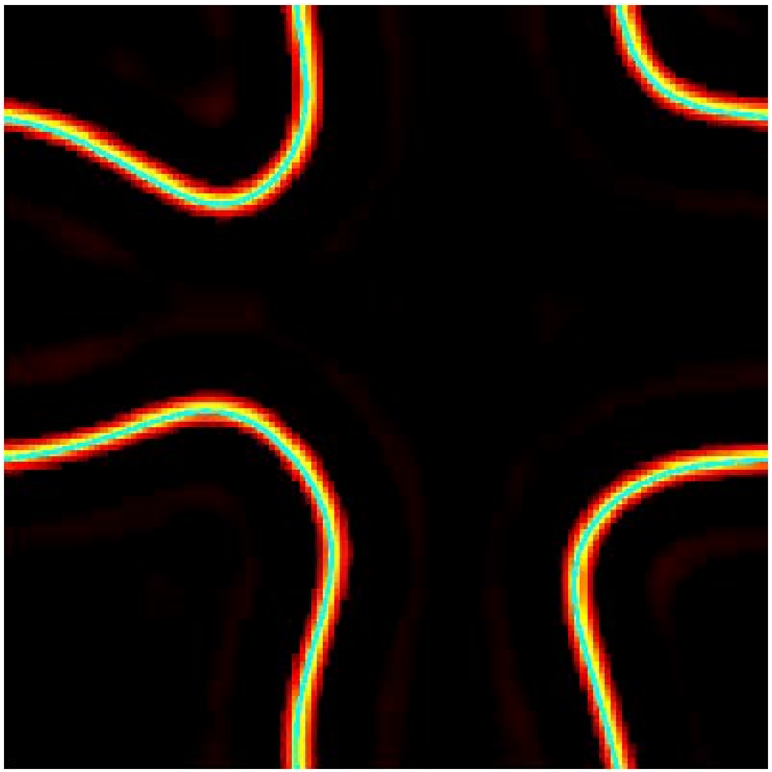
- If the flamelet is thin in the *Z* direction, an order-of-magnitude analysis similar to that for a boundary layer shows that

$$\left(\frac{\partial Z}{\partial x_i}\right)^2\frac{\partial^2 T}{\partial Z^2}$$

  is the dominating term of the spatial derivatives
- Equivalent to the assumption that temperature derivatives normal to the flame surface are much larger than those in tangential direction
- $\partial T/\partial \tau$ is important if very rapid changes, such as extinction, occur

Example

- Example from DNS of Non-Premixed Combustion in Isotropic Turbulence



- Temperature (color)
- Stoichiometric mixture fraction (line)

Flamelet Equations

- Same procedure for the mass fraction…
- Flamelet structure is to leading order described by the one-dimensional time-dependent equations

→

$$\rho\frac{\partial T}{\partial \tau} - \frac{\rho\chi_{st}}{2}\frac{\partial^2 T}{\partial Z^2} = \dot{\omega}_T$$
$$\rho\frac{\partial Y_\alpha}{\partial \tau} - \frac{\rho\chi_{st}}{2}\frac{\partial^2 Y_\alpha}{\partial Z^2} = \dot{m}'''_\alpha$$

$$\longrightarrow \quad \boxed{\rho\frac{\partial \psi_i}{\partial \tau} - \frac{\rho\chi_{st}}{2}\frac{\partial^2 \psi_i}{\partial Z^2} = \dot{\omega}_{\psi_i}}$$

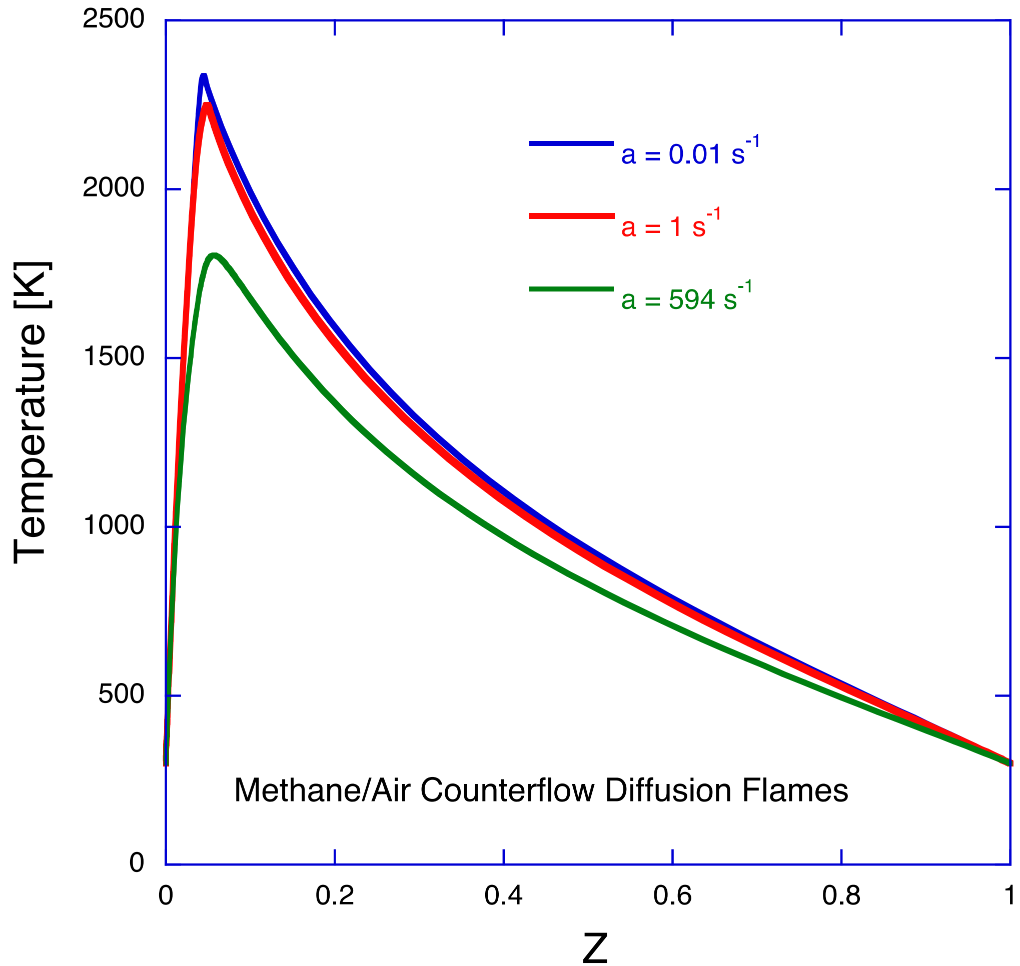
- Instantaneous scalar dissipation rate at stoichiometric conditions

$$\chi_{st} = 2D\left(\frac{\partial Z}{\partial x_i}\right)^2\Bigg|_{st}$$

→ $[\chi_{st}]$ = 1/s: may be interpreted as the inverse of a characteristic diffusion time

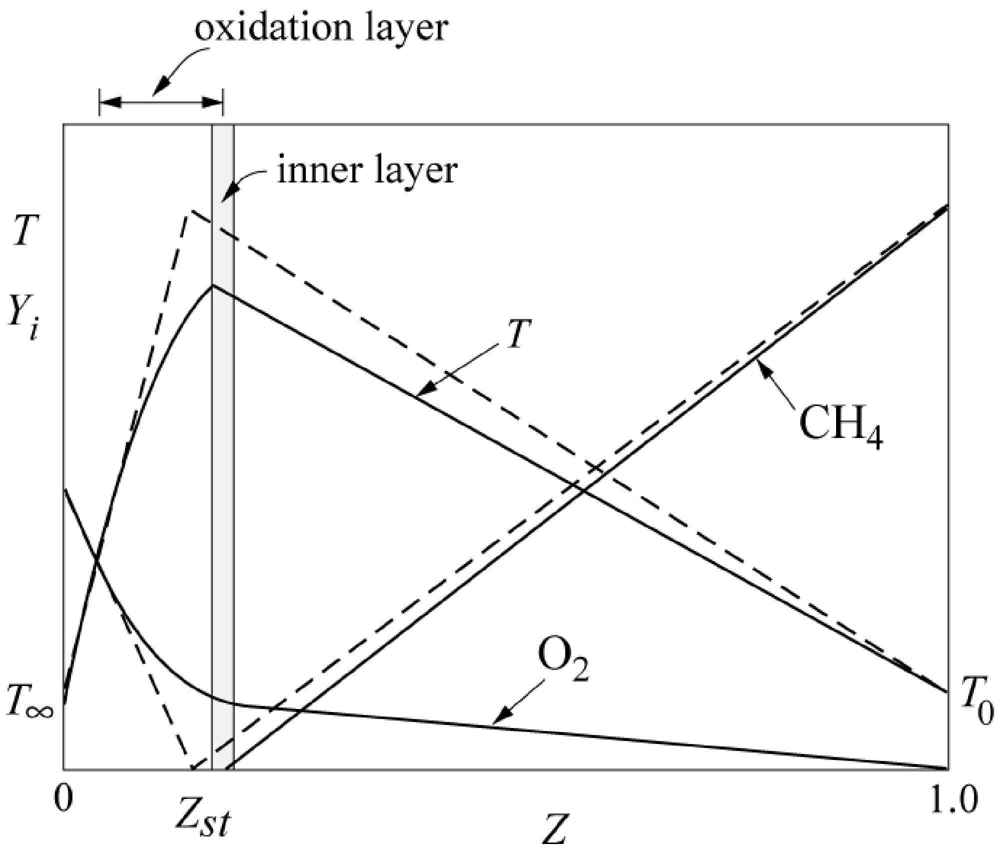
Temperature profiles for methane-air flames

- Temperature profiles for methane-air flames



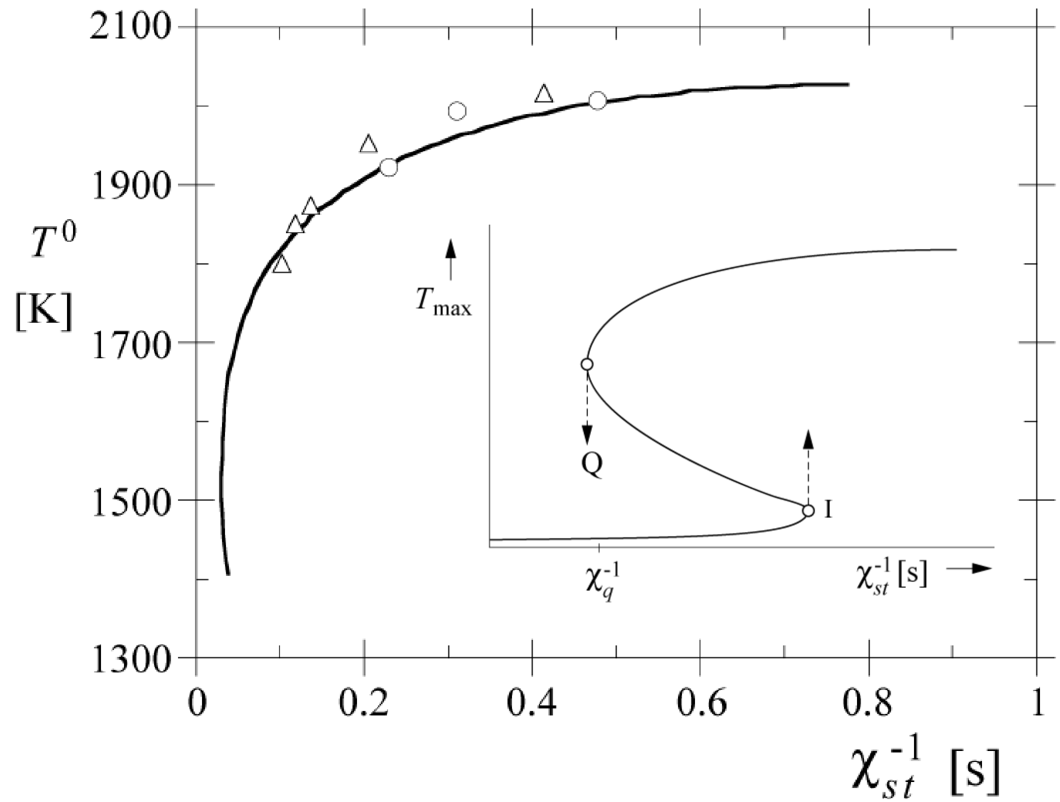
Flamelet Equations

- Asymptotic analysis by Seshadri (1988)
  - Based on four-step model
  - Close correspondence between layers identified in premixed diffusion flames



$$\begin{aligned}
CH_4 + 2H + H_2O &= CO + 4H_2 \\
CO + H_2O &= CO_2 + H_2 \\
H + H + M &= H_2 + M \\
O_2 + 3H_2 &= 2H + 2H_2O
\end{aligned}$$

- The calculations agree well with numerical and experimental data
- They also show the vertical slope of T^0 versus χ_{st} which corresponds to extinction



Flamelet Equations

- Steady state flamelet equations provide $\psi_i = f(Z, \chi_{st})$
- If joint pdf $\widetilde{P}(Z, \chi_{st})$ is known

  → Favre mean of ψ_i:

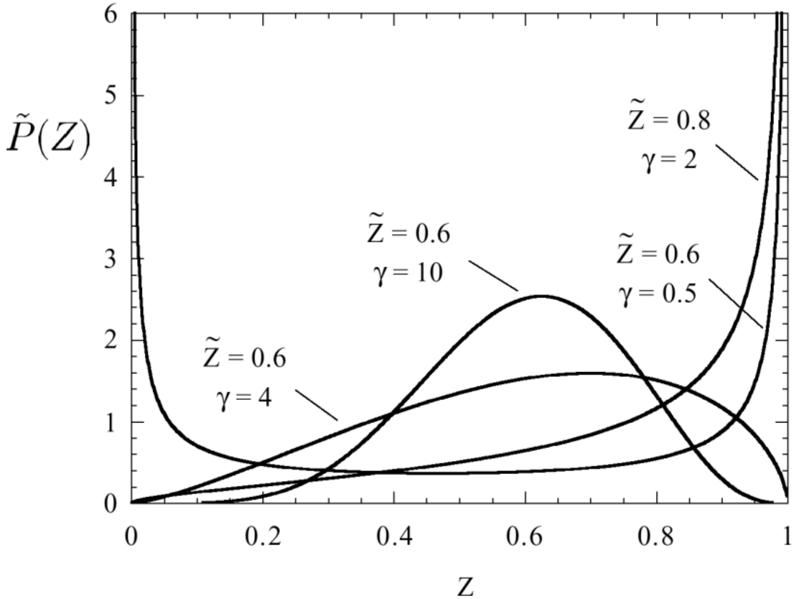
$$\widetilde{\psi}_i(x_j, t) = \int_0^1 \int_0^\infty \psi_i(Z, \chi_{st}) \widetilde{P}(Z, \chi_{st}; x_j, t) \mathrm{d}\chi_{st} \mathrm{d}Z$$

- If the unsteady term in the flamelet equation must be retained, joint statistics of Z and χ_{st} become impractical
- Then, in order to reduce the dimension of the statistics, it is useful to introduce multiple flamelets, each representing a different range of the χ-distribution
- Such multiple flamelets are used in the Eulerian Particle Flamelet Model (EPFM) by Barths et al. (1998)
- Then the scalar dissipation rate can be formulated as function of the mixture fraction

Flamelet Equations

- Modeling the conditional Favre mean scalar dissipation rate

$$\widetilde{\chi}_Z = \frac{\langle \rho\chi | Z \rangle}{\langle \rho | Z \rangle}$$



- Flamelet equations

$$\rho \frac{\partial \psi_i}{\partial t} - \frac{\rho}{Le_i} \frac{\chi_Z}{2} \frac{\partial^2 \psi_i}{\partial Z^2} = \dot{\omega}_{\psi_i} \longrightarrow \psi_i(Z, \widetilde{\chi}_Z, t)$$

- Favre mean

$$\widetilde{\psi}_i(x_j, t) = \int_0^1 \psi_i(Z, \widetilde{\chi}_Z, t) \widetilde{P}(Z; x_j, t) \mathrm{d}Z, \quad \text{with} \quad \widetilde{P}(Z; x_j, t) = \frac{Z^{\alpha-1}(1-Z)^{\beta-1}\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}$$

Flamelet Equations

- Model for conditional scalar dissipation rate $\widetilde{\chi}_Z$
- One relates the conditional scalar dissipation rate to that at a fixed value Z_{st} by

$$\widetilde{\chi}_Z = \boxed{\widetilde{\chi}_{st}} \frac{f(Z)}{f(Z_{st})}$$

– With

$$\boxed{\widetilde{\chi}} = c_\chi \frac{\widetilde{\varepsilon}}{\widetilde{k}} \widetilde{Z''^2}$$

$$\widetilde{\chi} = \int_0^1 \widetilde{\chi}_Z \widetilde{P}(Z) \mathrm{d}Z = \widetilde{\chi}_{st} \int_0^1 \frac{f(Z)}{f(Z_{st})} \widetilde{P}(Z) \mathrm{d}Z \quad \rightarrow \quad \boxed{\widetilde{\chi}_{st}} = \frac{\boxed{\widetilde{\chi}} f(Z_{st})}{\int_0^1 f(Z) \widetilde{P}(Z) \mathrm{d}Z}$$

Representative-Interactive-Flamelet-Modell (RIF)

- Flamelet equations are unsteady
- RIF model solves unsteady flamelet equations coupled with CFD code[1]
- Describes ignition, combustion, and pollutant formation for non-premixed combustion
  → Typical application for diesel engines

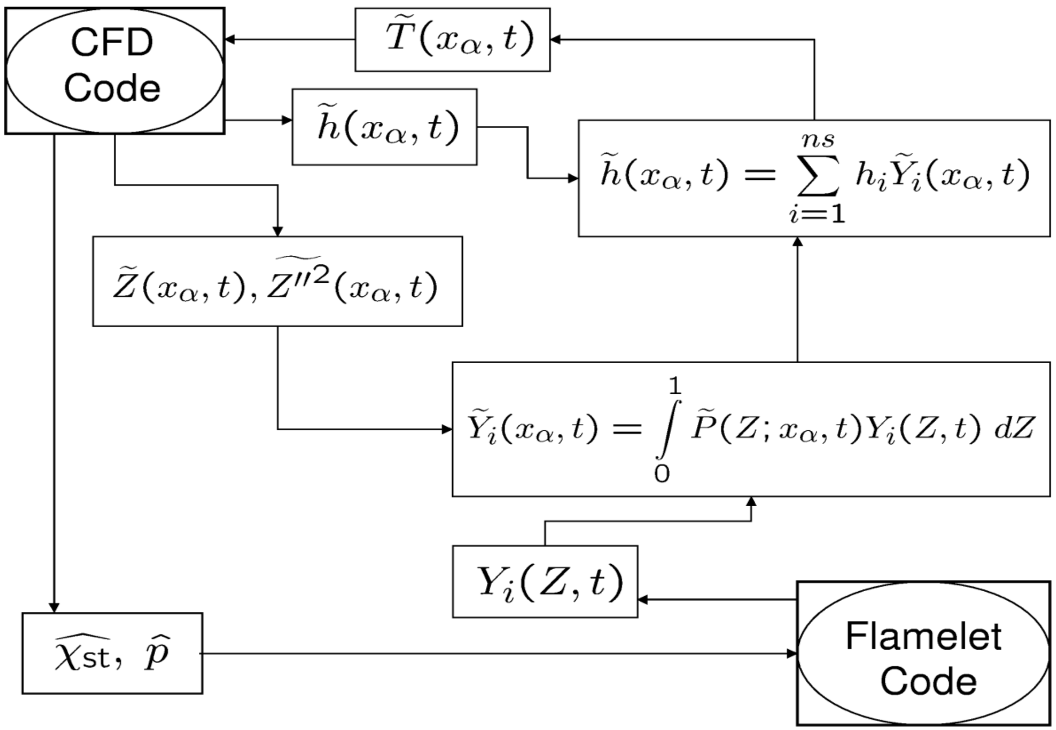
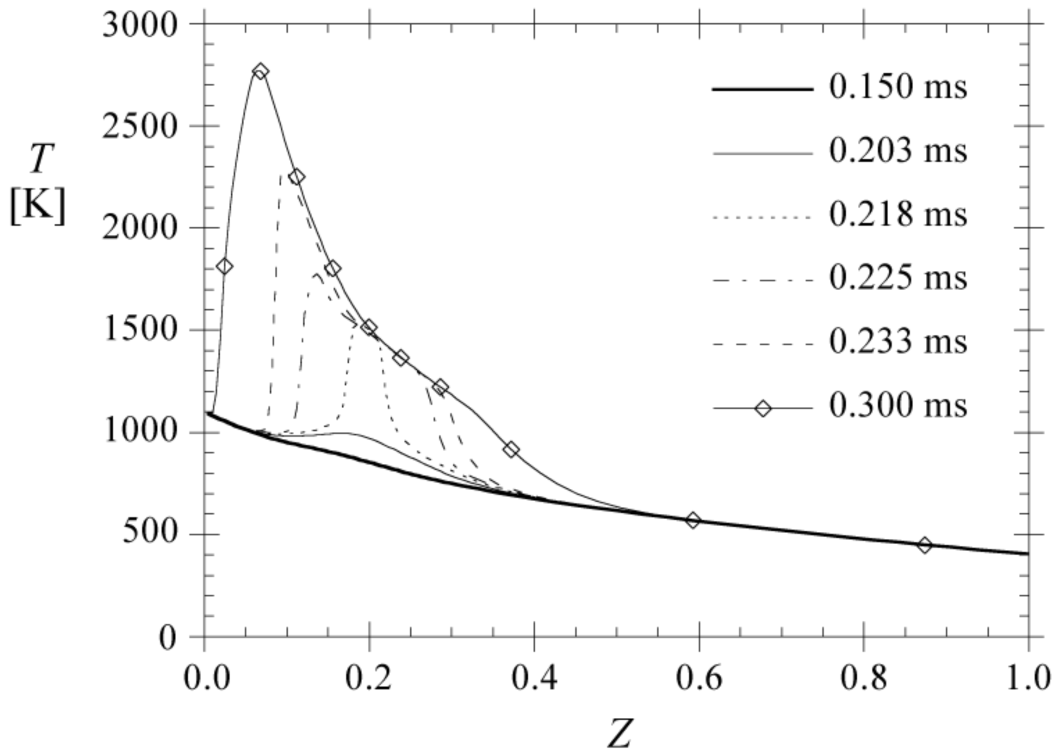


Illustration of coupling between RIF code and CFD code

[1] Barths, H., Pitsch, H., Peters, N., 3D Simulation of DI Diesel Combustion and Pollutant Formation Using a Two-Component Reference Fuel, Oil & Gas Science and Technology Rev. IFP 54, pp. 233-244, 1999.

n-Heptane Air Ignition

- The initial air temperature is 1100 K and the initial fuel temperature is 400 K.



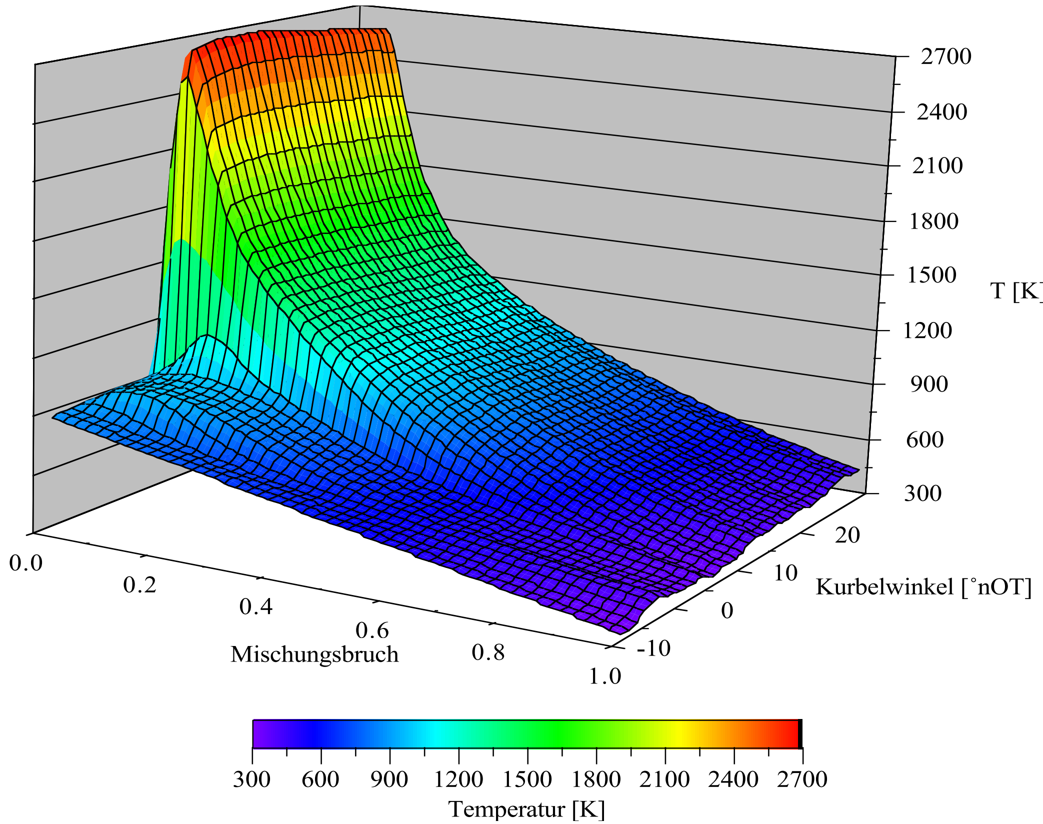
Example: Diesel engine simulation

- VW 1,9 l DI-Diesel engine (Fuel: *n*-Heptan)
- Simulation:
  - KIVA-Code
  - RIF-Model
  - *n*-Heptan detailed chemistry
  - Soot and No_x as function of EGR

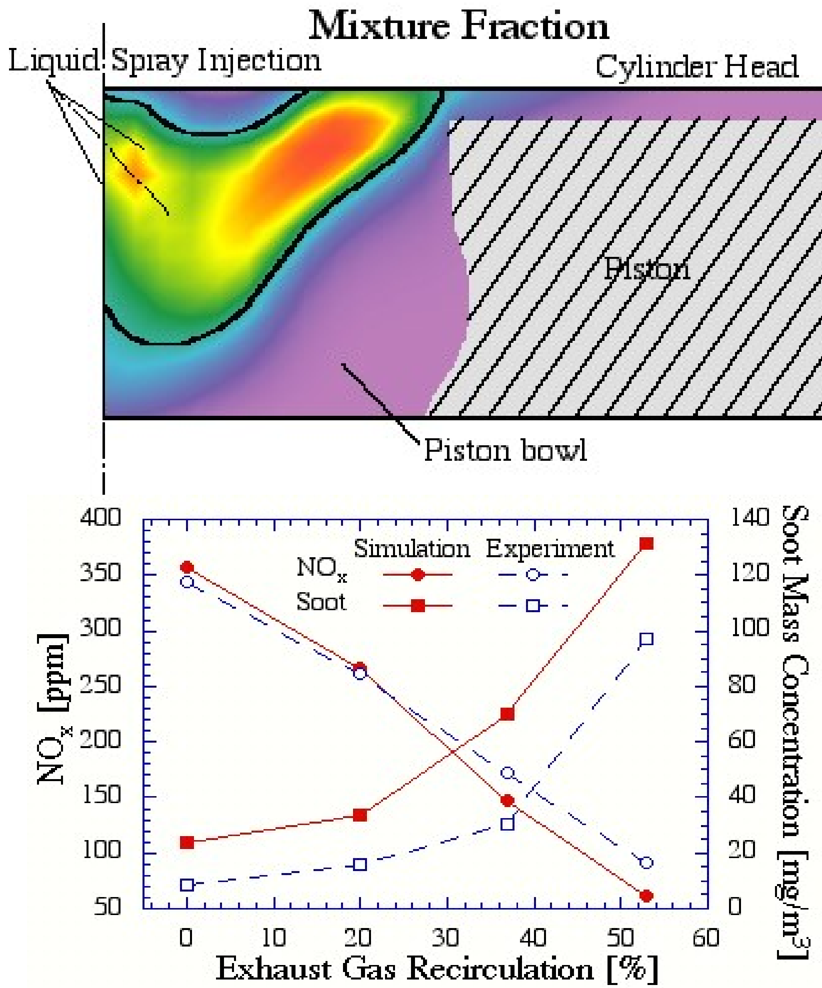
Model:	Volkswagen DI 1.9 l
Piston Displacement:	1896 cm^3
Bore:	79.5 mm
Stroke:	95.0 mm
Connecting Rod Length:	144.0 mm
Compression Ratio:	17.5:1
Nozzle:	5-Hole
Hole Diameter:	0.194 mm
Opening Pressure:	250 bar
Injection Angle:	150°
Operation Point:	2000 rpm
Fuel:	*n*-Heptane
Injected Fuel Mass:	8 mg

Example: Diesel engine simulation

- RIF-Temperature



Example: Diesel engine simulation

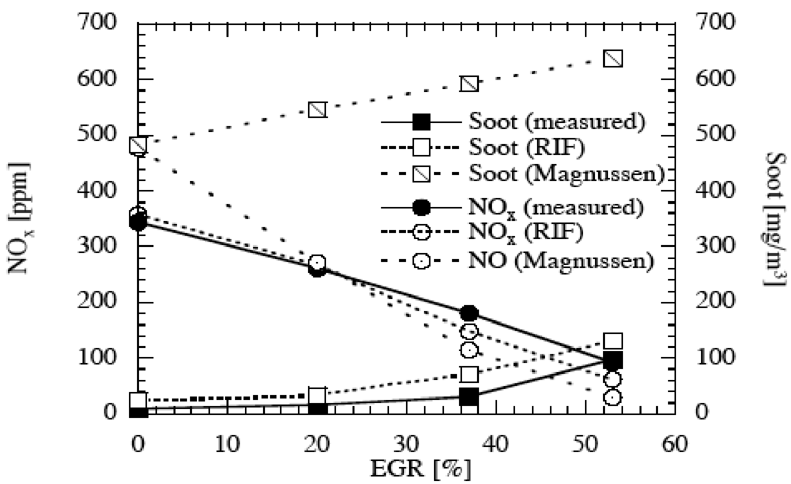


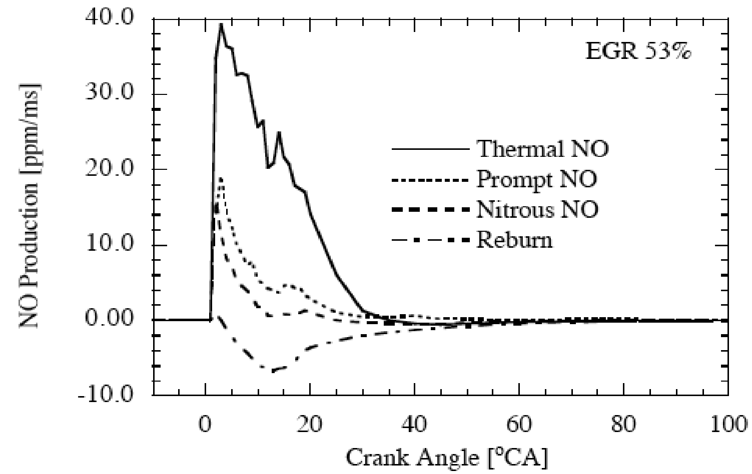
Mischungsbruch-
verteilung

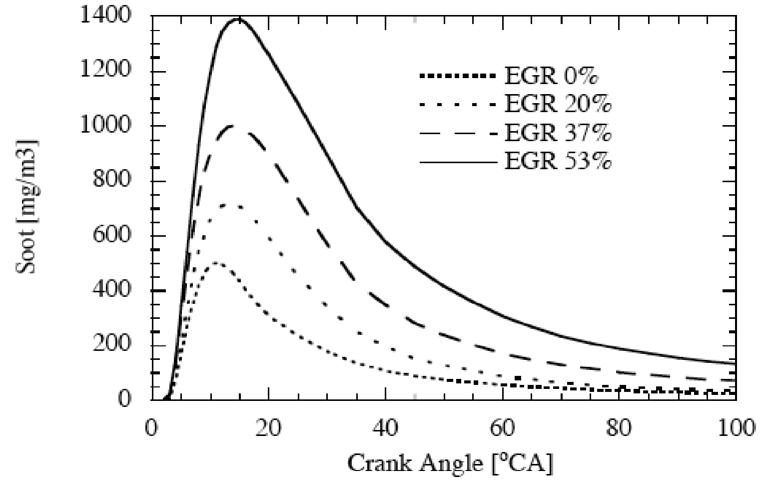
Schadstoff-
bildung

Example: Diesel engine simulation

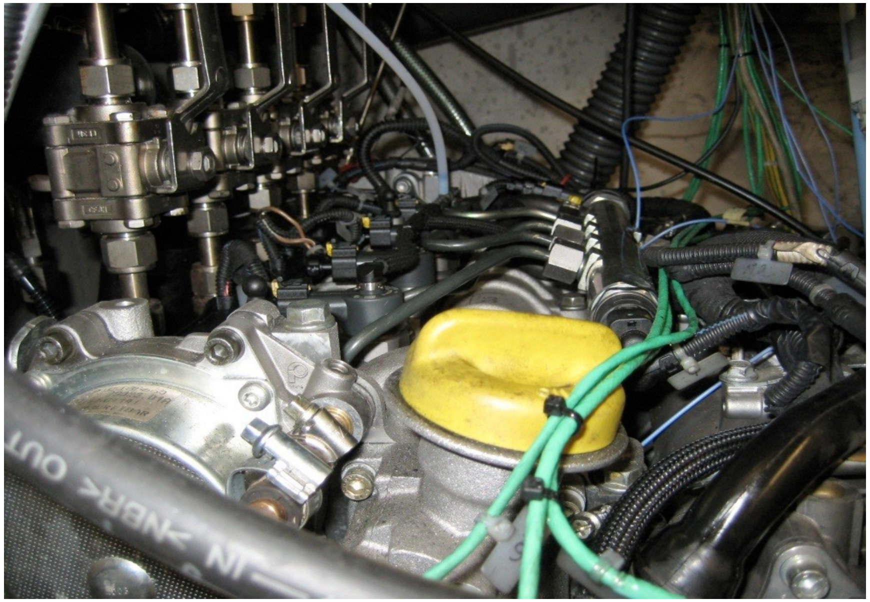
- Comparison with Magnussen-/ Hiroyasu-Model







Example: ITV Diesel Engine Test Bench

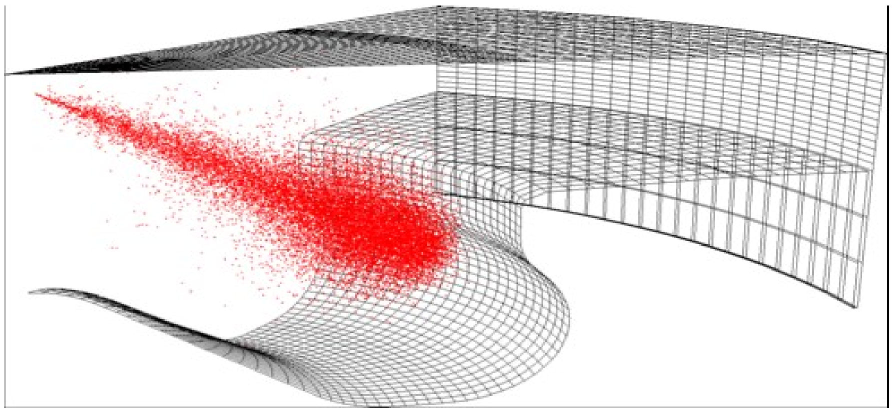


Engine type	4 cylinder diesel engine
Bore	82.0 mm
Stroke	90.4 mm
Displacement	1910 mm^3
Pistons	Reentrant type
Compression ratio	17.5:1
Valves	16 V
Max. Power	110 kW (150 PS)
Swirl number	2.5
Injection system	Bosch Common-Rail (2nd generation), central injector position, 7 holes nozzle

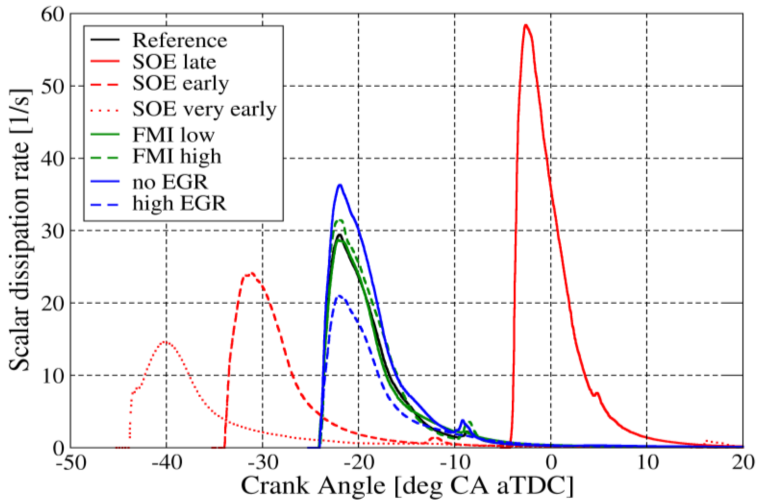
- The range of operation was extended for partially homogenized conditions (PCCI)
- High performance measurement equipment
  - Rapid and dynamic measurement of EGR
  - Fast sensors with cycle-to-cycle resolution for NO_x and uHC
  - Stationary measurement of soot, CO, CO2, ...

Numerical Setup

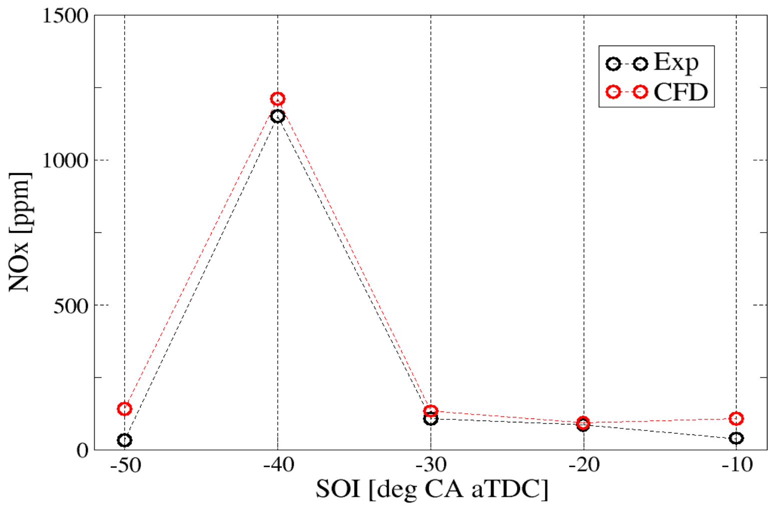
- Multidimensional CFD-RANS code AC-FLuX
- Computations performed for variations in
  - Start of energizing (SOE): 10, 20, 30, 40 and 50 deg CA bTDC
  - Fuel mass injected (FMI): 11, 12, 13.5 and 17.5 mm3/cycle
  - Exhaust gas recirculation (EGR): 0, 15, 26, 33 and 34 %
- Computations from IVC to EVO
- Sector grid of the combustion chamber (~ 50000 cells)
- Two different meshes for compression and combustion
- RIF combustion model initialized at start of injection

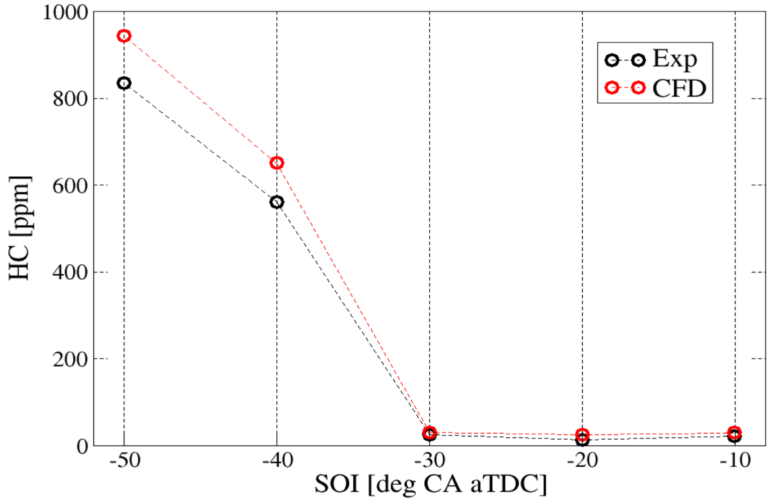


Multi-Zone Model Results

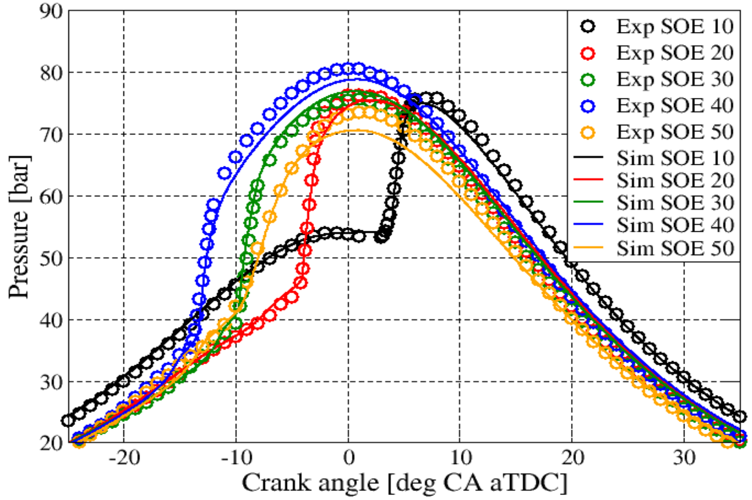


- Scalar dissipation rate:
  - Strong influence of SOE on position and maximum
  - FMI and EGR only affect the maximum value
- IMEP:
  - Good qualitative agreement
  - Noticeable deviation at SOE 50
- CA50:
  - Even better agreement
  - Only minor deviations observable

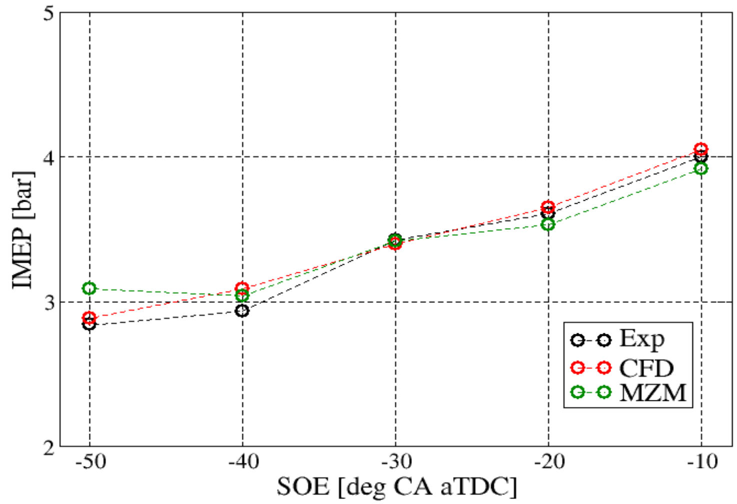


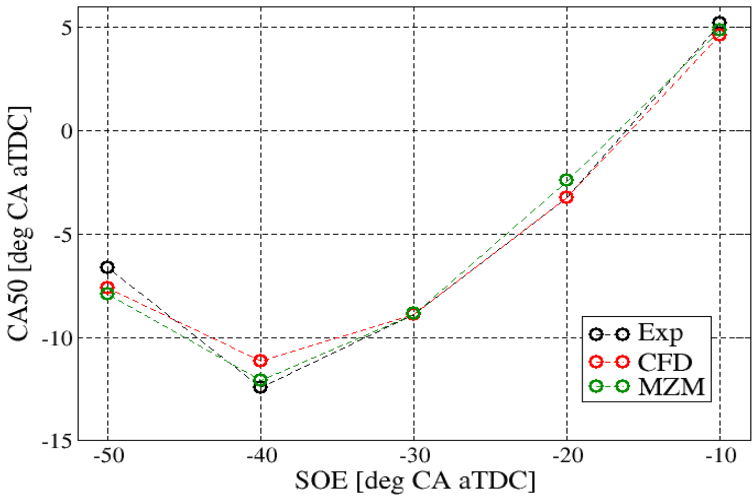


Results

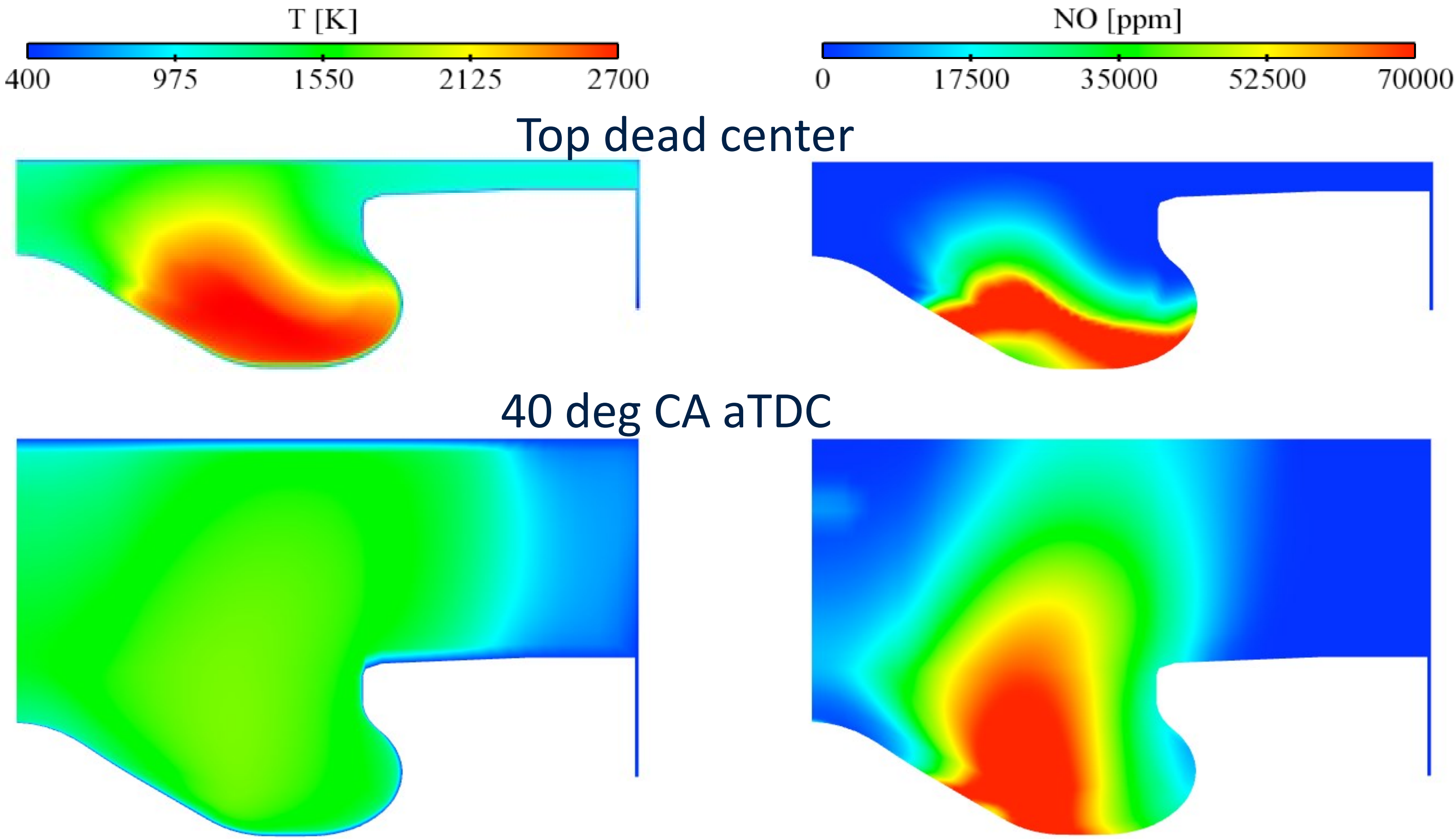


- Good agreement in terms of in-cylinder pressure
  - Ignition delay
  - Combustion
  - Peak pressure
  - Expansion
- Nitrogen oxides (NOx) and unburned hydrocarbons (HC):
  - Simulation captures experimental trend
  - Minor deviations for latest injection timing (NO_x) and early injection timings (HC)

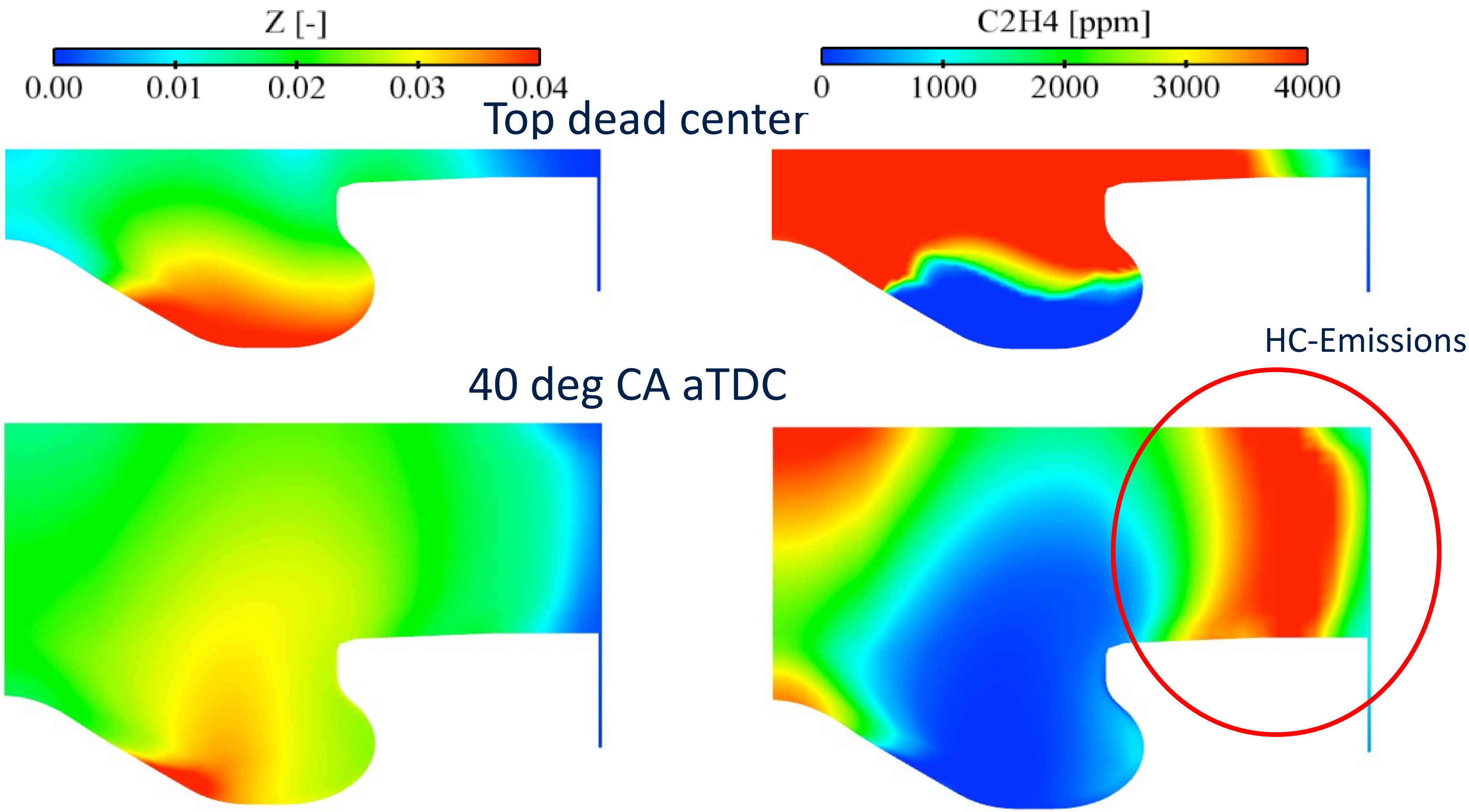


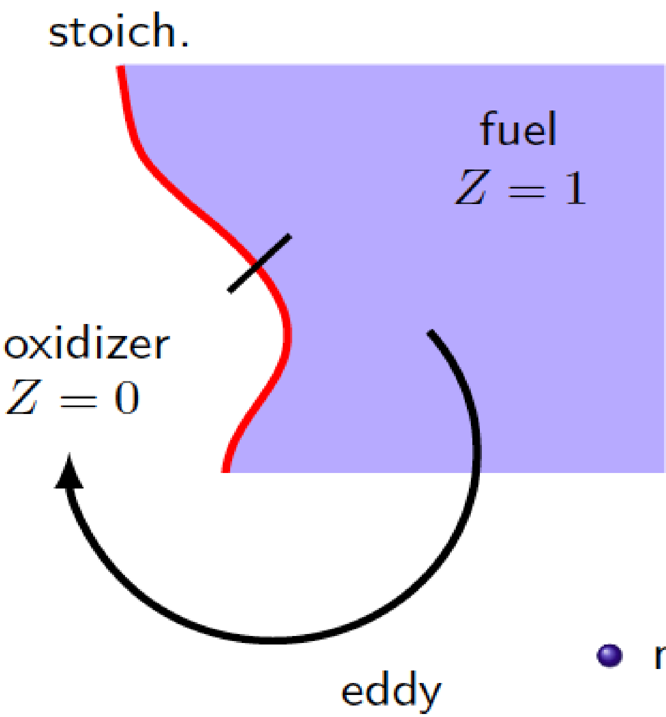


Injector cut plane SOE 40



Injector cut plane SOE 50





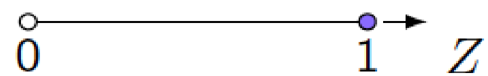
mixing

$(\chi = 2D|\nabla Z|^2)$

chemistry

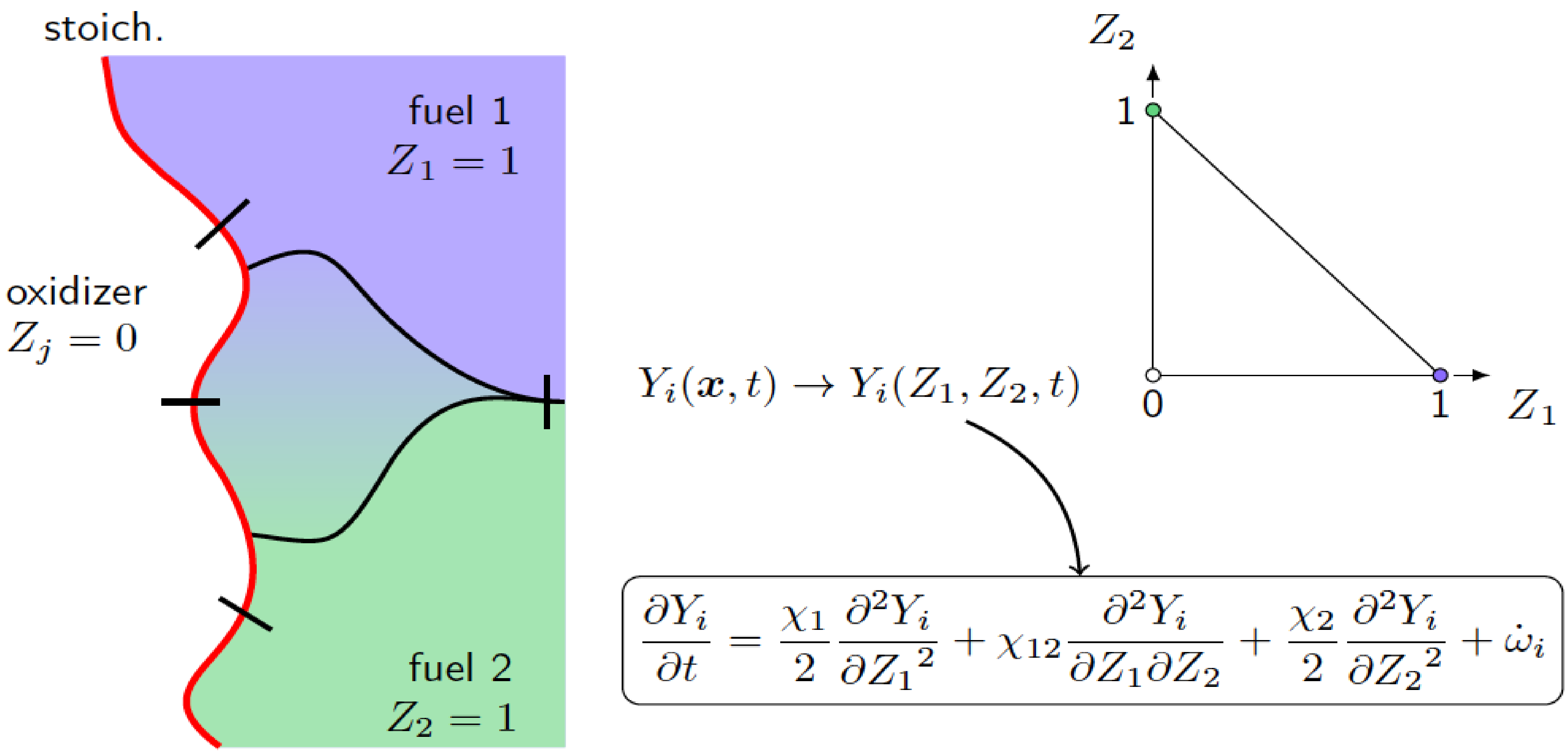
$$\frac{\partial Y_i}{\partial t} = \frac{\chi}{2}\frac{\partial^2 Y_i}{\partial Z^2} + \dot{\omega}_i$$

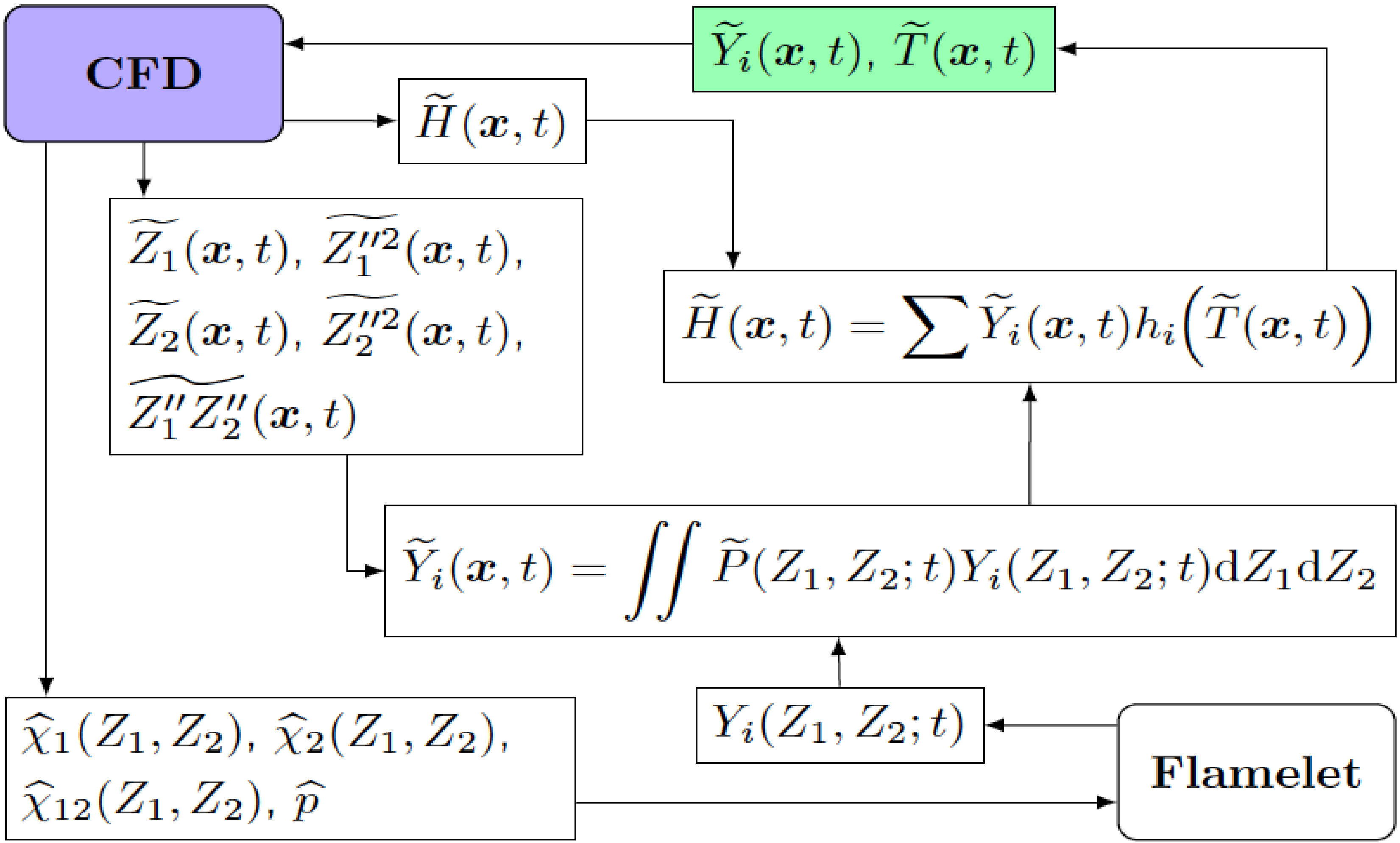
$$Y_i(\boldsymbol{x}, t) \rightarrow Y_i(Z, t)$$

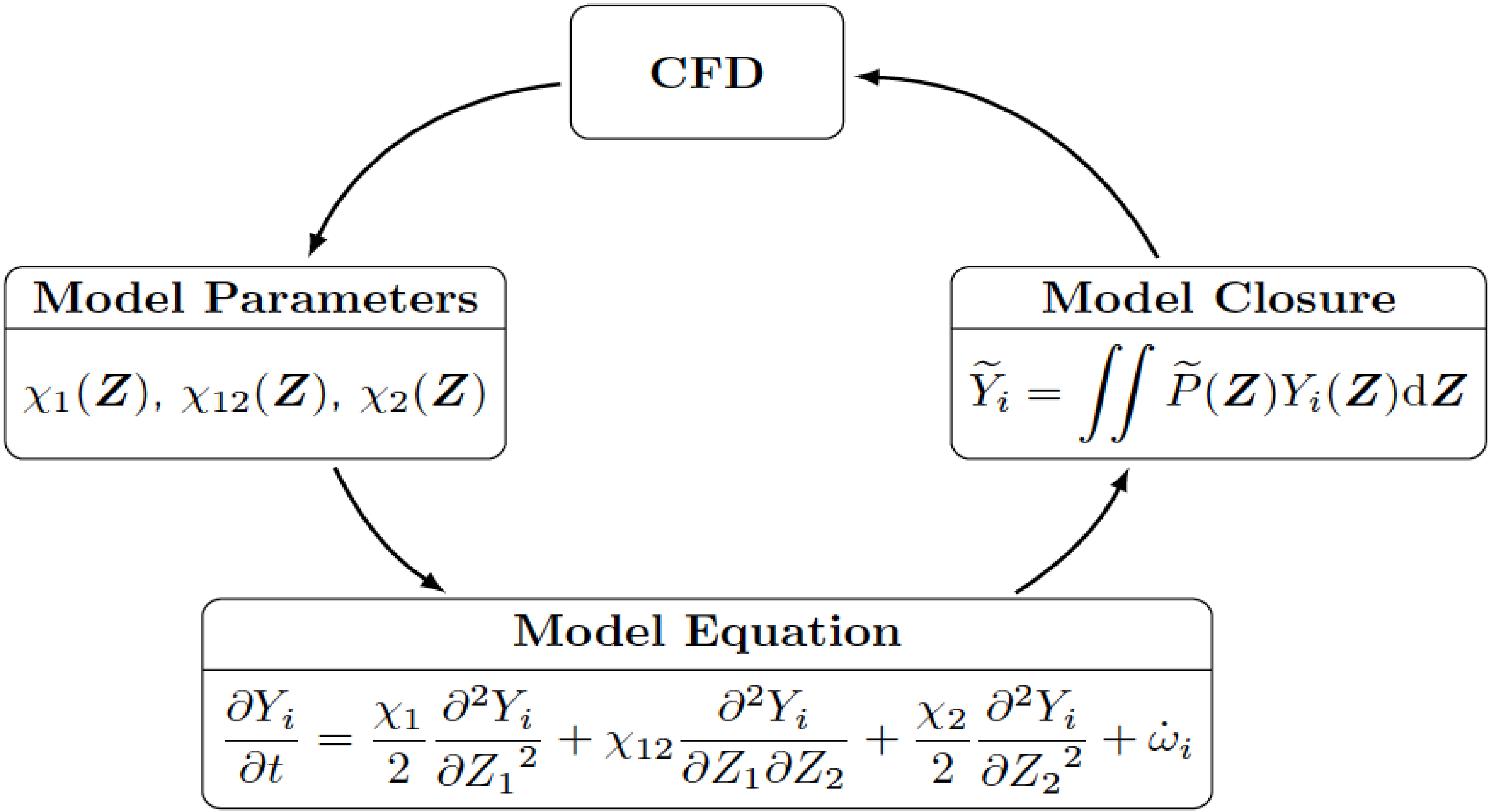


- mixing state described by composition space, Z
- allows for detailed chemistry

- 3


stoich.
fuel 1
$Z_1 = 1$
oxidizer
$Z_j = 0$
fuel 2
$Z_2 = 1$
Z_2
1
0
1
Z_1
$Y_i(\boldsymbol{x}, t) \rightarrow Y_i(Z_1, Z_2, t)$
$\boxed{\frac{\partial Y_i}{\partial t} = \frac{\chi_1}{2}\frac{\partial^2 Y_i}{\partial {Z_1}^2} + \chi_{12}\frac{\partial^2 Y_i}{\partial Z_1 \partial Z_2} + \frac{\chi_2}{2}\frac{\partial^2 Y_i}{\partial {Z_2}^2} + \dot{\omega}_i}$


CFD
$\widetilde{Y}_i(\boldsymbol{x},t)$, $\widetilde{T}(\boldsymbol{x},t)$
$\widetilde{H}(\boldsymbol{x},t)$
$\widetilde{Z}_1(\boldsymbol{x},t)$, $\widetilde{Z_1''^2}(\boldsymbol{x},t)$,
$\widetilde{Z}_2(\boldsymbol{x},t)$, $\widetilde{Z_2''^2}(\boldsymbol{x},t)$,
$\widetilde{Z_1''Z_2''}(\boldsymbol{x},t)$
$\widetilde{H}(\boldsymbol{x},t) = \sum \widetilde{Y}_i(\boldsymbol{x},t) h_i\Big(\widetilde{T}(\boldsymbol{x},t)\Big)$
$\widetilde{Y}_i(\boldsymbol{x},t) = \iint \widetilde{P}(Z_1,Z_2;t) Y_i(Z_1,Z_2;t)\,\mathrm{d}Z_1\mathrm{d}Z_2$
$\widehat{\chi}_1(Z_1,Z_2)$, $\widehat{\chi}_2(Z_1,Z_2)$,
$\widehat{\chi}_{12}(Z_1,Z_2)$, $\widehat{p}$
$Y_i(Z_1,Z_2;t)$
Flamelet


CFD
Model Parameters
$\chi_1(\boldsymbol{Z}),\ \chi_{12}(\boldsymbol{Z}),\ \chi_2(\boldsymbol{Z})$
Model Closure
$\widetilde{Y}_i = \iint \widetilde{P}(\boldsymbol{Z}) Y_i(\boldsymbol{Z}) \mathrm{d}\boldsymbol{Z}$
Model Equation
$\frac{\partial Y_i}{\partial t} = \frac{\chi_1}{2} \frac{\partial^2 Y_i}{\partial {Z_1}^2} + \chi_{12} \frac{\partial^2 Y_i}{\partial Z_1 \partial Z_2} + \frac{\chi_2}{2} \frac{\partial^2 Y_i}{\partial {Z_2}^2} + \dot{\omega}_i$

Example: High Fidelity Modeling of Multi-Injection Diesel Engine Application

Specifications

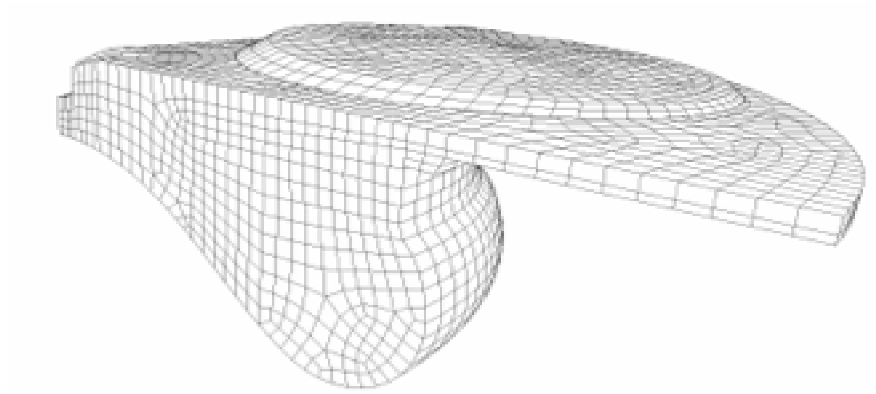
- Bore: 84.7 mm
- Stroke: 90 mm
- Displacement: 0.5 L
- Compression Ratio: 16

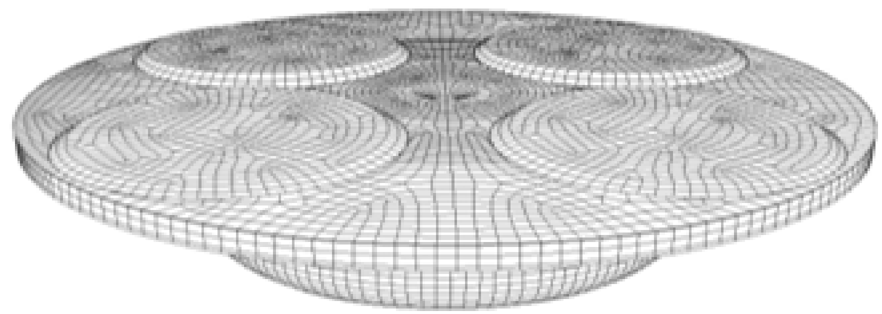
Operating Conditions

- Engine Speed: 2000 RPM
- IMEP: 8 bar
- Swirl Ratio: 2
- EGR: 20-30%

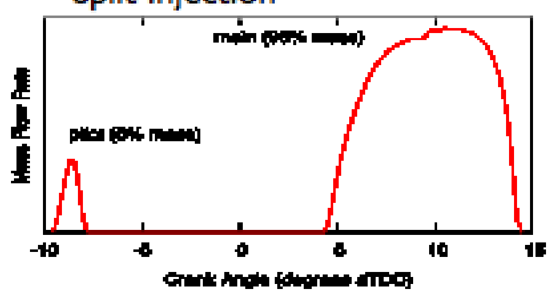
Bosch 7 hole Injector (CRI3.0/CRI3.2)

- Rail Pressure: 1500 bar
- Spray Angle: 160 degrees





Split Injection



Solver and Modeling Approaches

Combustion Model

- Multi-dimensional flamelet model

CFD

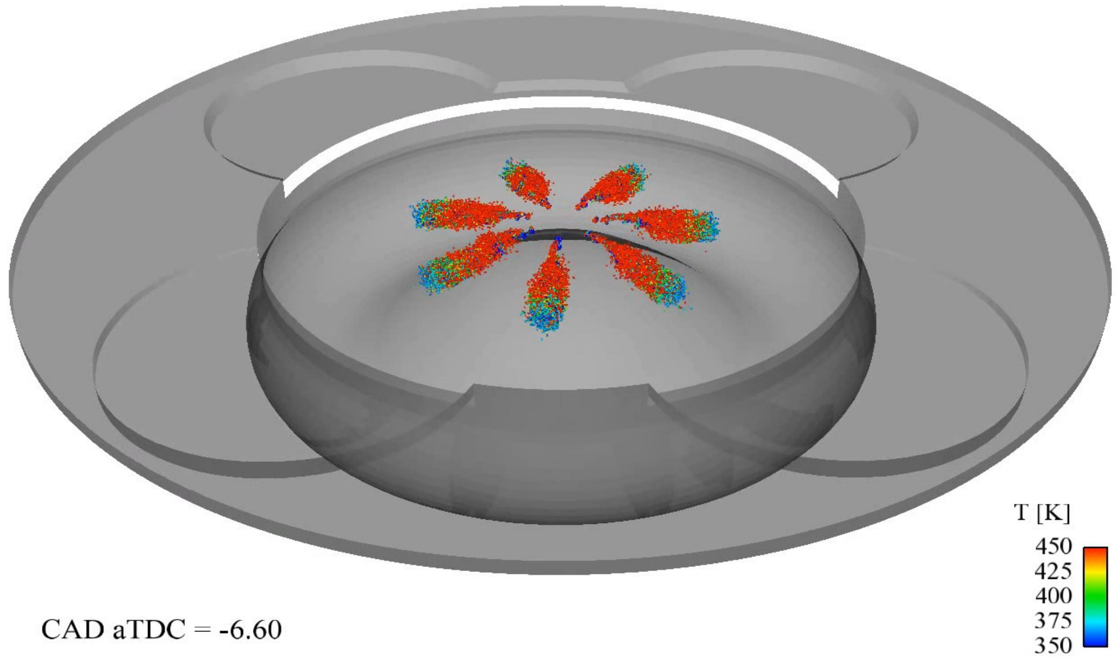
- Fluent Turbulent RANS
- k-epsilon realizable

Spray Model

- Discrete phase
- WAVE breakup model

Mechanism[1]

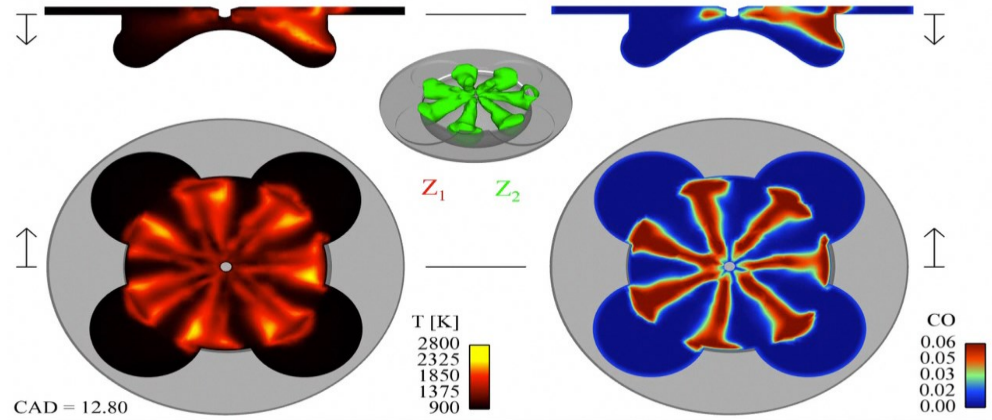
- n-heptane
- 36 species

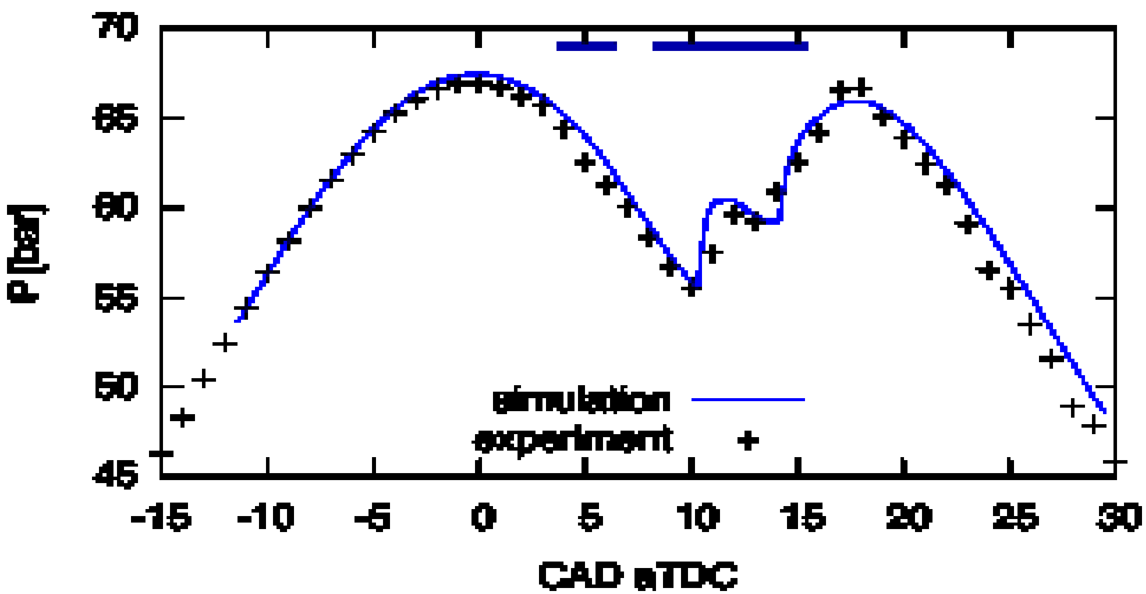


[1] S. Liu, J.C. Hewson, J.H. Chen, and H. Pitsch, *Combustion and Flame*, 2004

Close Pilot Injection

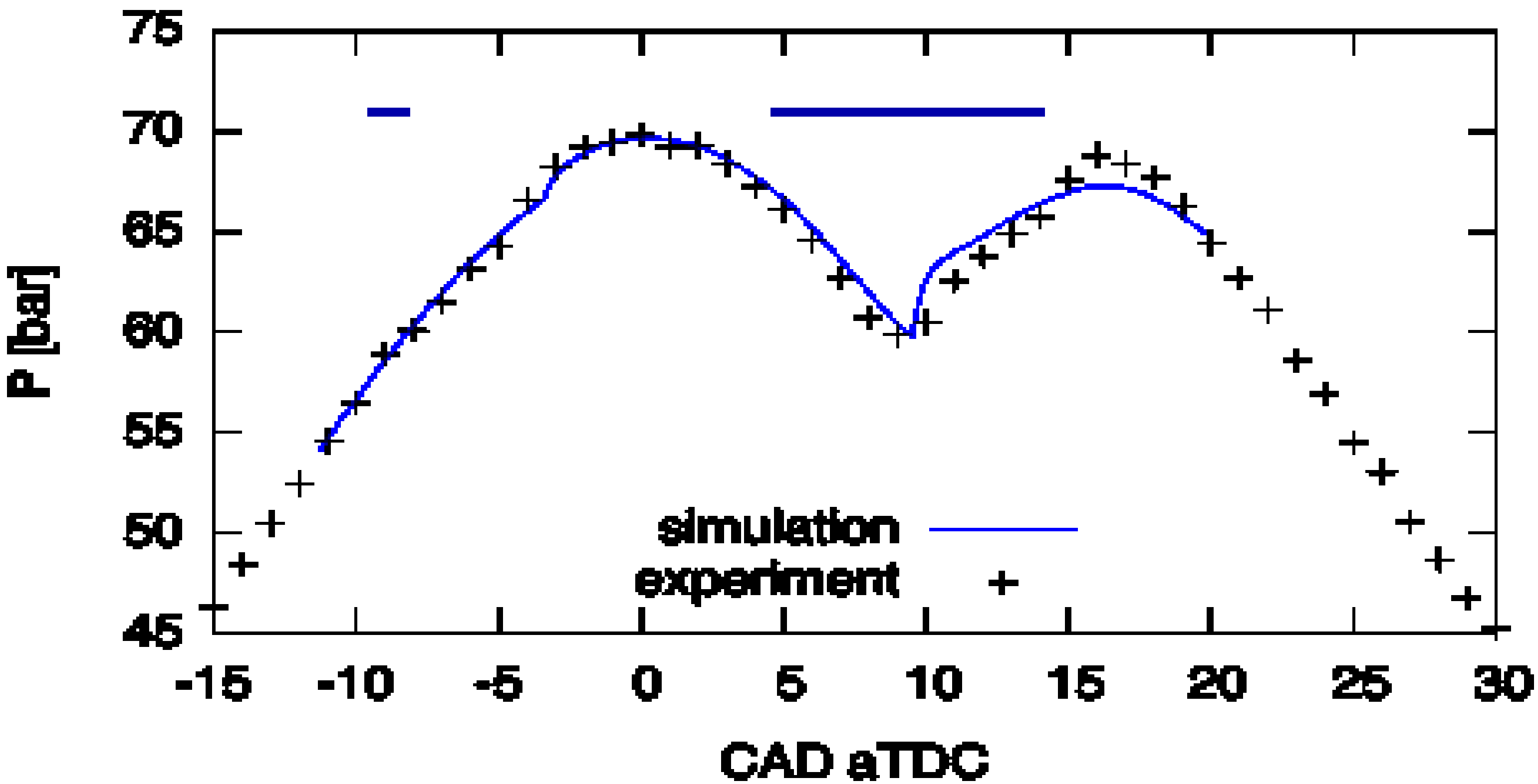
- Close pilot injection:
  - IMEP: 8 bar
  - 28% EGR





Classic Pilot Injection

- Classic pilot injection:
  - IMEP: 8 bar
  - 24% EGR



Steady Laminar Flamelet Model

- Assumption that flame structure is in steady state

$$\cancel{\rho \frac{\partial T}{\partial \tau}} - \frac{\rho \chi_{st}}{2} \frac{\partial^2 T}{\partial Z^2} = \dot{\omega}_T$$

$$\cancel{\rho \frac{\partial Y_\alpha}{\partial \tau}} - \frac{\rho \chi_{st}}{2} \frac{\partial^2 Y_\alpha}{\partial Z^2} = \dot{m}'''_\alpha$$

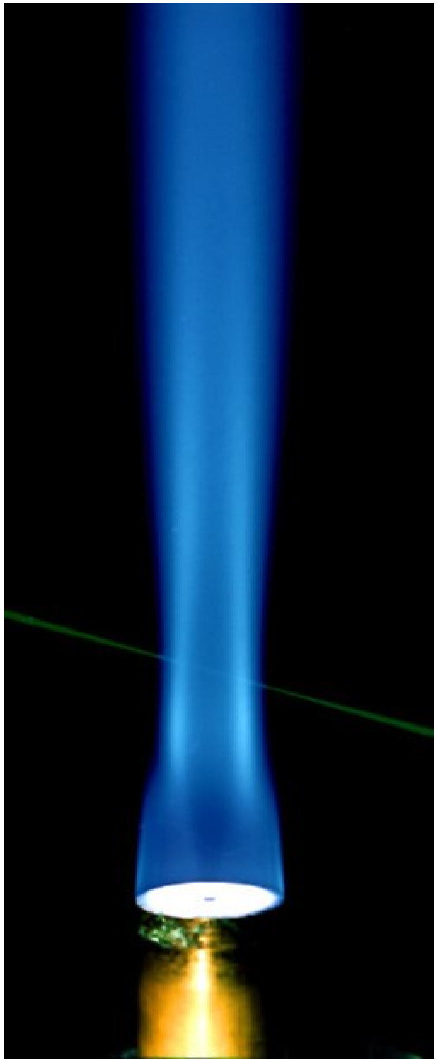
- Assumption often good, except slow chemical and physical processes, such as
  - Pollutant formation
  - Radiation
  - Extinction/re-ignition

- Model formulation
  - Solve steady flamelet equations with varying χ_{st}
  - Tabulate in terms of χ_{st} or progress variable C, e.g. $C = Y_{CO2} + Y_{HO2} + Y_{CO} + Y_{H2}$
  - Presumed PDF, typically beta function for Z, delta function for dissipation rate or reaction progress parameter

Example: LES of a Bluff-Body Stabilized Flame

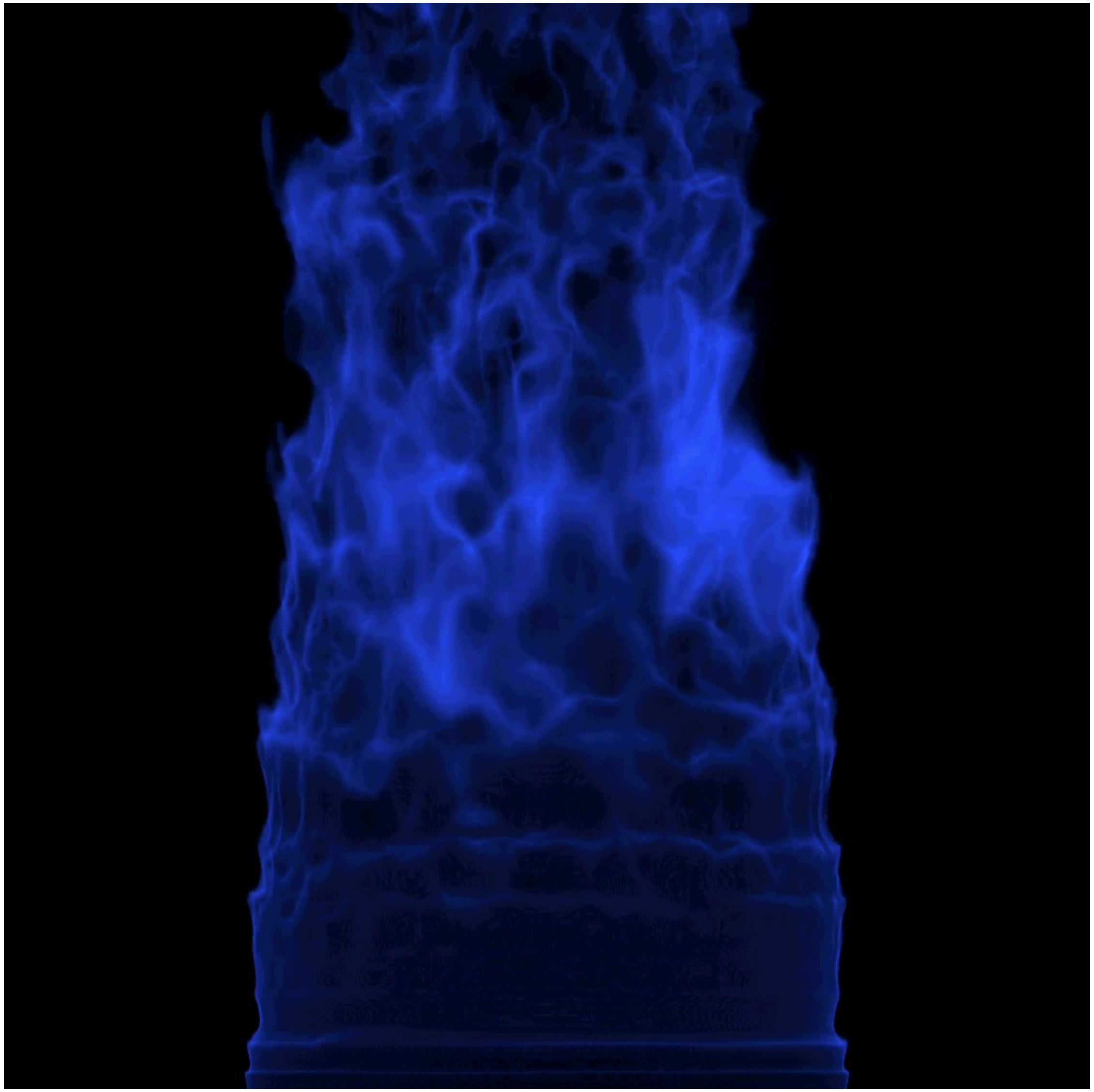
- Bluff-body stablized methane/air flame
- Fuel issues through center of bluff body
- Flame stabilization by complex recirculating flow
- RANS models where unsuccessful in predicting experimental data

- Here, LES using simple steady flamelet model
- New recursive filter refinement method
- Accurate models for scalar variance and scalar dissipation rate



Exp. by Masri et al.

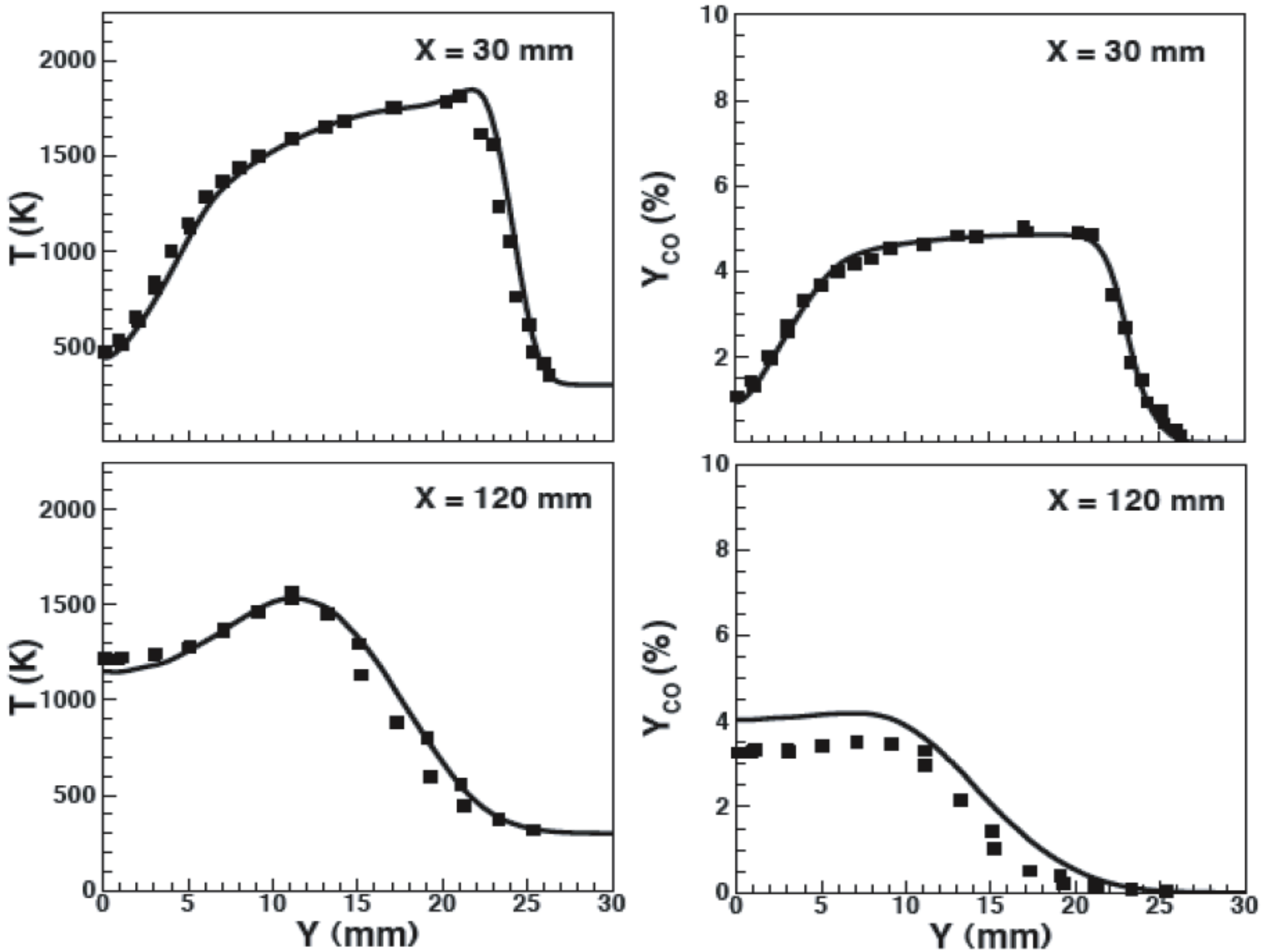
Example: LES of a Bluff-Body Stabilized Flame

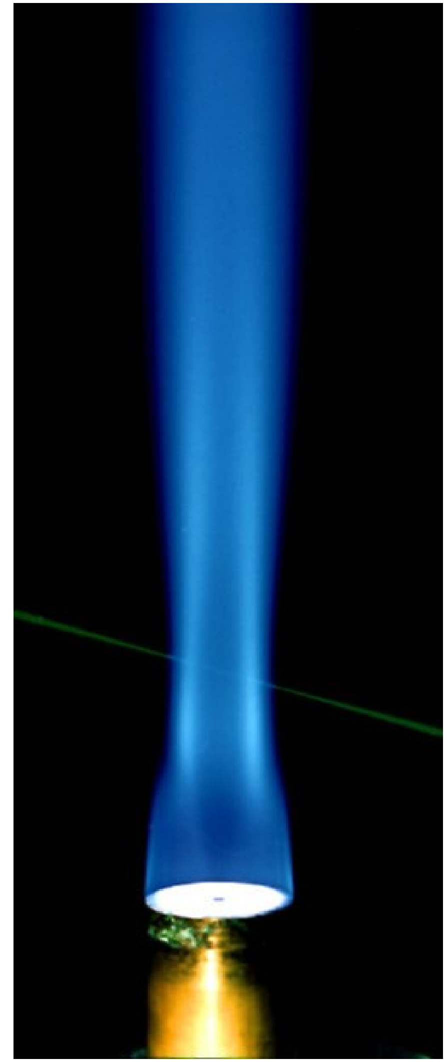


Example: LES of a Bluff-Body Stabilized Flame

Temperature

CO Mass Fraction

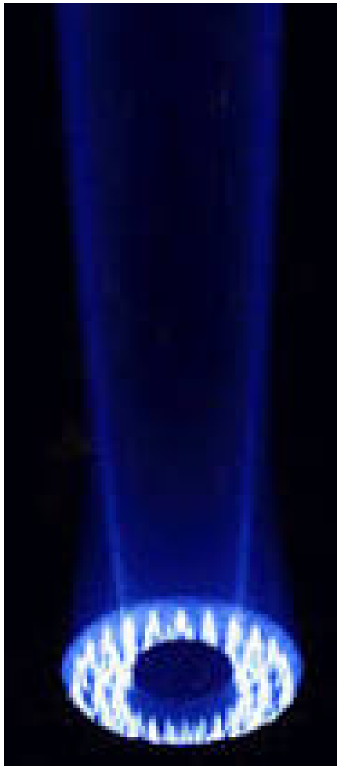




Flamelet Model Application to Sandia Jet Flames

Flamelet model application to jet flame with extinction and reignition

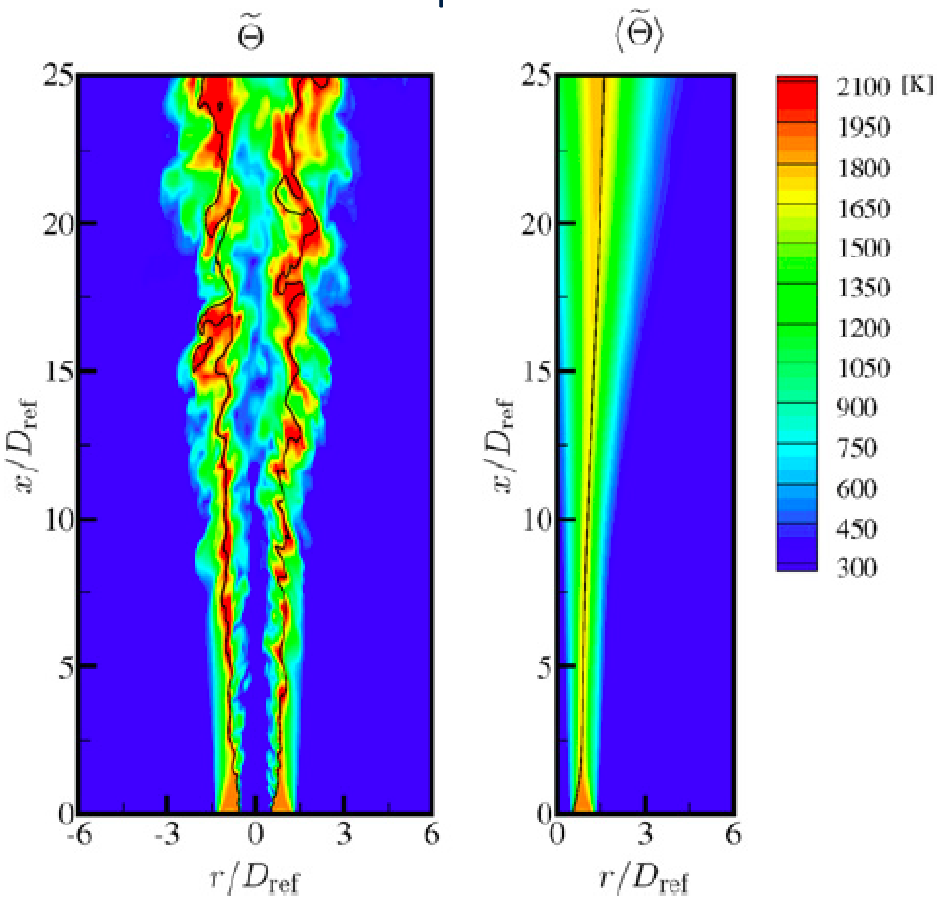
- Flamelet/progress variable model (Ihme & Pitsch, 2008)
- Definition of reaction progress parameter
  - Based on progress variable *C*
  - Defined to be independent of *Z*
- Joint pdf of *Z* and λ
  - Z and λ independent
  - Beta function for *Z*
  - Statistically most likely distribution for λ



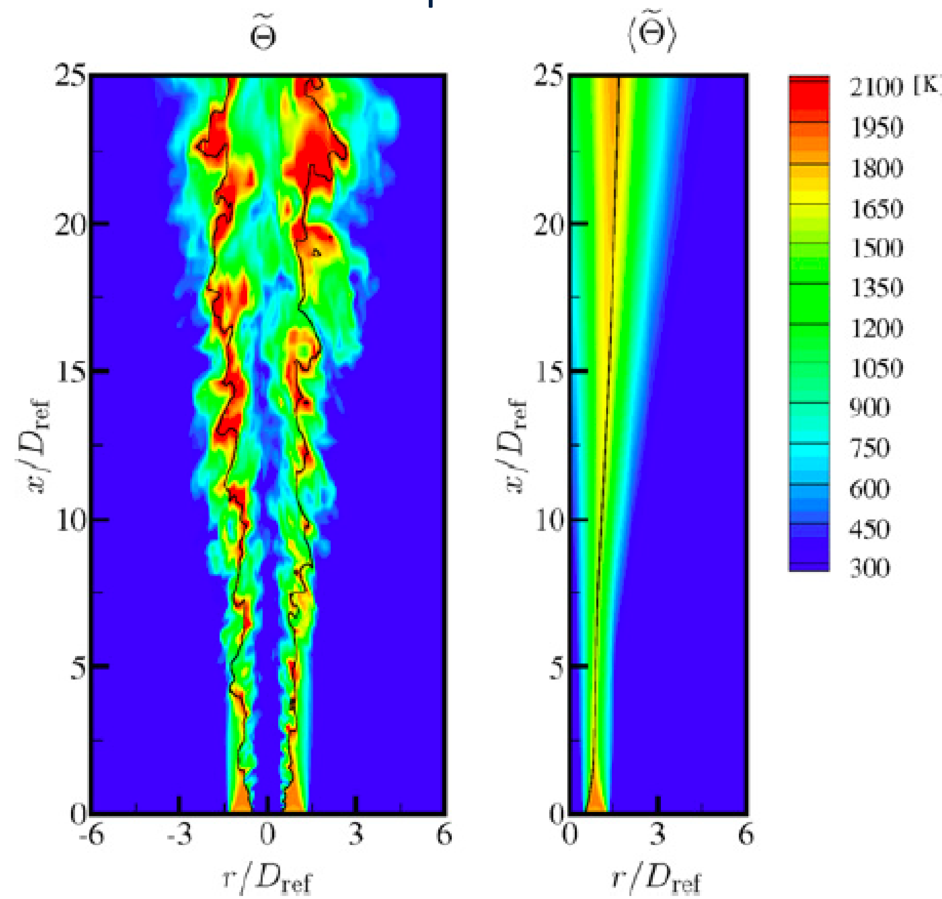
Exp. by Barlow et al.

Flamelet Model Application to Sandia Jet Flames

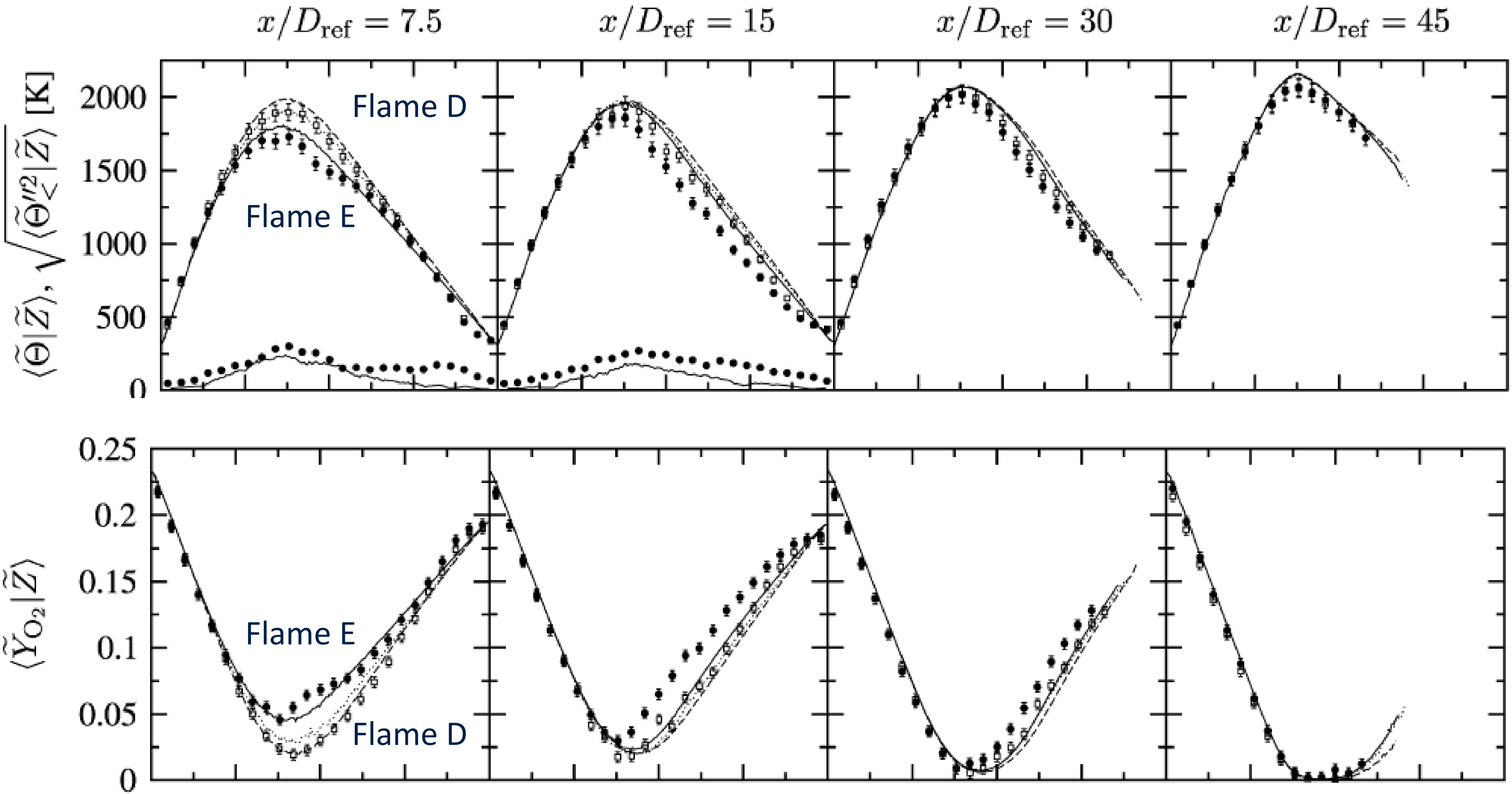
Flame D:
Temperature



Flame E:
Temperature



Flamelet Model Application to Sandia Jet Flames



Summary

Part II: Turbulent Combustion

- Turbulence
- Turbulent Premixed Combustion
- Turbulent Non-Premixed Combustion
- Turbulent Combustion Modeling
- Applications

- Moment Methods for reactive scalars
- Simple Models in Fluent: EBU,EDM, FRCM, EDM/FRCM
- Introduction in Statistical Methods: PDF, CDF,...
- Transported PDF Model
- Modeling Turbulent Premixed Combustion
  - BML-Model
  - Level Set Approach/G-equation
- Modeling Turbulent Non-Premixed Combustion
  - Conserved Scalar Based Models for Non-Premixed Turbulent Combustion
  - Flamelet-Model
  - Application: RIF, steady flamelet model