



# Modellierung der turbulenten Verbrennung für Wasserstoff-Antriebe

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1. Introduction – the turbulent combustion problem
2. Modeling of premixed turbulent flames
3. Validation of premixed combustion model (methane)
4. Modeling of non-premixed turbulent flames
5. Validation of non-premixed flame model (hydrogen)
6. Real gas effects – rocket motors
7. Conclusions



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## Favre-averaged Conservation Equations

Mass:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial (\bar{\rho} \tilde{u}_i)}{\partial x_i} = 0$$

Momentum:

$$\frac{\partial}{\partial t}(\bar{\rho} \tilde{u}_i) + \frac{\partial}{\partial x_j}(\bar{\rho} \tilde{u}_i \tilde{u}_j) = \bar{\rho} g_i - \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \bar{\tau}_{ij}}{\partial x_j} - \frac{\partial}{\partial x_j}(\bar{\rho} \widetilde{\tilde{u}_i \tilde{u}_j})$$

Species:

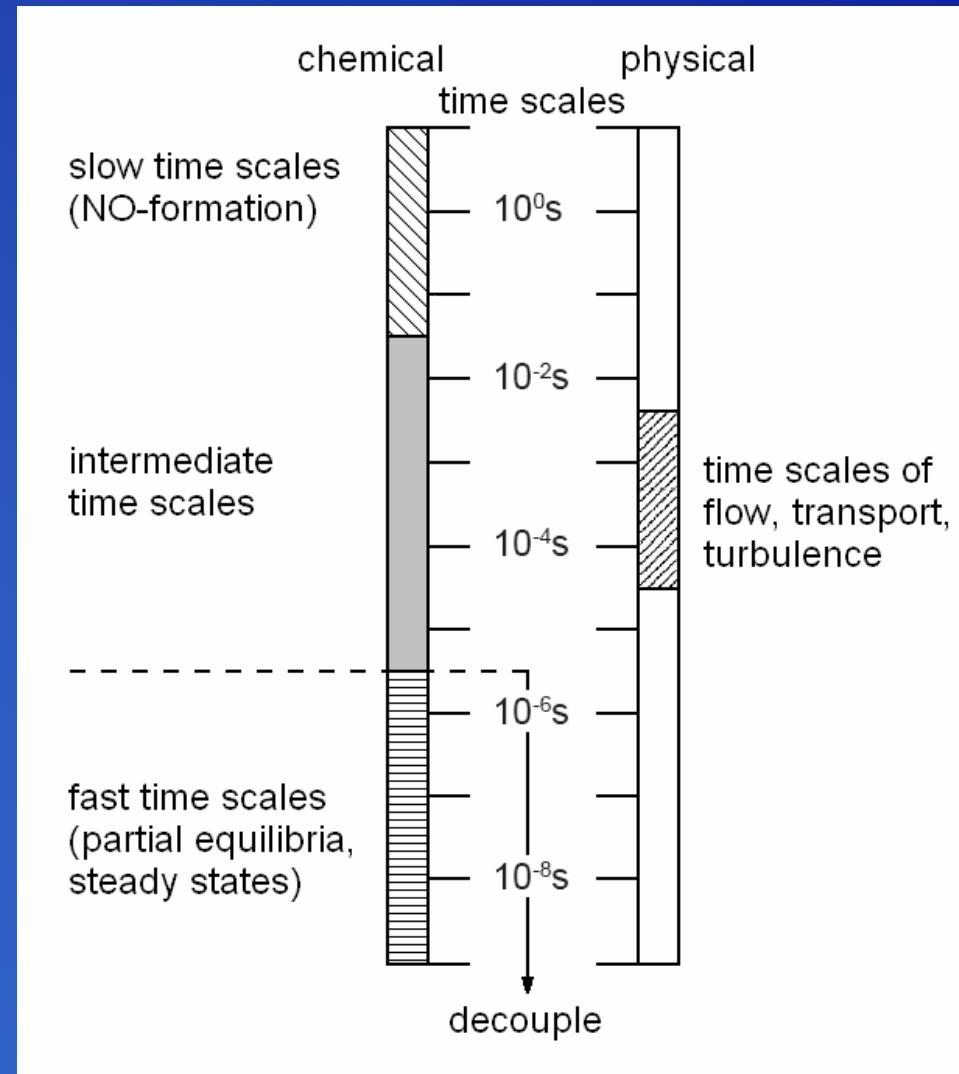
$$\frac{\partial}{\partial t}(\bar{\rho} \tilde{Y}_\alpha) + \frac{\partial}{\partial x_i}(\bar{\rho} \tilde{u}_i \tilde{Y}_\alpha) = \frac{\partial}{\partial x_i} \left( \bar{\rho} D_\alpha \frac{\partial \tilde{Y}_\alpha}{\partial x_i} \right) - \frac{\partial}{\partial x_i} \bar{\rho} \widetilde{\tilde{u}_i \tilde{Y}_\alpha} + \tilde{R}_\alpha$$

Enthalpy:

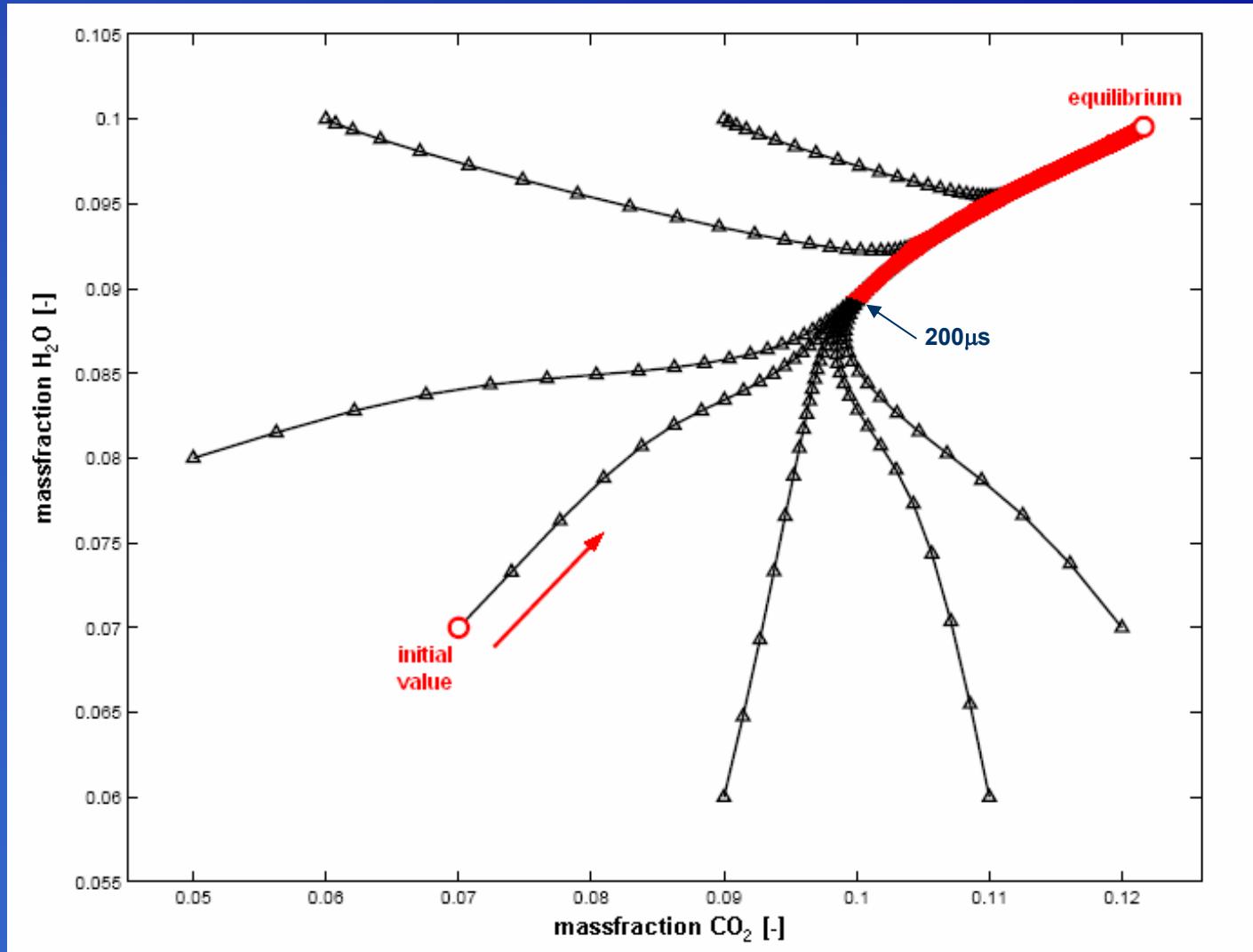
$$\frac{\partial}{\partial t}(\bar{\rho} \tilde{h}) + \frac{\partial}{\partial x_i}(\bar{\rho} \tilde{u}_i \tilde{h}) = \frac{\partial}{\partial x_i} \left( \bar{\rho} D_h \frac{\partial \tilde{h}}{\partial x_i} \right) - \frac{\partial}{\partial x_i} \bar{\rho} \widetilde{\tilde{u}_i \tilde{h}} + \dot{q}_{str}$$

→ **unclosed** Terms need modelling, reaction source term very nonlinear:

$$\widetilde{R}_\alpha \neq f(\widetilde{c}_i, \widetilde{T})$$



## Timescales of Chemical and Physical Processes

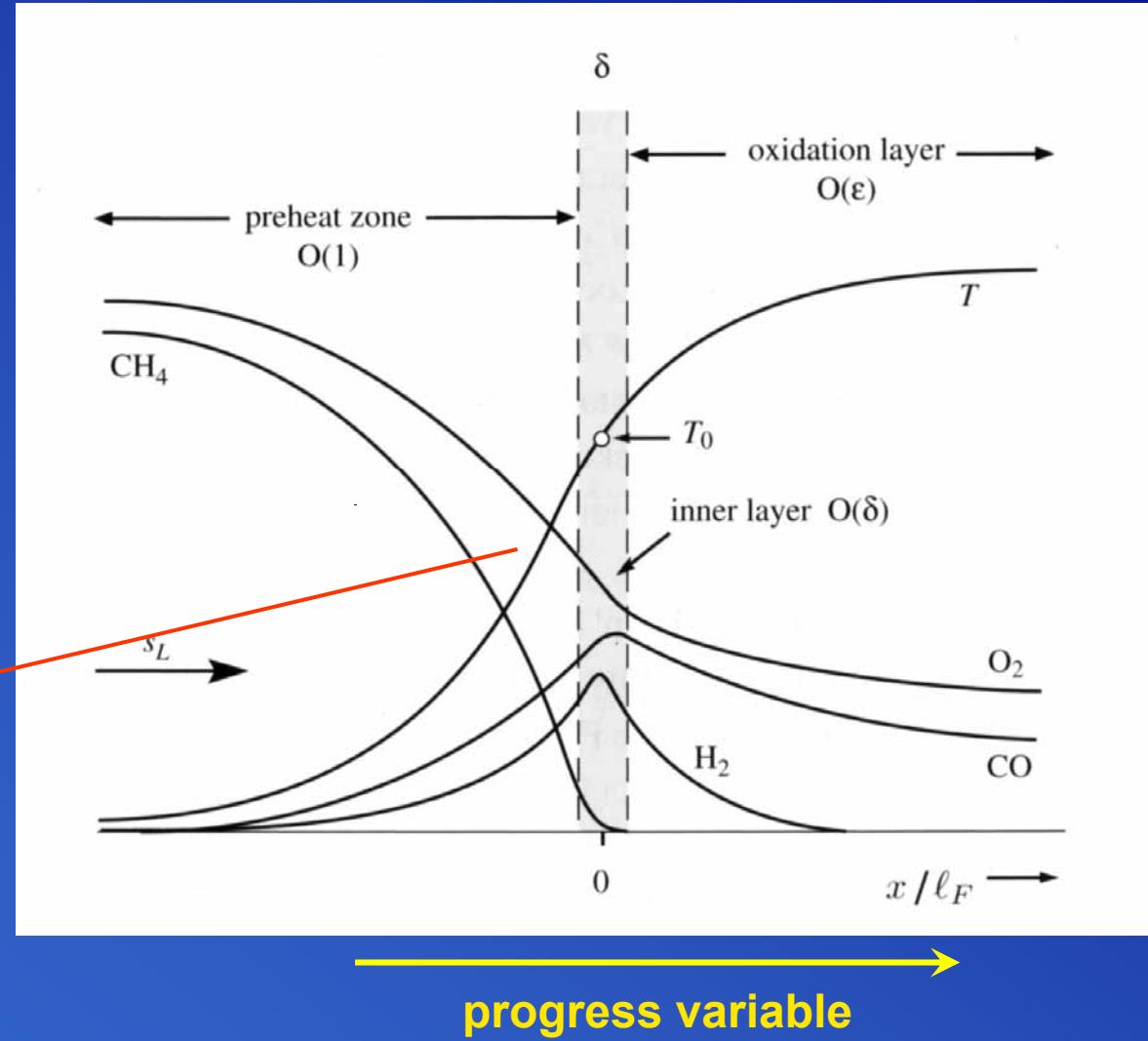
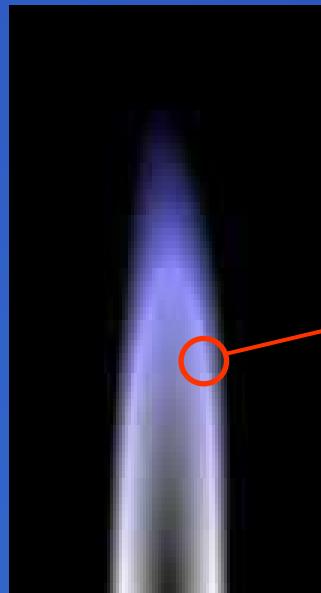


Trajectories of a Methane-Air Reaction → use tables



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thin reaction zone

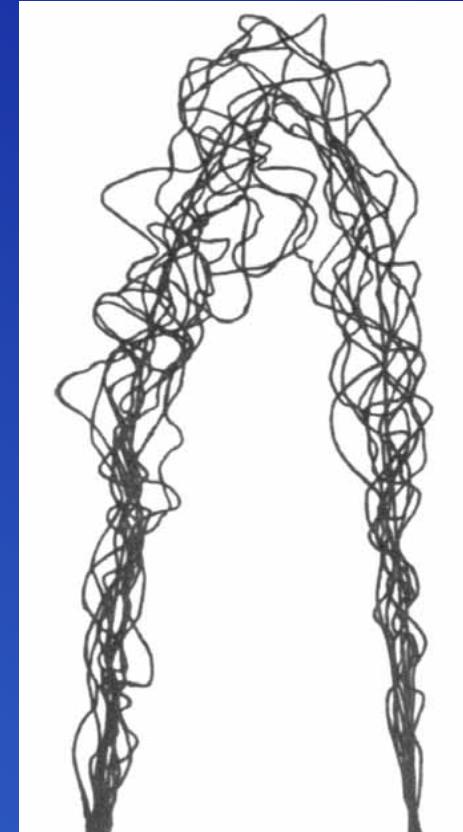


Structure of a premixed laminar methan-air flame

## Increase of burning rate through folding of flame



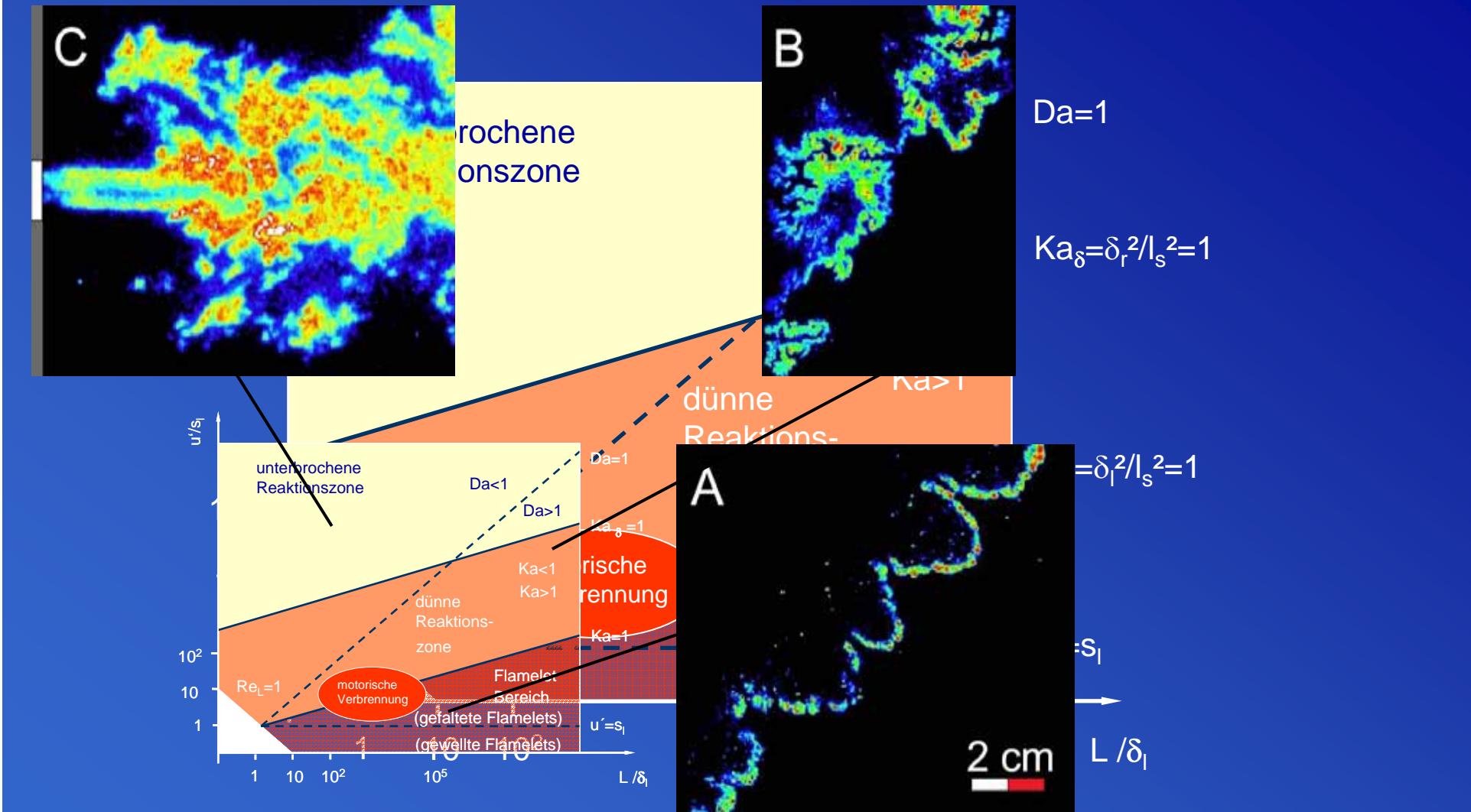
Schlieren picture



Instantaneous flame front

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**Visualisations of a turbulent premixed Bunsen flame**

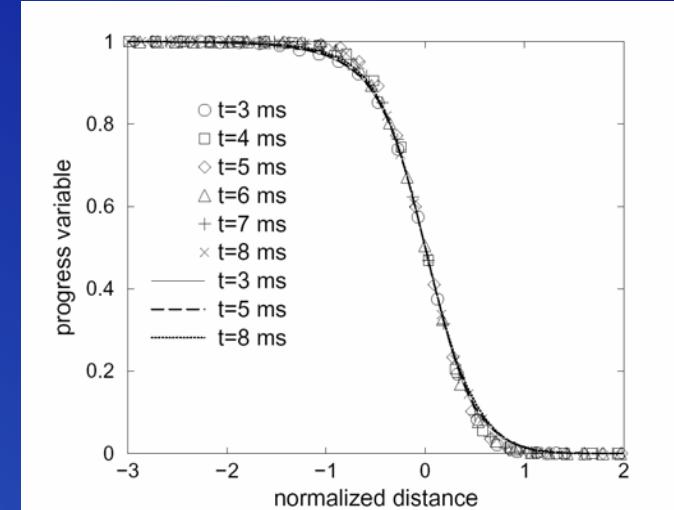


## Regime-Diagramm turbulent premixed combustion



OH visualisation flame front

Transport equation for Favre-averaged progress variable:



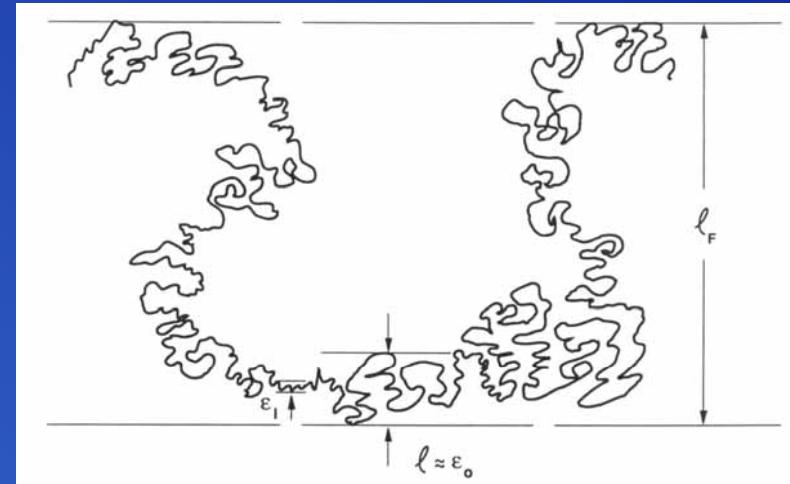
Reaction progress turbulent premixed flame

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{c}) + \frac{\partial}{\partial x_i}(\bar{\rho}\tilde{u}_i\tilde{c}) = -\frac{\partial}{\partial x_i}\left(\bar{\rho}\widetilde{u_i'c'}\right) + \bar{S}_c$$

Constant pressure:

$$\tilde{c} = \frac{\tilde{T} - T_u}{T_b - T_u}$$

## Reaction progress variable transport equation



fractal flame front

- $\rho_u$  density of unburnt gases
- $s_{l,0}$  laminar flame speed
- $\Sigma$  flame surface density  $\Sigma$  (fractal theory, Gouldin):

Turbulent burning rate:

$$\bar{S}_c = \rho_u \cdot s_{l,0} \cdot \Sigma$$

$$\bar{S}_c = C_R \cdot \rho_u \cdot \frac{s_l}{V_u^{1/4}} \cdot \frac{\tilde{\epsilon}^{3/4}}{\tilde{k}} \cdot \tilde{c} \cdot (1 - \tilde{c})$$

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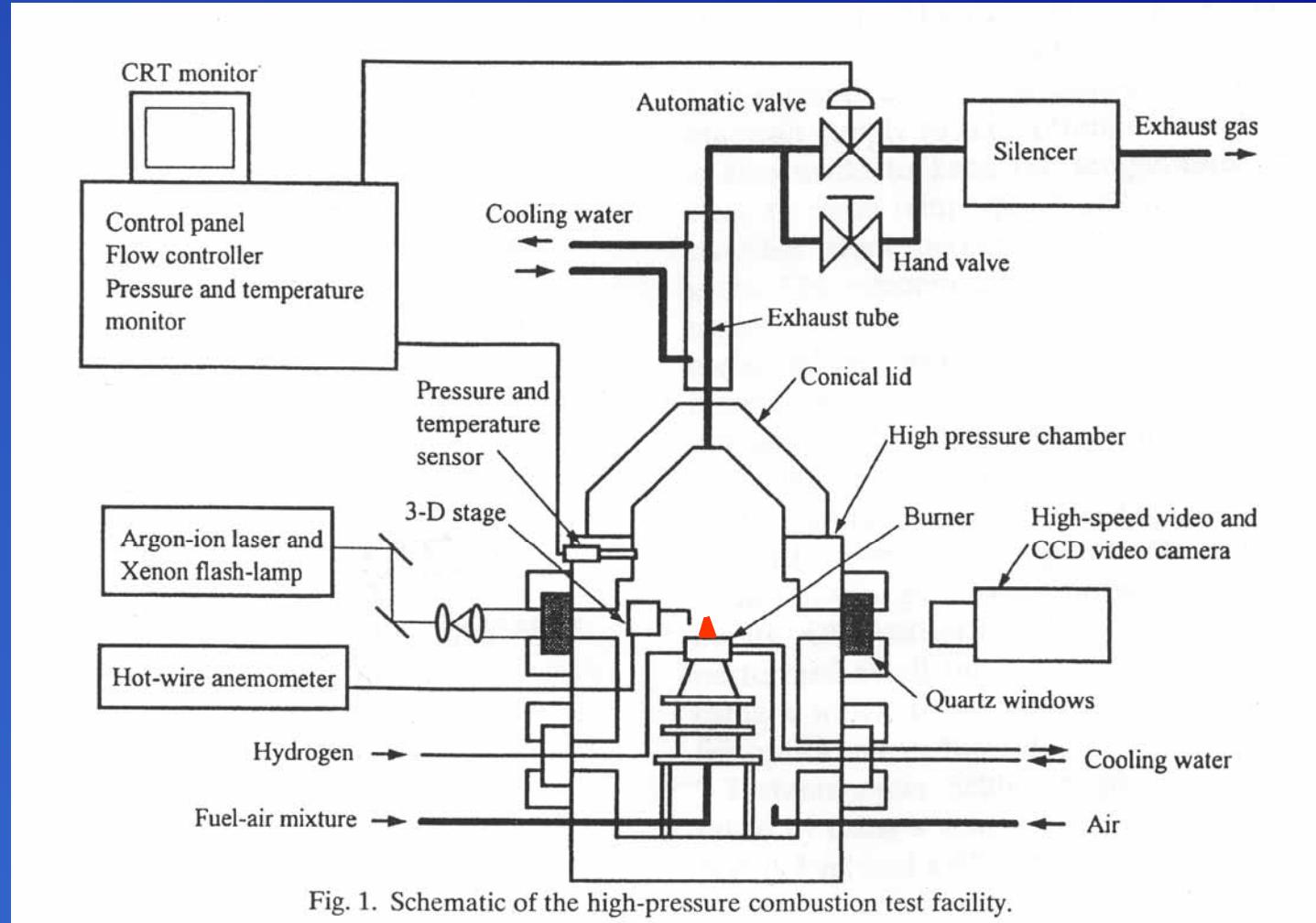
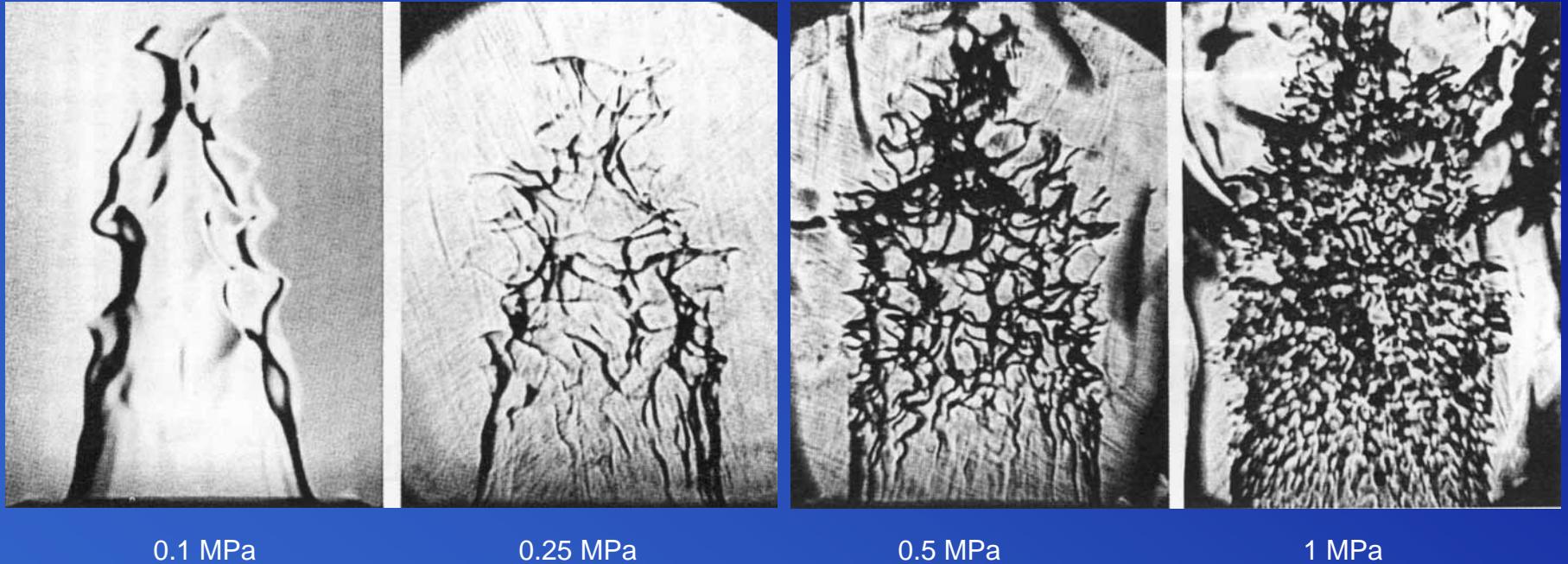


Fig. 1. Schematic of the high-pressure combustion test facility.

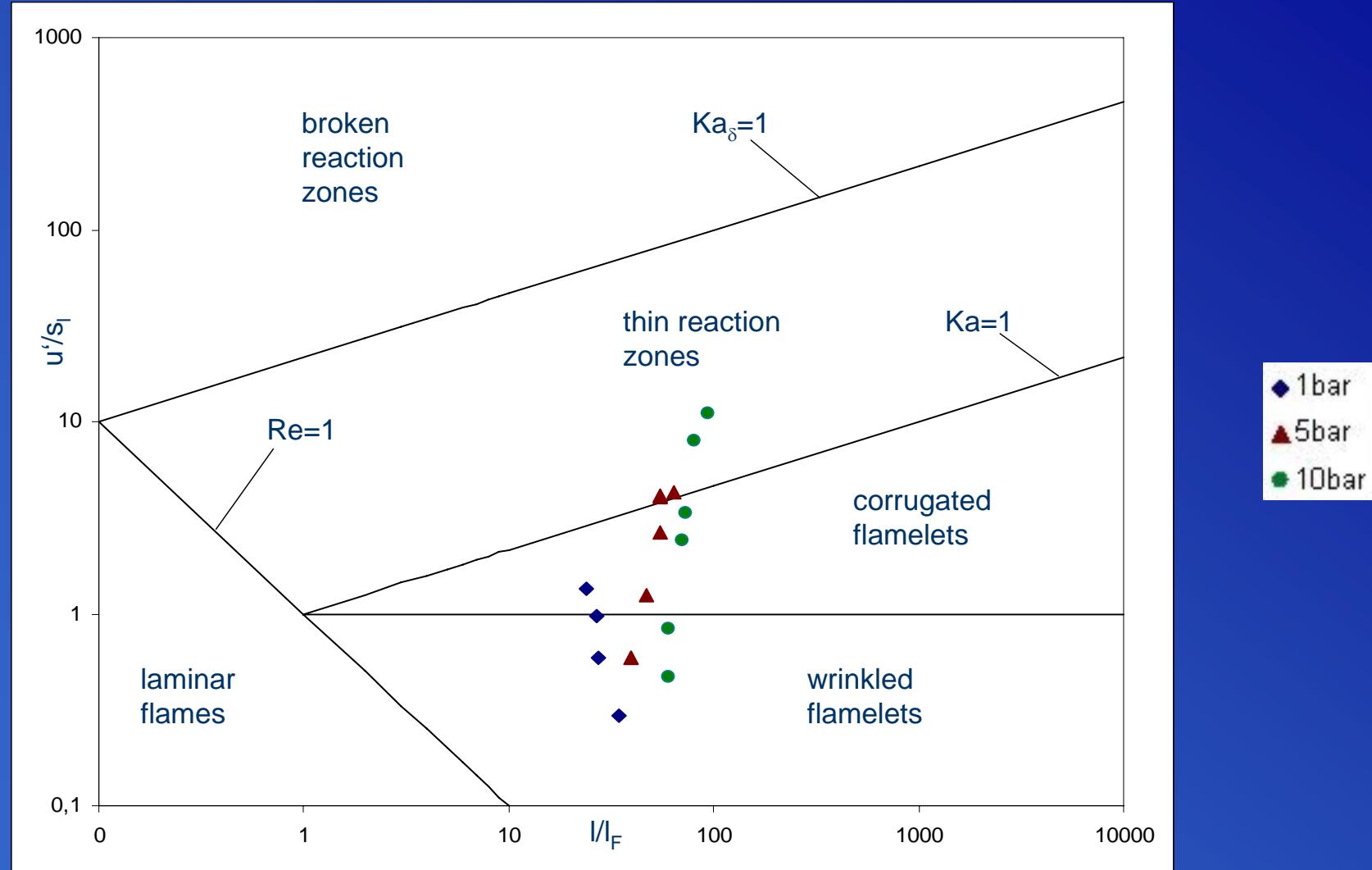
## Validation configuration (Kobayashi)



$\text{Re} \uparrow$  : fractal flame structure more pronounced

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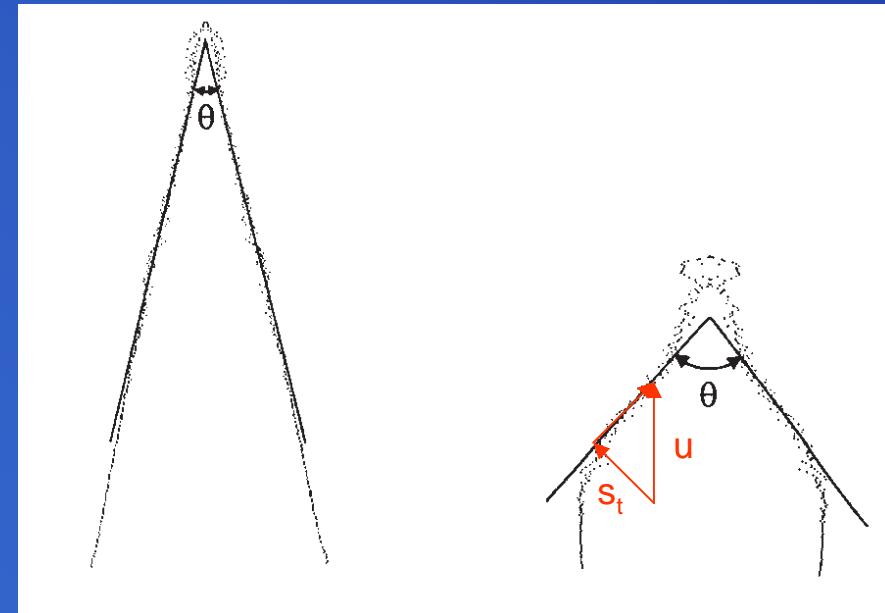
**Schlieren pictures of methane Bunsen flame (variation of pressure)**



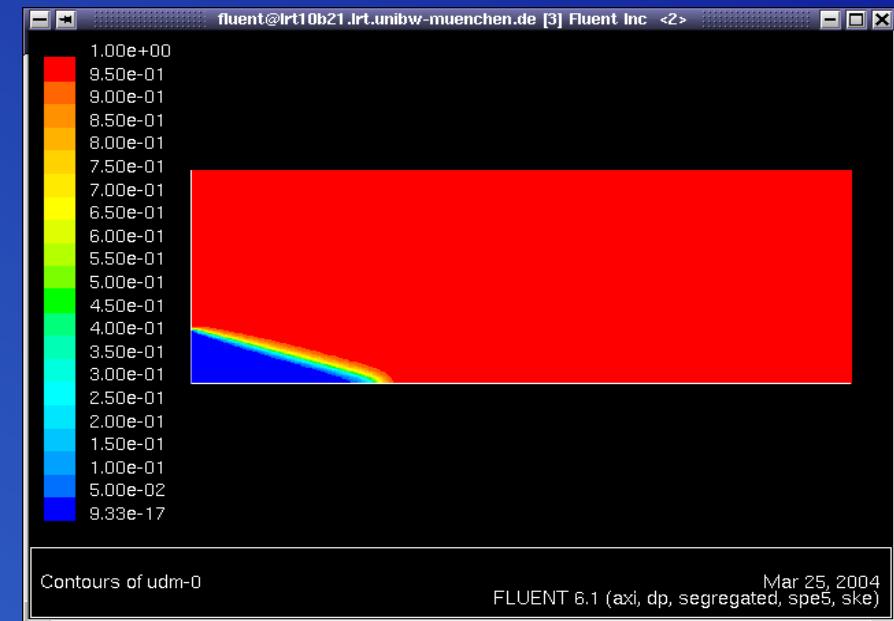
Experimental conditions in Borghi-Peters-regime-diagram

Flame angle from flame conus:  $s_t = u \cdot \sin\left(\frac{\theta}{2}\right)$

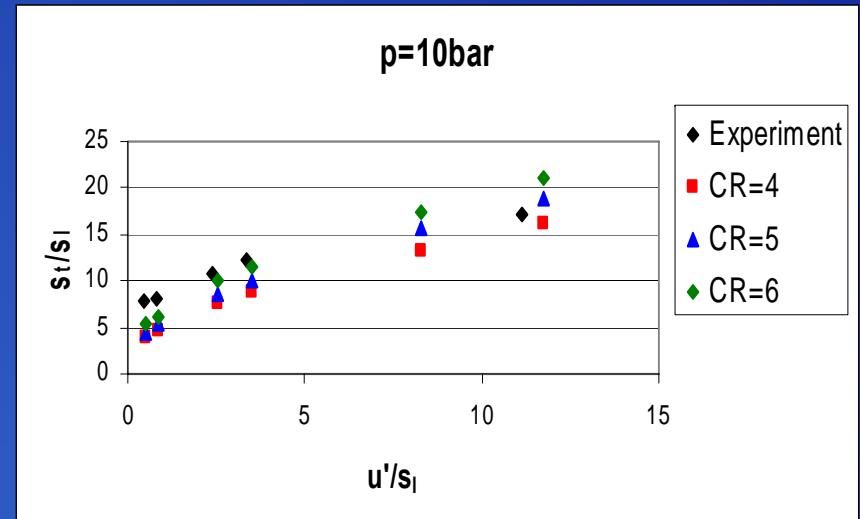
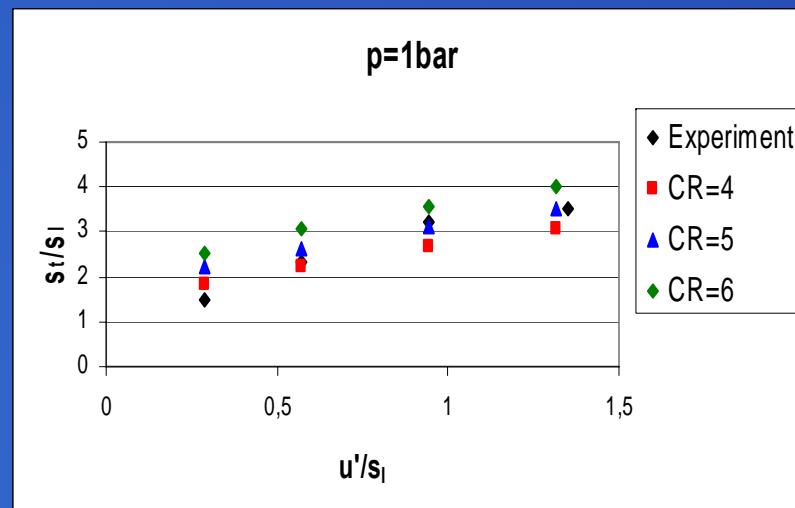
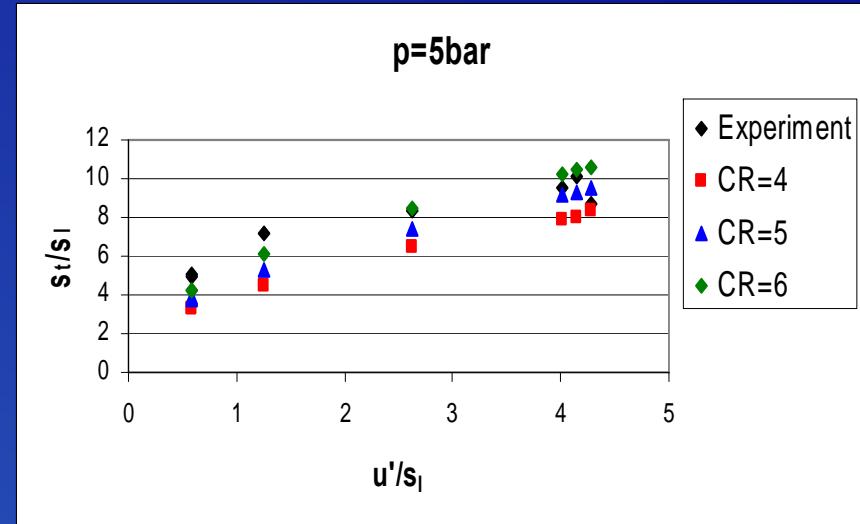
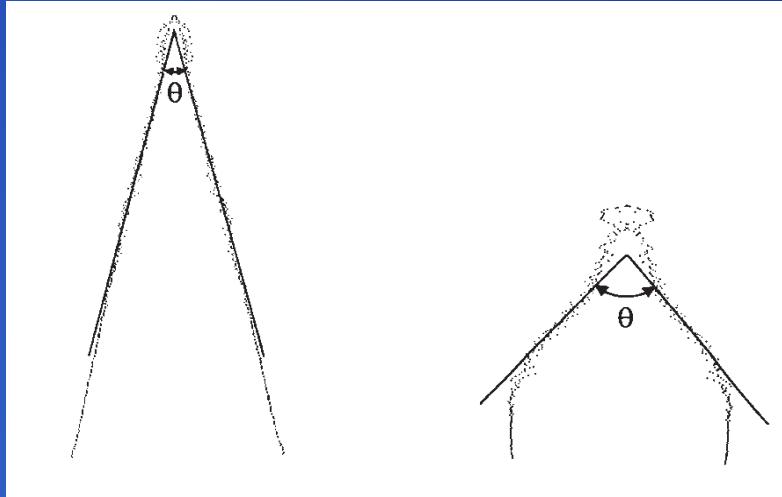
Experiment



Simulation:  $\bar{c} = \frac{(1+\tau)\tilde{c}}{1+\tau\tilde{c}}$

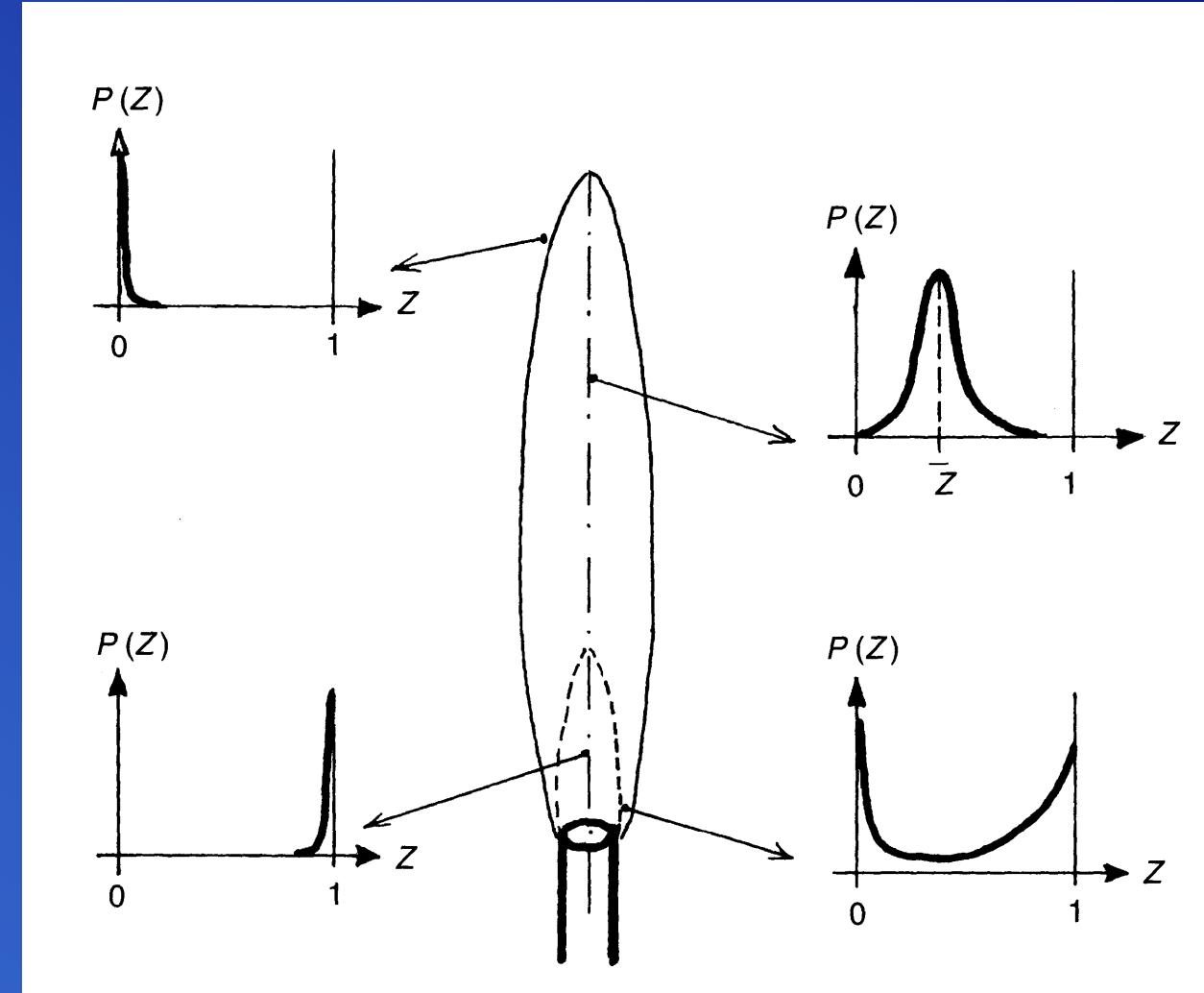


Validation of combustion model using flame cone angle



Results with Lindstedt-Vaos-Model (Methane/Air  $\Phi=0.9$ )

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PDF's of mixture fraction in non-premixed flame

## Balance equation for the mixture fraction and its variance

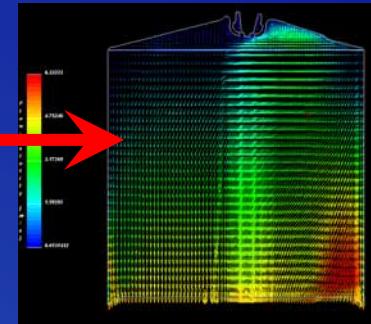
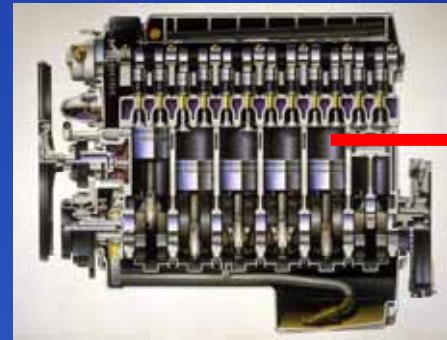
$$\frac{\partial(\bar{\rho}\tilde{Z})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\tilde{Z})}{\partial x_j} = \frac{\partial}{\partial x_j} \left\{ \left( \bar{\mu} + \frac{\mu_t}{\sigma_Z} \right) \frac{\partial \tilde{Z}}{\partial x_j} \right\}$$

and its variance

$$\frac{\partial(\bar{\rho}\widetilde{Z''^2})}{\partial t} + \frac{\partial(\bar{\rho}\widetilde{u}_j\widetilde{Z''^2})}{\partial x_j} = \frac{\partial}{\partial x_j} \left\{ \left( \bar{\mu} + \frac{\mu_t}{\sigma_{Z''^2}} \right) \frac{\partial \widetilde{Z''^2}}{\partial x_j} \right\} + 2 \frac{\mu_t}{\sigma_Z} \left( \frac{\partial Z}{\partial x_j} \right)^2 - \bar{\rho}\tilde{\chi}$$

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## Transport equation for mixture fraction



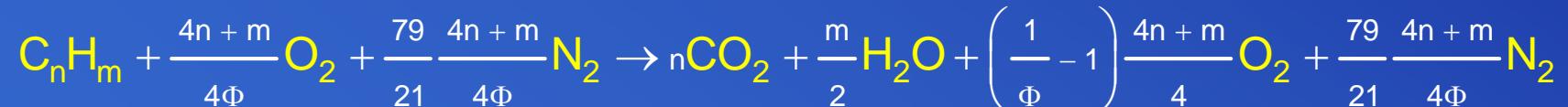
Mass fraction transport  
equation for partial premixing:

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{Y}_i) + \frac{\partial}{\partial x_i}(\bar{\rho}\tilde{u}_i\tilde{Y}_i) = -\frac{\partial}{\partial x_i}\bar{\rho}\widetilde{u_i''Y_i''} + \bar{R}_i$$

$$\tilde{c} = \frac{\tilde{Y}_p - Y_u}{Y_b - Y_u}$$

$$\bar{R}_i = \bar{S}_c \cdot (Y_b - Y_u)$$

1-step global reaction:



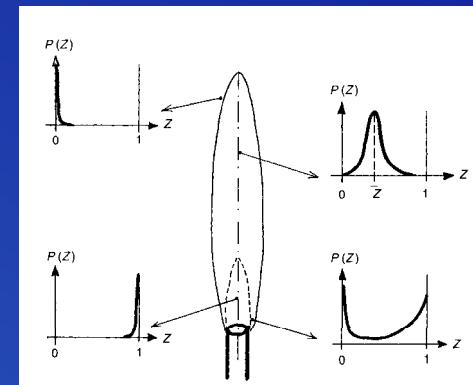
## Changes through partial premixing

Lindstedt-Vaos model:

$$\bar{S}_c = C_R \cdot \rho_u \cdot \frac{s_l}{\nu^{1/4}} \cdot \frac{\tilde{\epsilon}^{3/4}}{\tilde{k}} \cdot \tilde{c} \cdot (1 - \tilde{c})$$

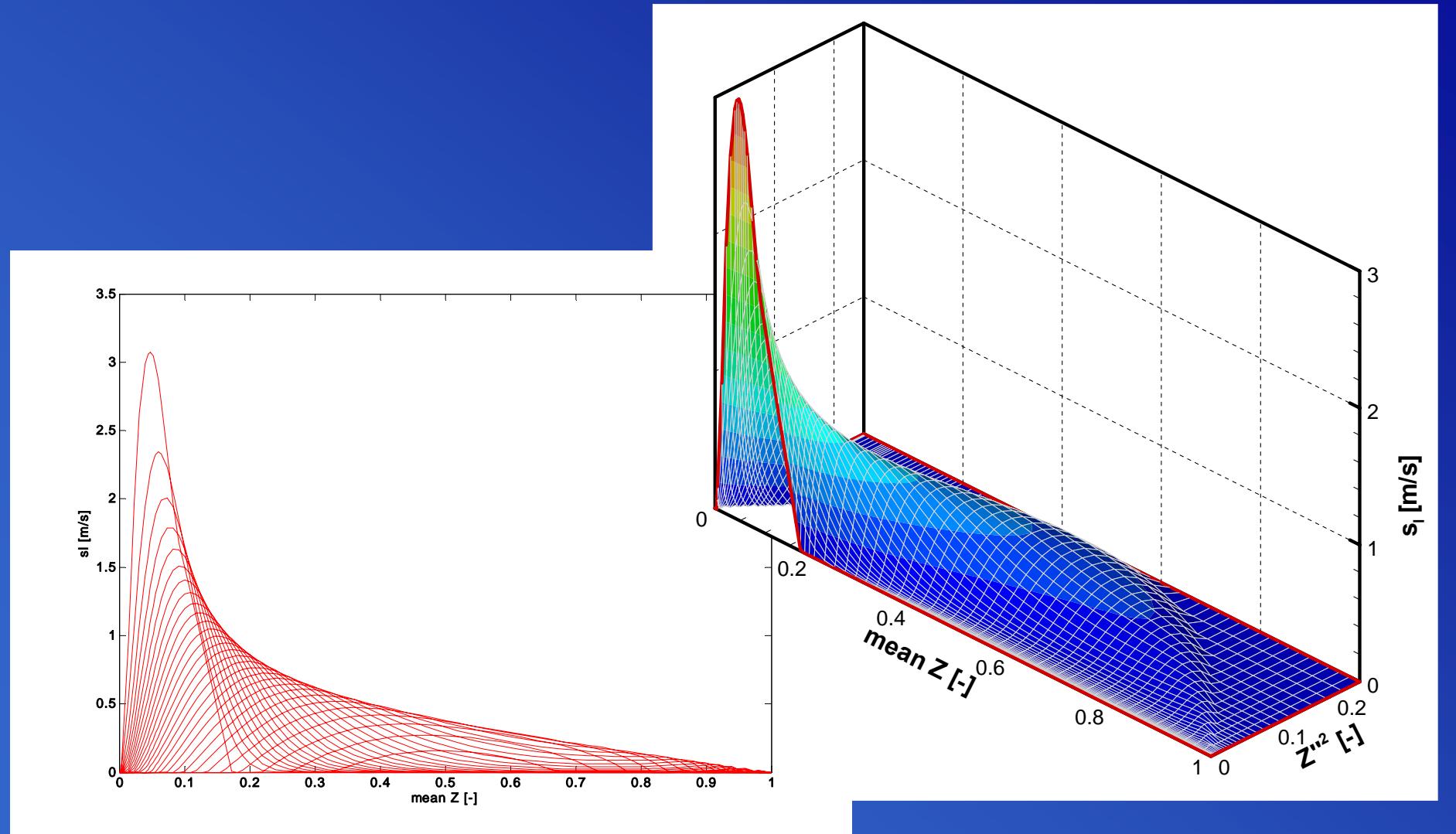


local flame speed:  $s_l = s_l(\tilde{Z}(x, t))$



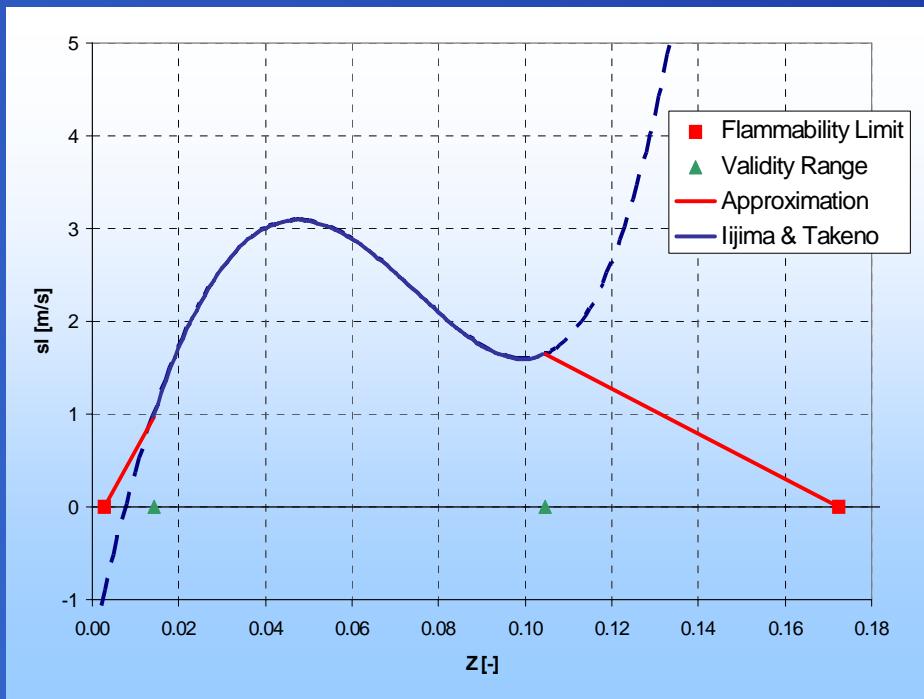
turbulence effect:  $\tilde{s}_l(\vec{x}, t) = \int s_{l_{\tilde{Z}, \tilde{Z}''^2}}(Z) \tilde{P}_{\tilde{Z}, \tilde{Z}''^2}(Z; \vec{x}, t) dZ$

**Turbulent burning rate in partially premixed flame**

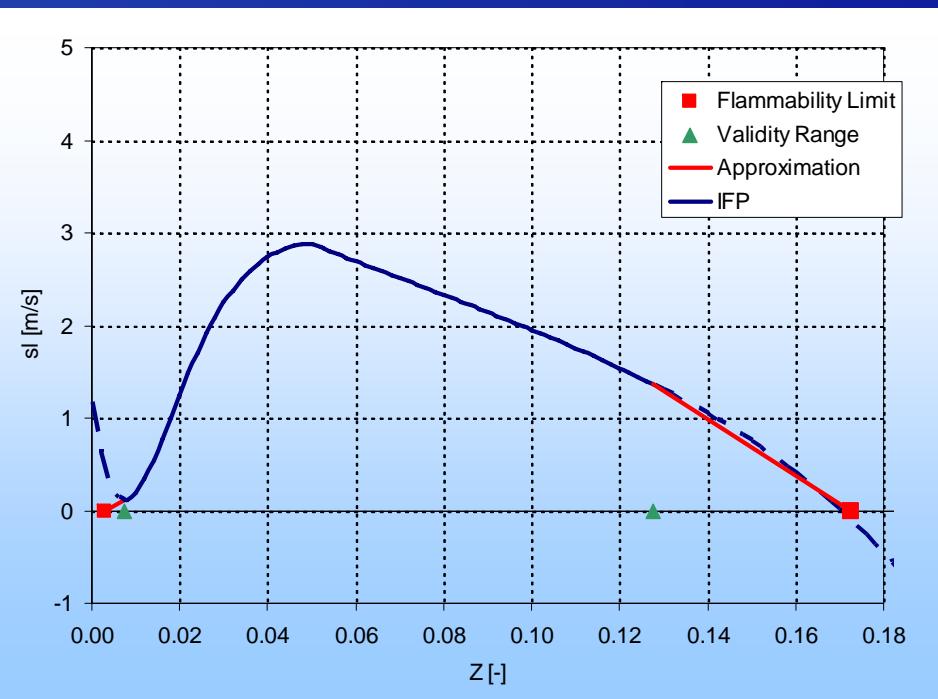


Laminar Flame Speed Table (Hydrogen,  $p = 1$  Bar)

## Correlation of Iijima & Takeno

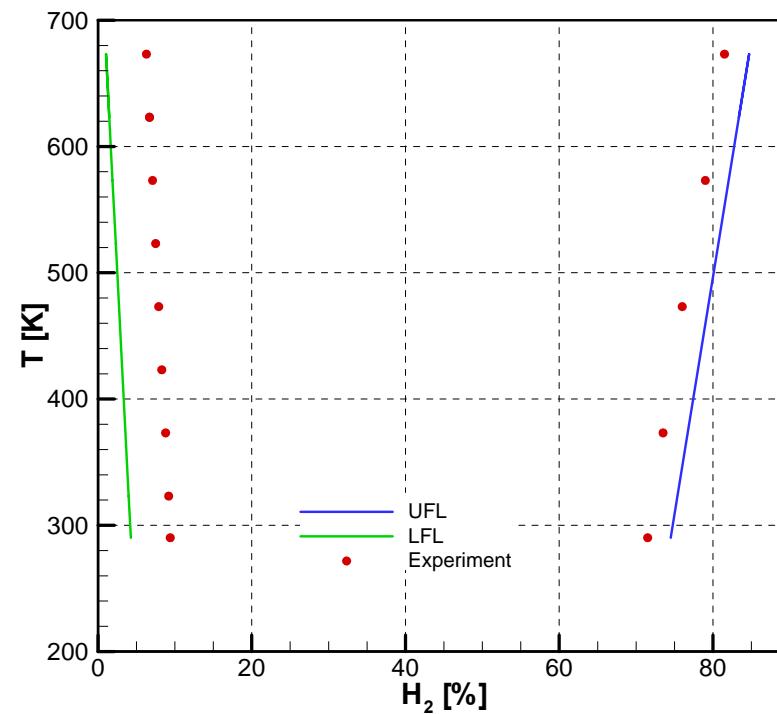
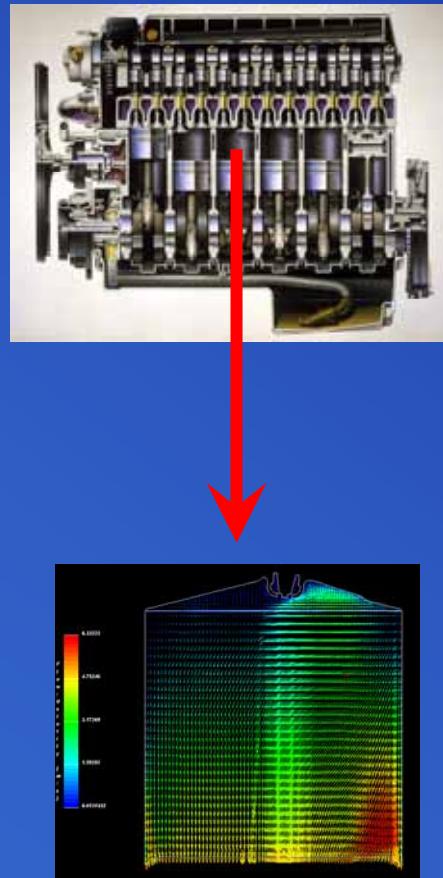


## Correlation of IFP



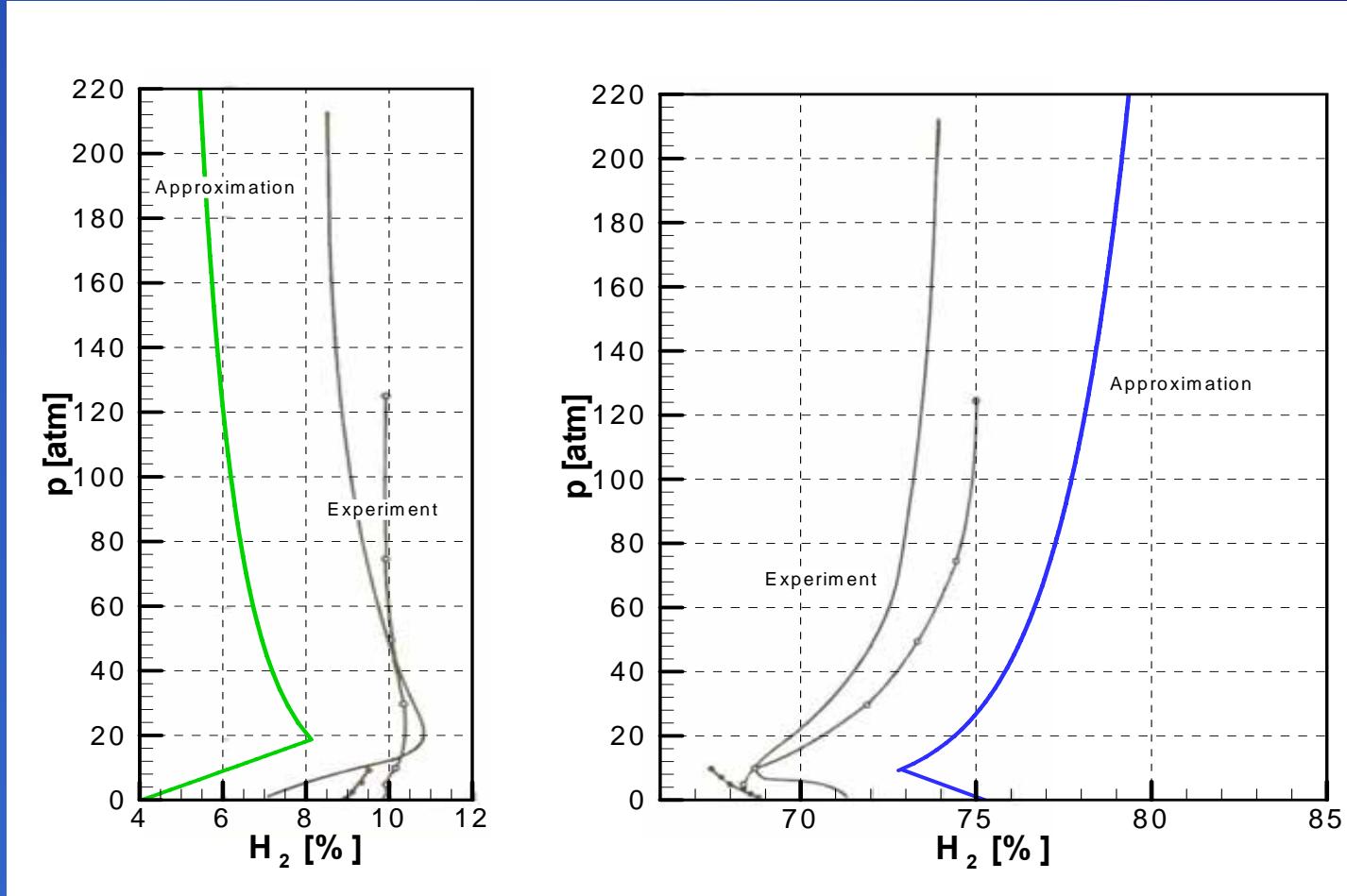
**Extension of laminar flame speed correlations**

## ICE application: $p$ , $T_{u,f}$ , $T_{u,ox}$ changes during simulation, partial premixing



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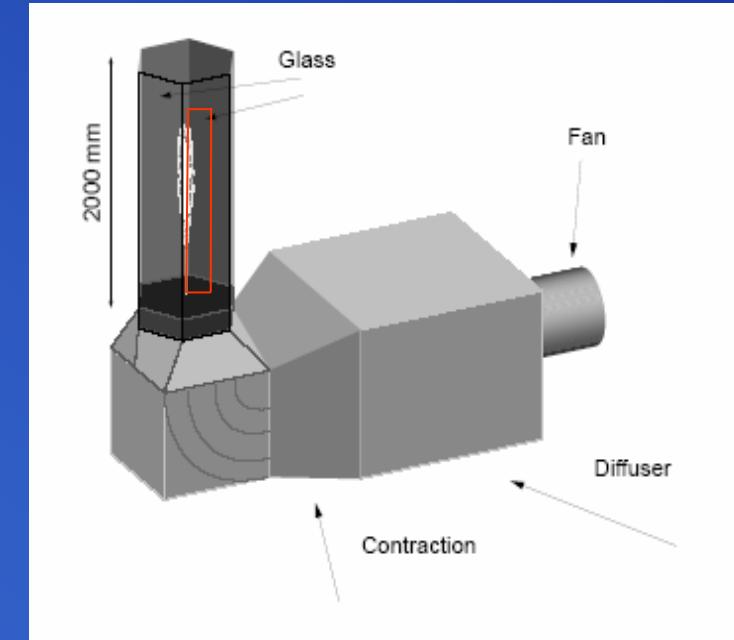
## Flammability Limits – Temperature Dependence



Experiment  
Bureau of Mines  
Bulletin 503

## Flammability Limits – Pressure Dependence

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Elements: 131518

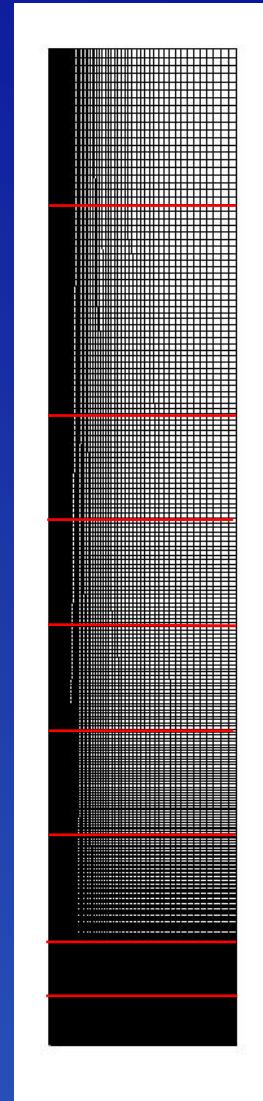
Nodes: 87200

Grid dimension:

150 mm x 800 mm

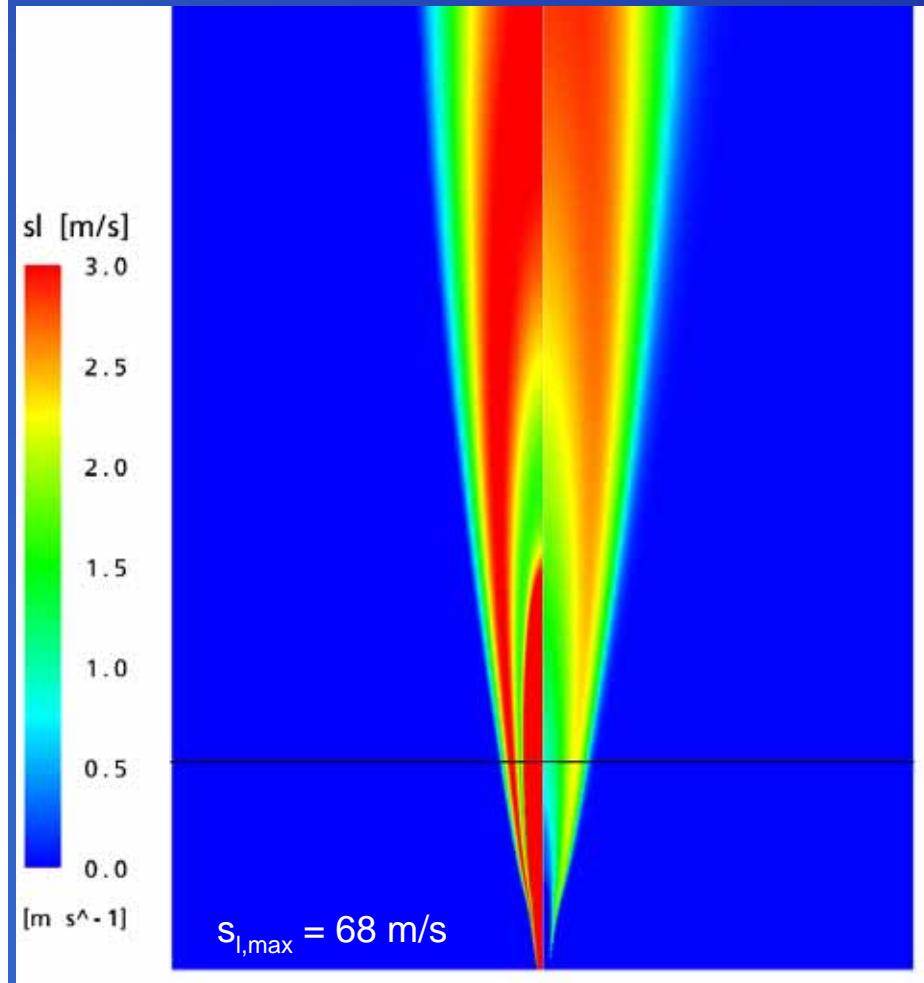


y [mm]	y/L	y/D
675	1/1	180
506	3/4	135
422	5/8	113
338	1/2	90
253	3/8	68
169	1/4	45
84	1/8	23
42	1/16	11

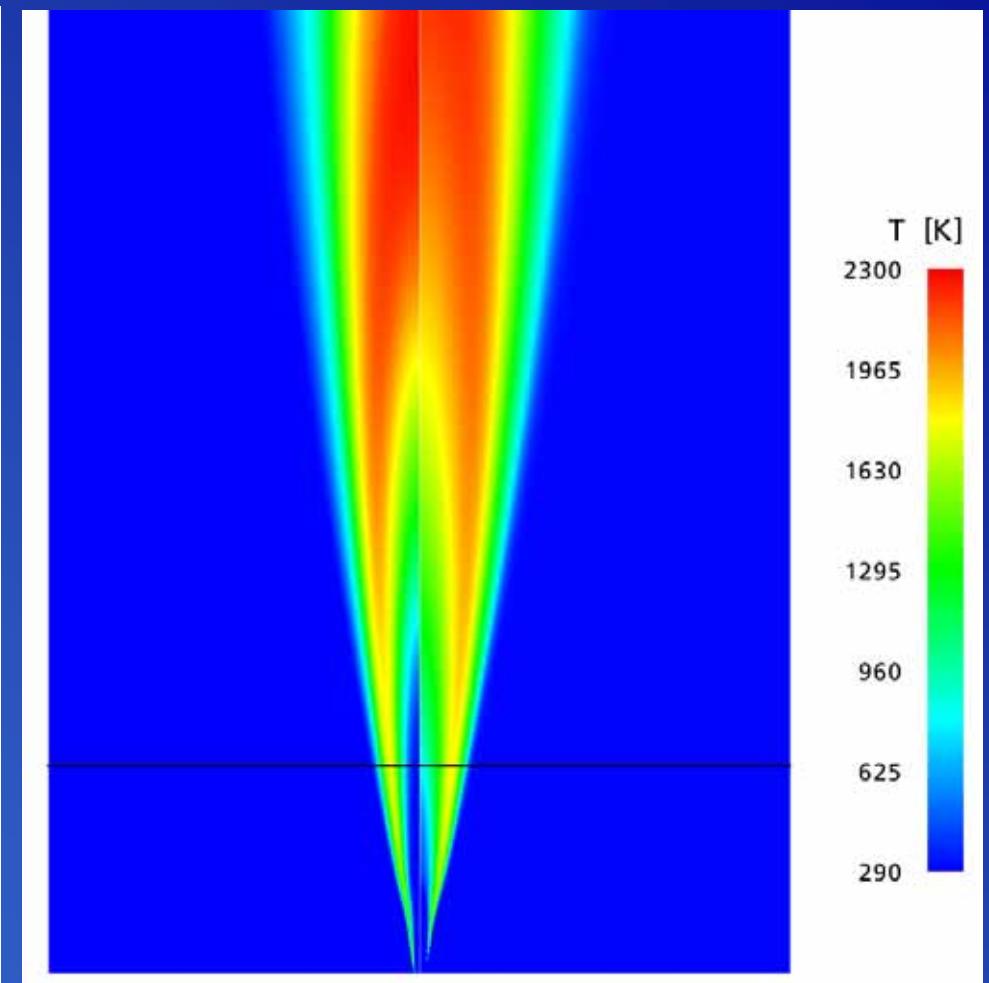


## Hydrogen Jet Flame

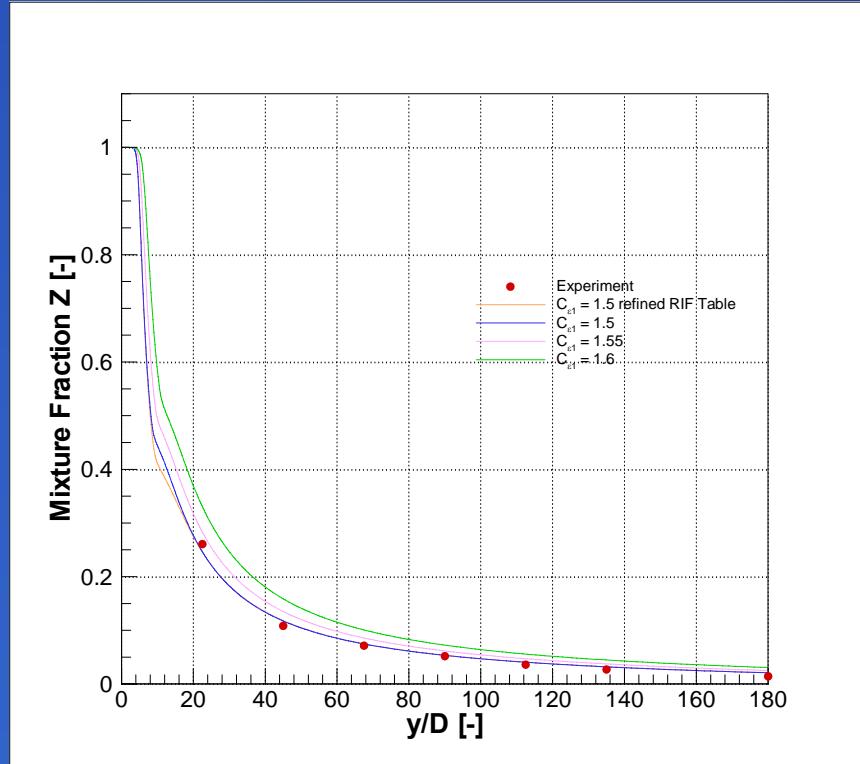
## Iijima &amp; Takeno Correlation



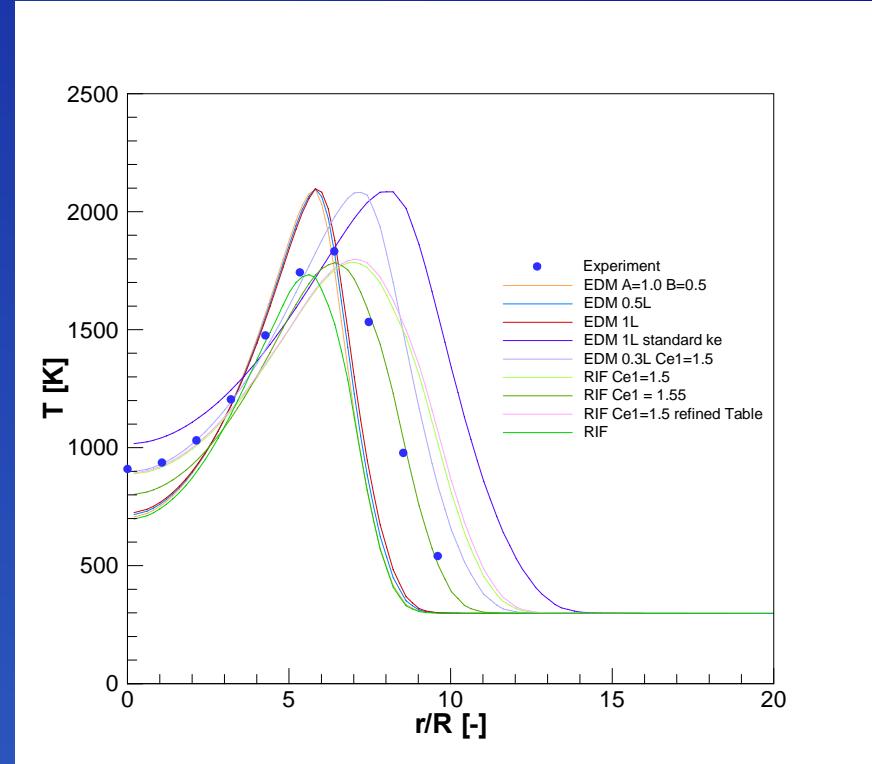
## Iijima &amp; Takeno Table



## Results



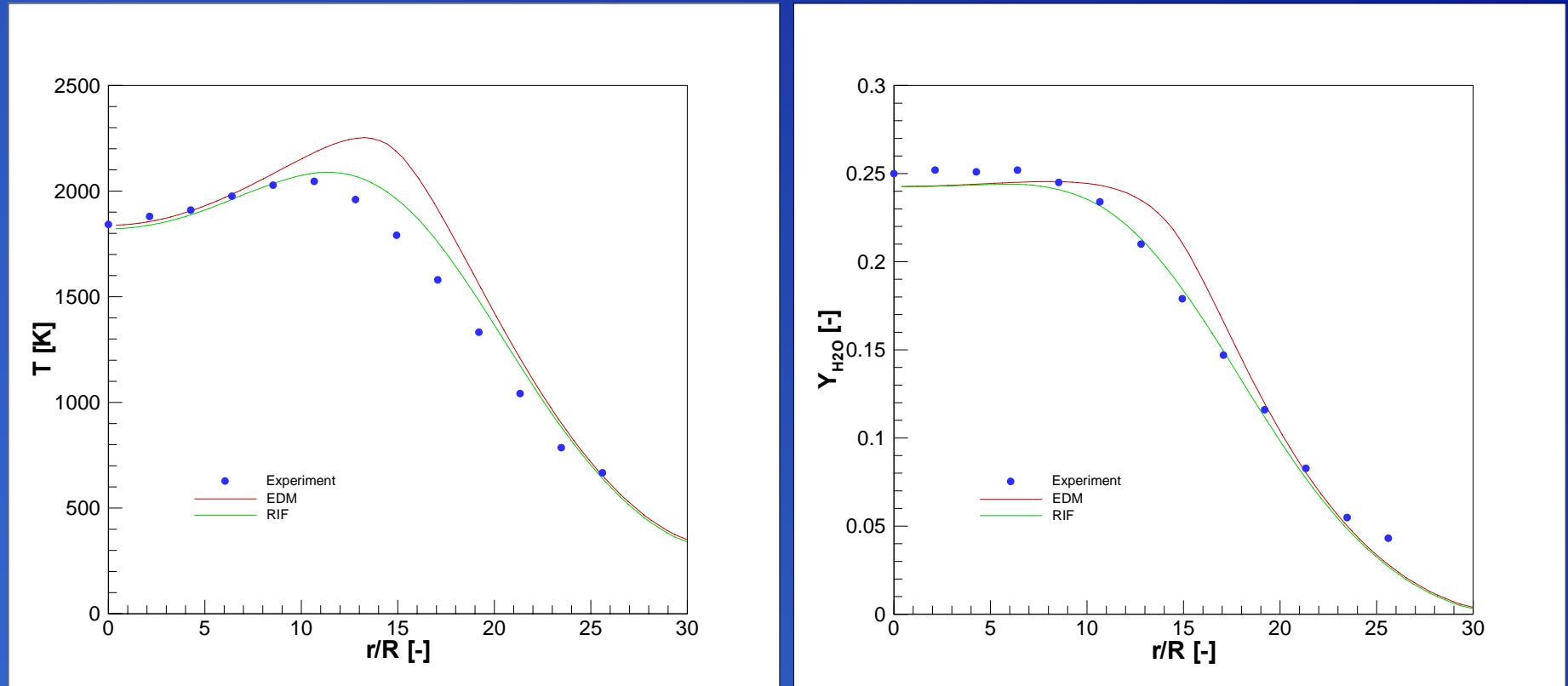
Mixture fraction on axis



Radial temperature profile  
 $(y/D = 23)$

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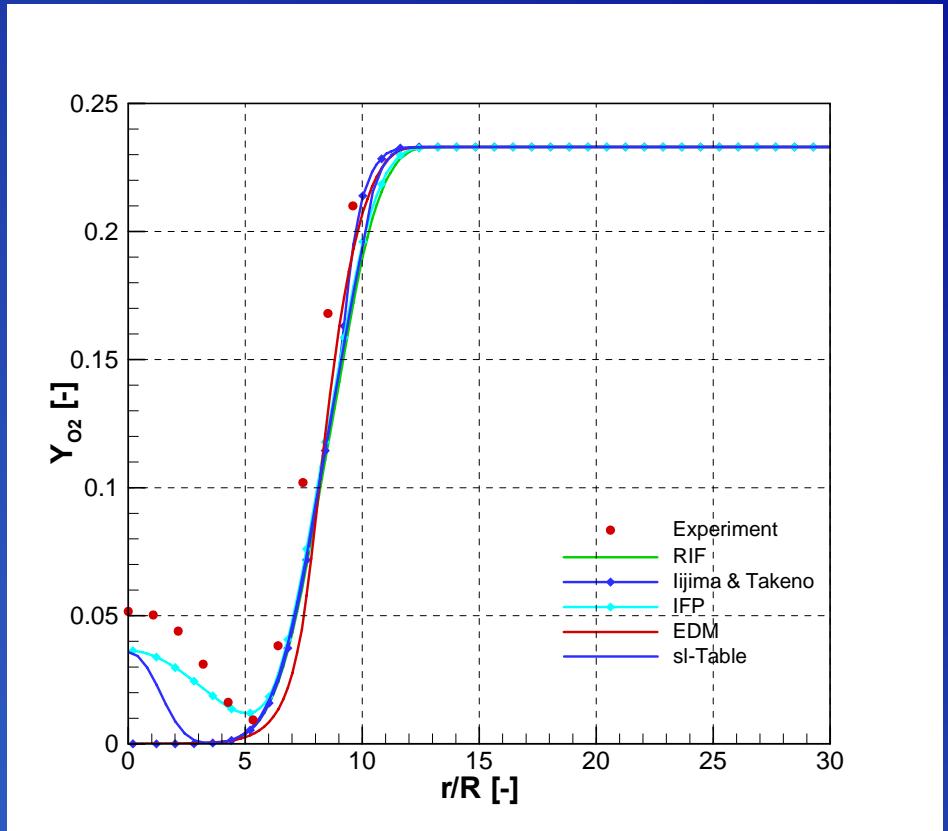
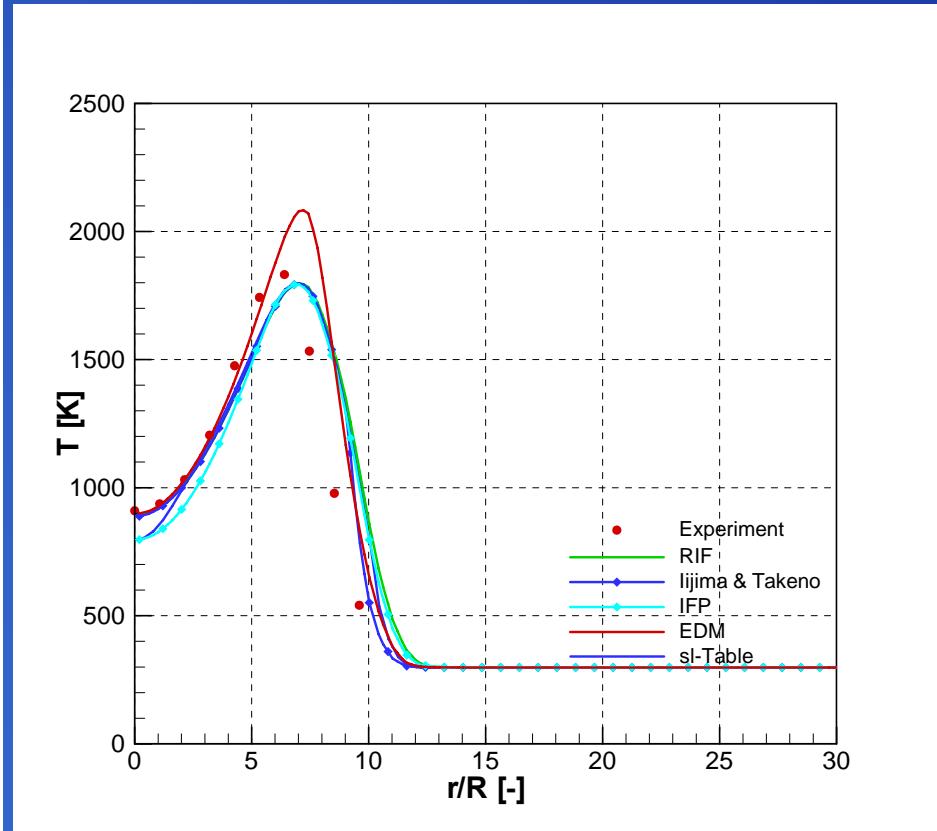
**H<sub>2</sub> Jet Flame – Influence from turbulence model**



$$C_{\varepsilon 1} = 1.5$$

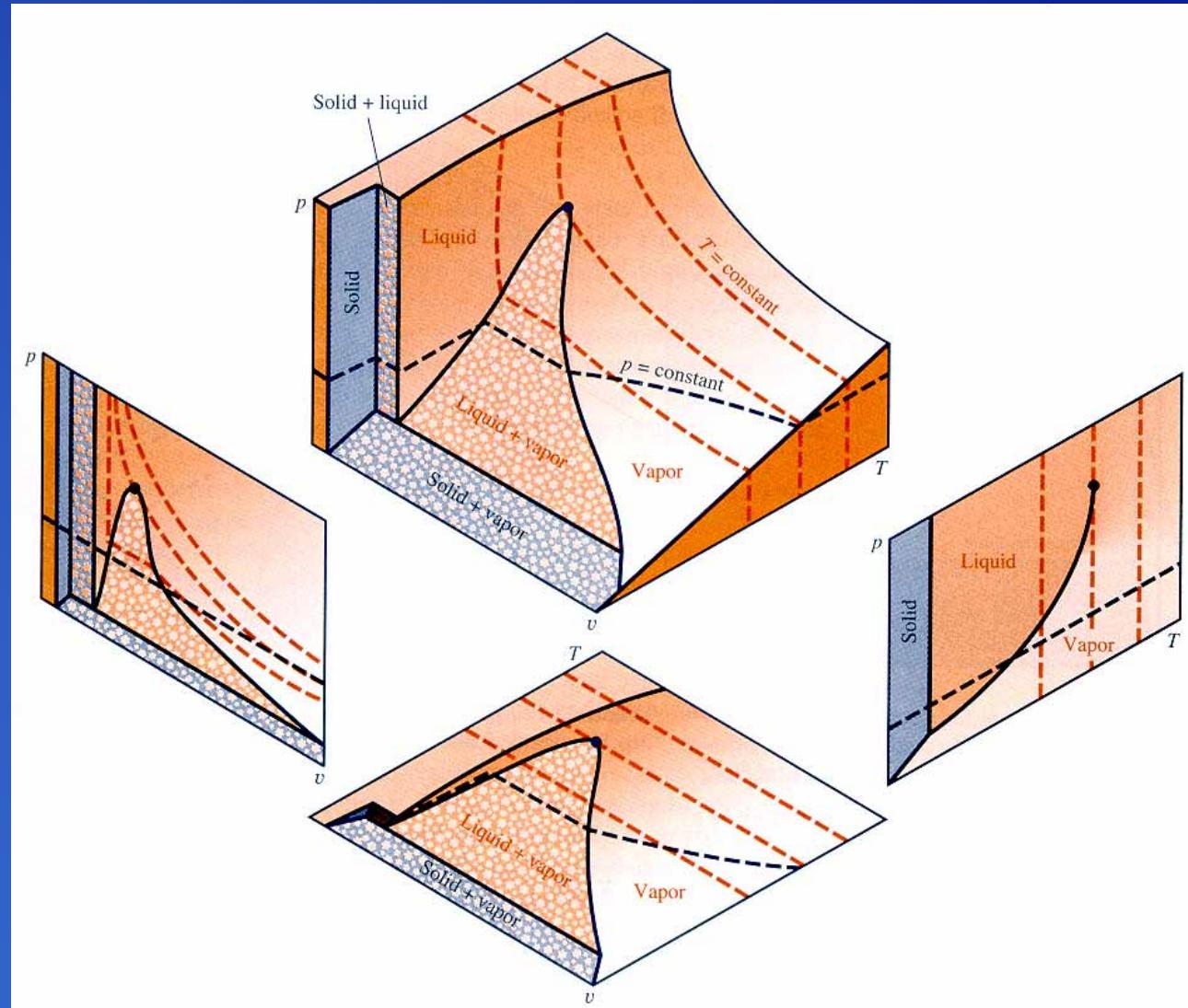
Axial Position 253 mm ( $y/D = 68$ )

$$y/L = 1/8$$

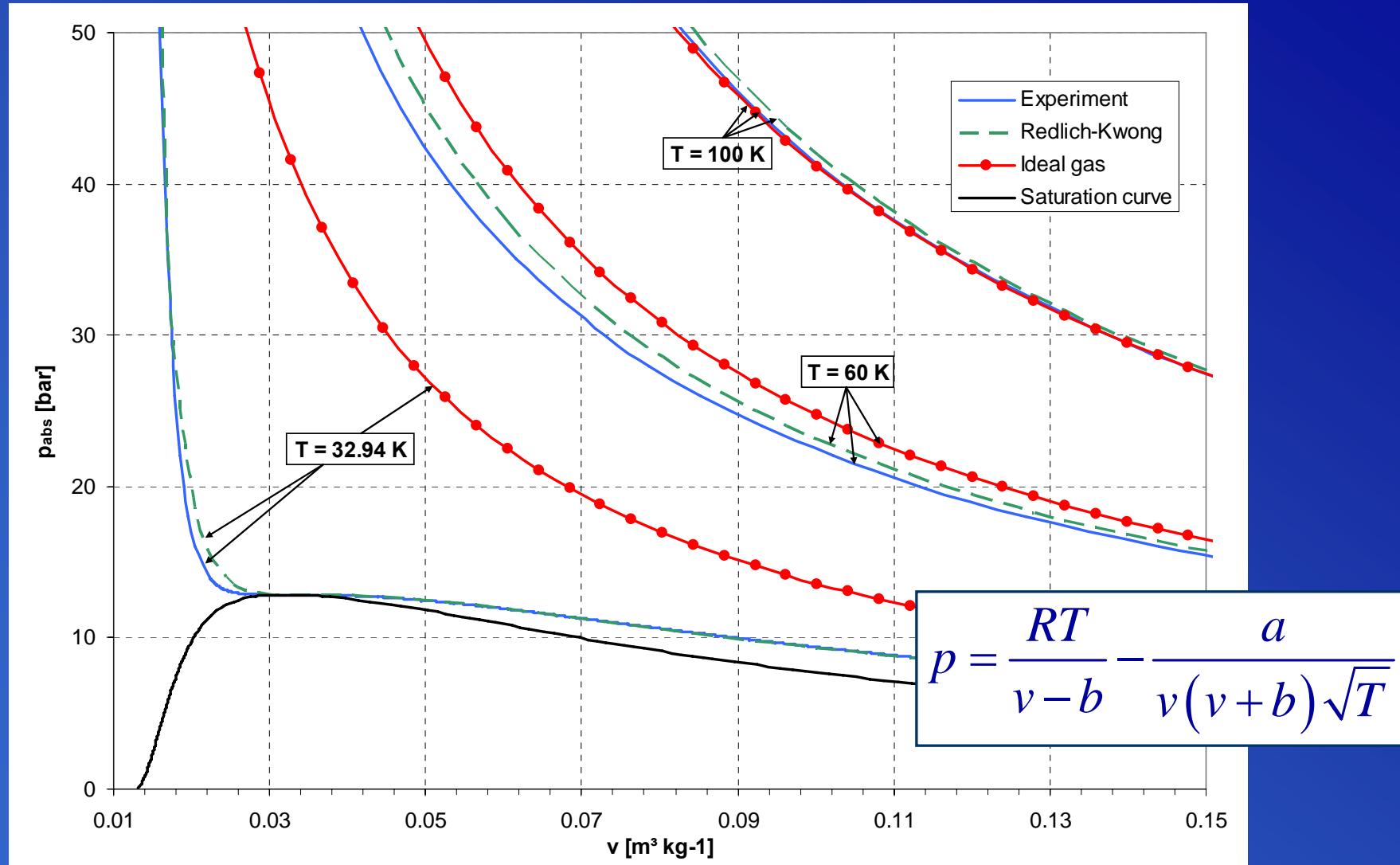


## Results

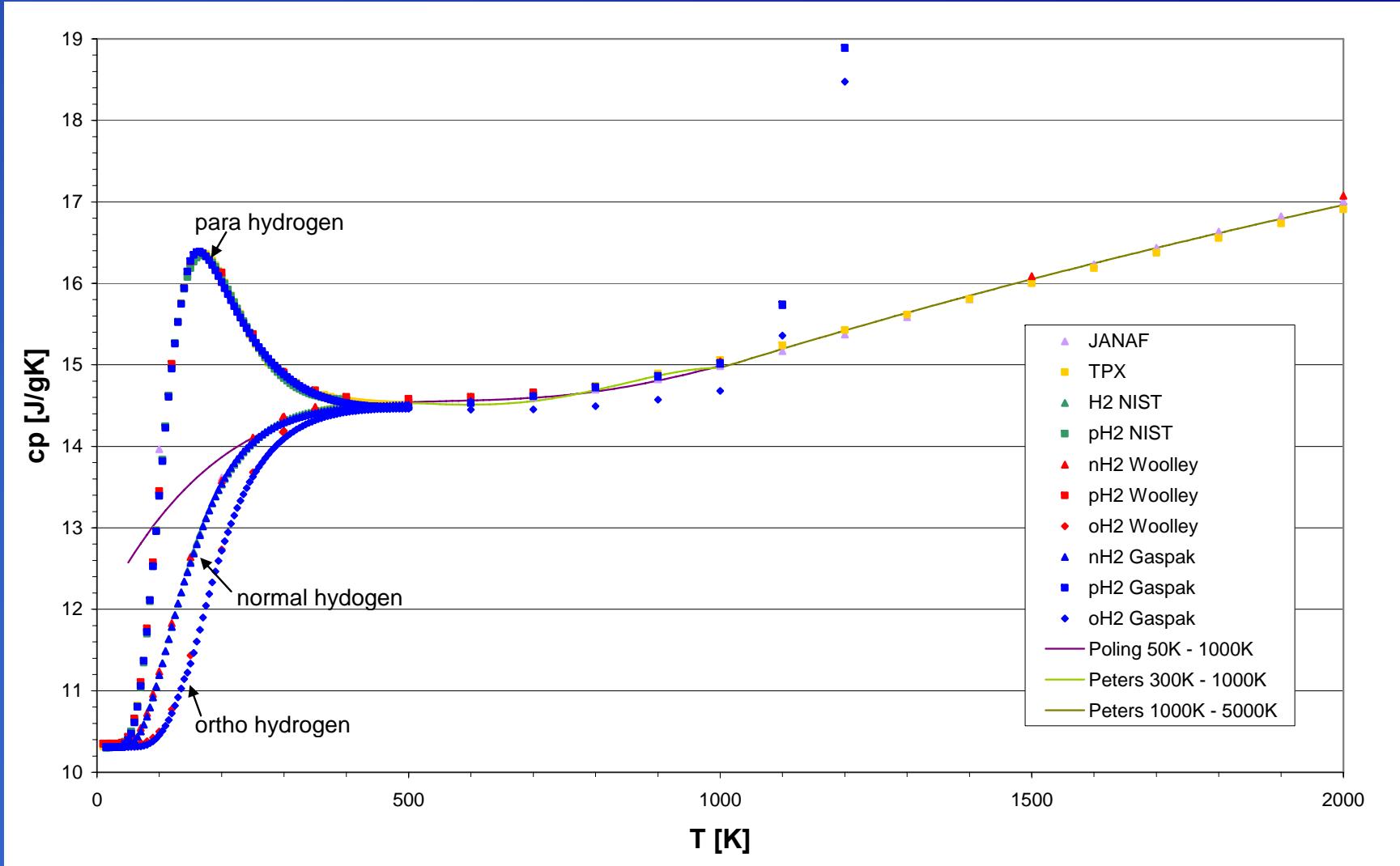
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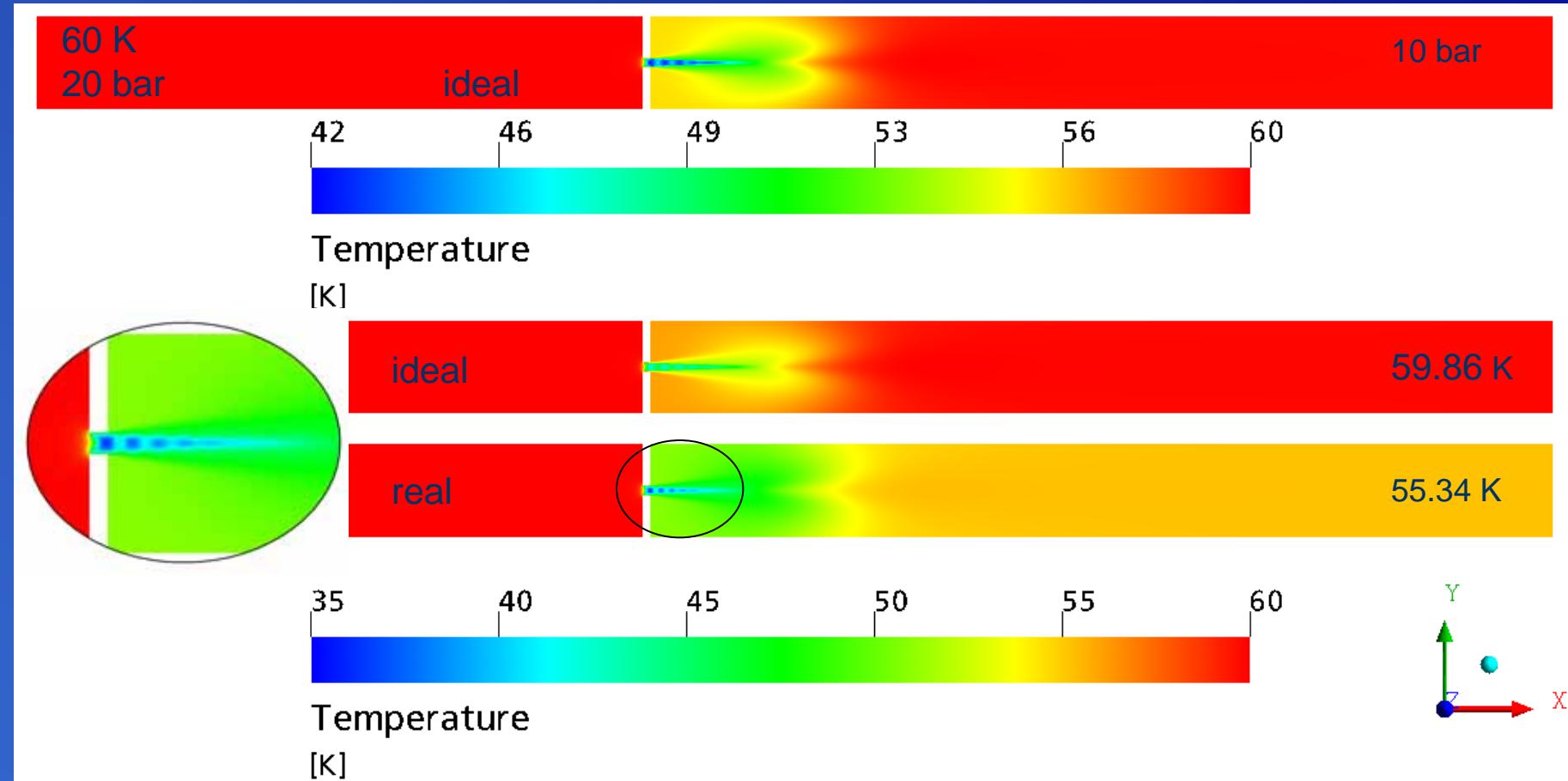
Real gas effects:  $pVT$ -surface of pure normal substances



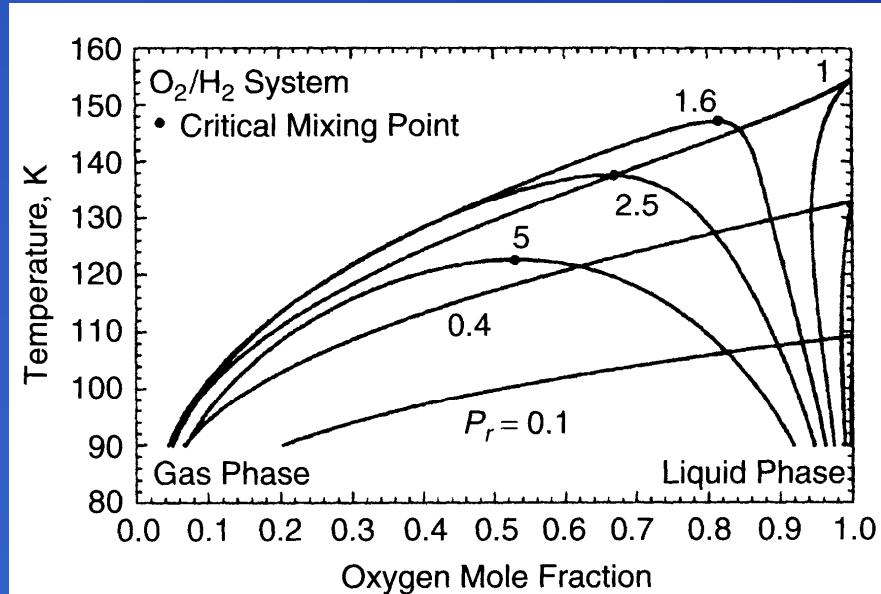
**pvT-data for hydrogen**



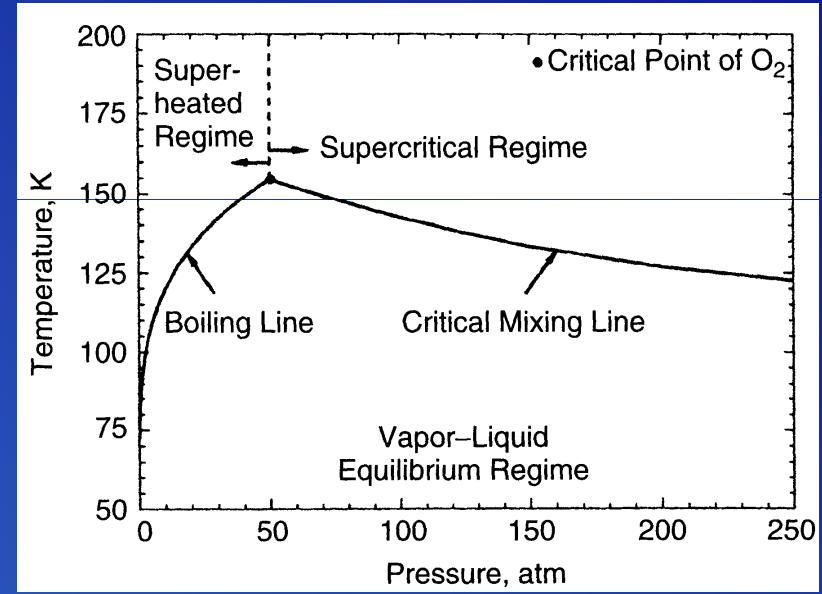
## H<sub>2</sub> specific heat at low temperatures



## Hydrogen Joule-Thomson effect

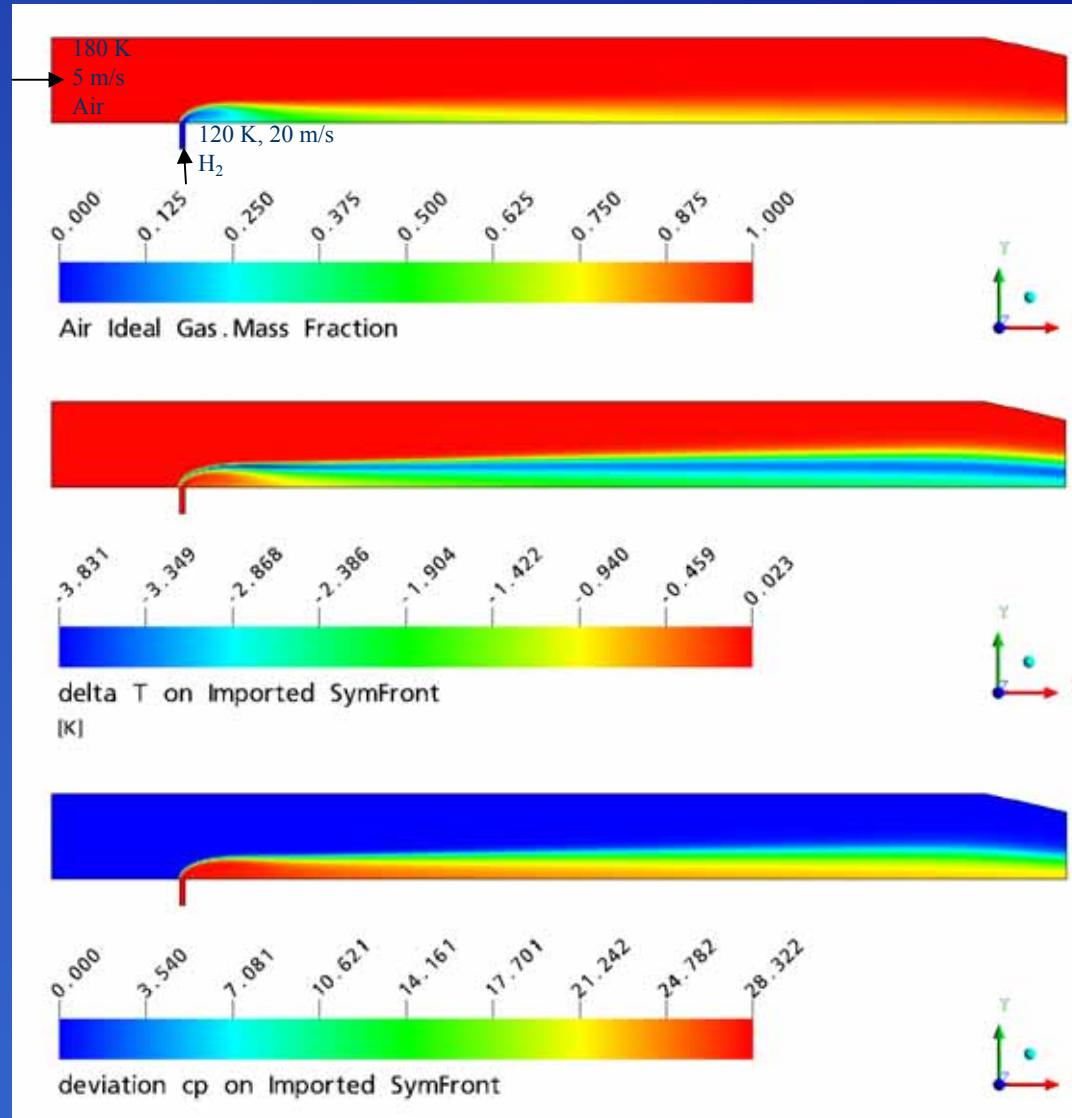


Critical mixture temperature

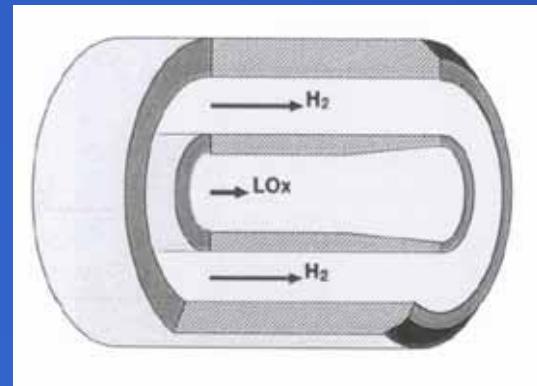
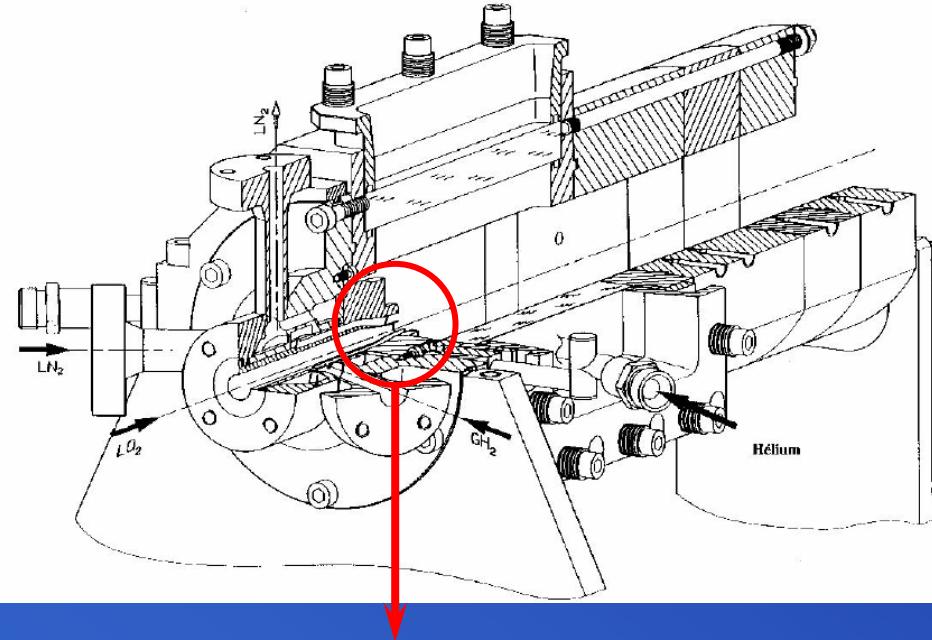


Critical mixture regime

## H<sub>2</sub>-O<sub>2</sub> Supercritical mixing regime

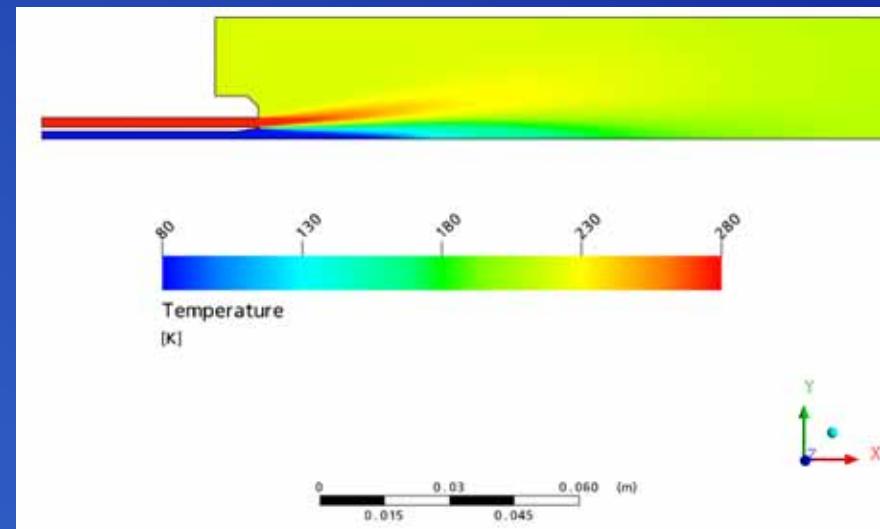
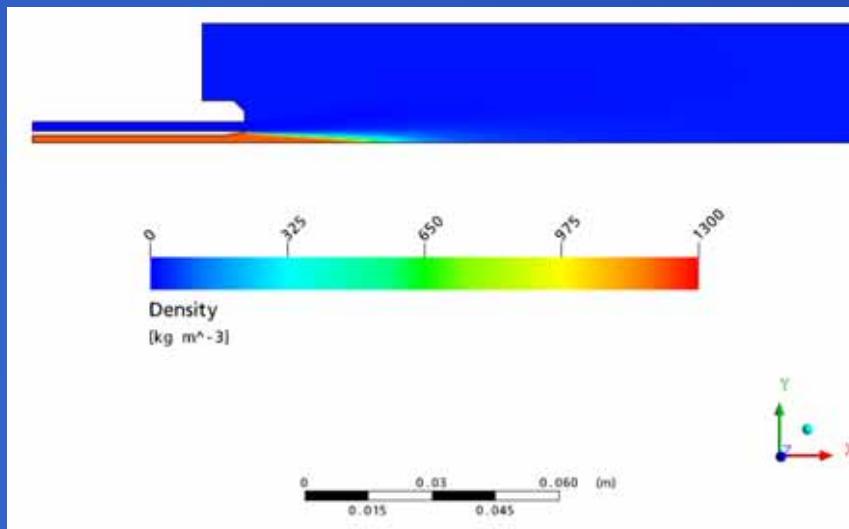
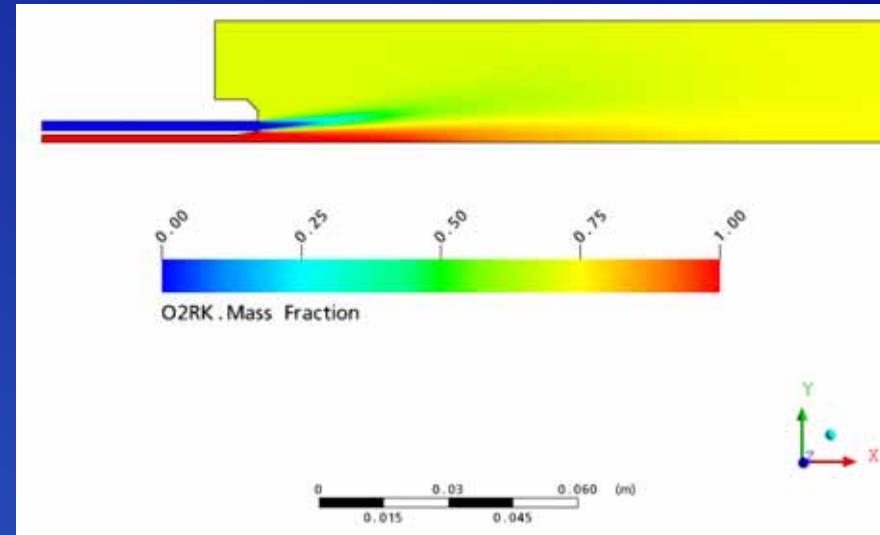
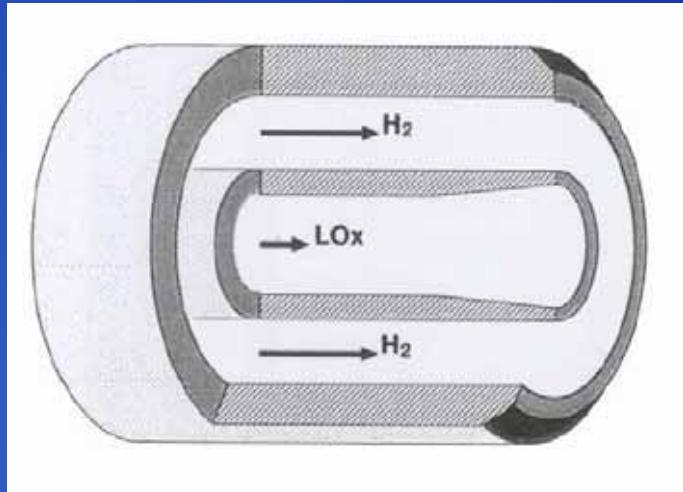


Injection of para and ortho hydrogen in air



Conditions	H2	O2
Pressure [MPa]	6	6
Massflow [g/s]	42	105
Temperature [K]	275	83
Density [kg/m <sup>3</sup> ]	5.66	1188.3
Cp [J/kg/K]	14412	1663
Velocity [m/s]	138	4.5
Viscosity [kg/m/s]	8.61e-4	2.57e-4

Mascotte single injector validation case



## Mascotte real gas cold mixing results

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- Modelling of partially premixed turbulent flames by combination of premixed and non-premixed concepts
- Reduced chemistry if only temperature / main species required
- Models validated at atmospheric / medium pressure
- Application to gas turbine / ICE / rocket motor combustion
- Real gas effects: important in rocket motors
- additional equations → new effects → extended models

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## Conclusions