Enabling Advanced Modeling and Simulations for Fuel-Flexible Combustors

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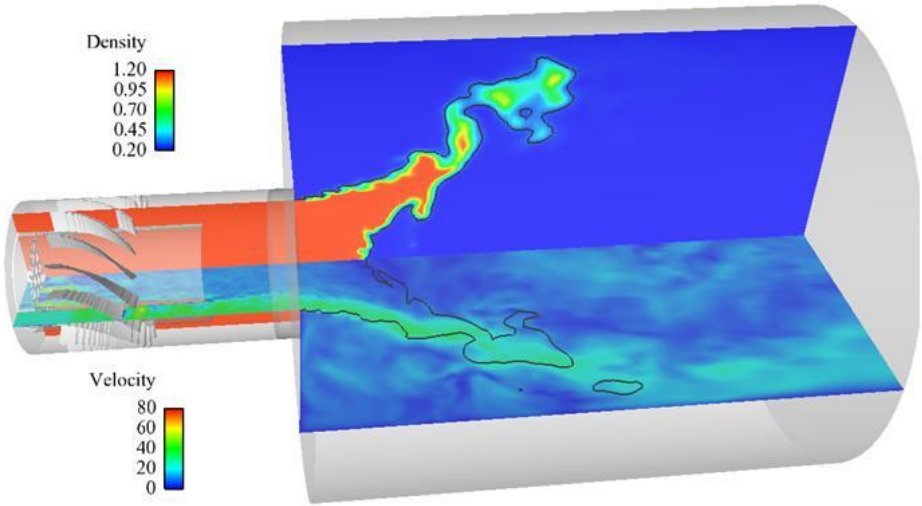
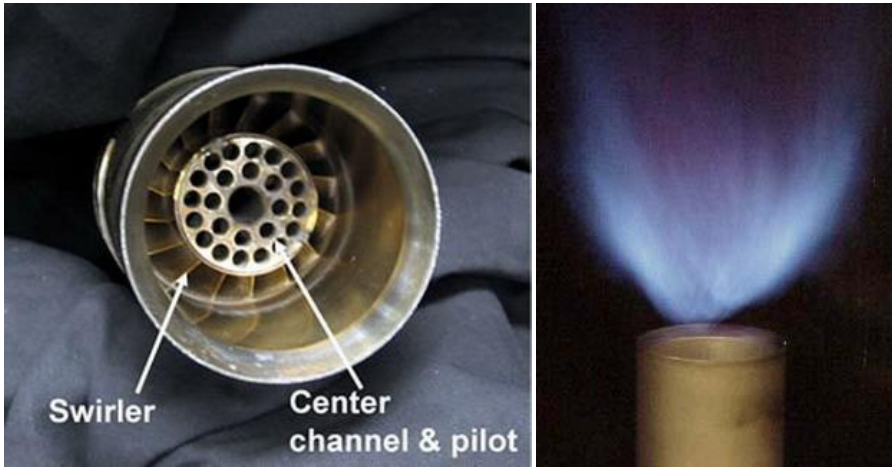
Stanford University

Grant #: DE-FG26-08NT43325



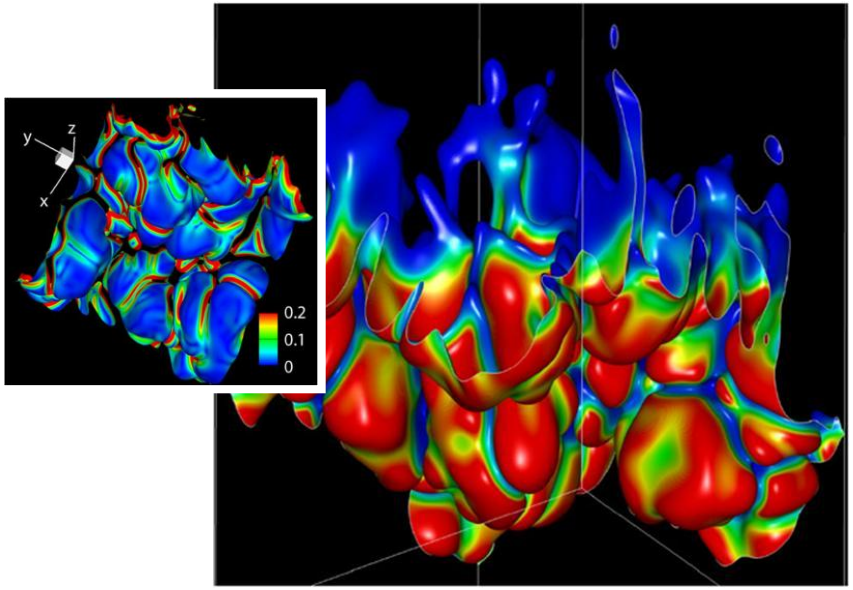
Motivation



http://eetd.lbl.gov/aet/combustion/LSC-info

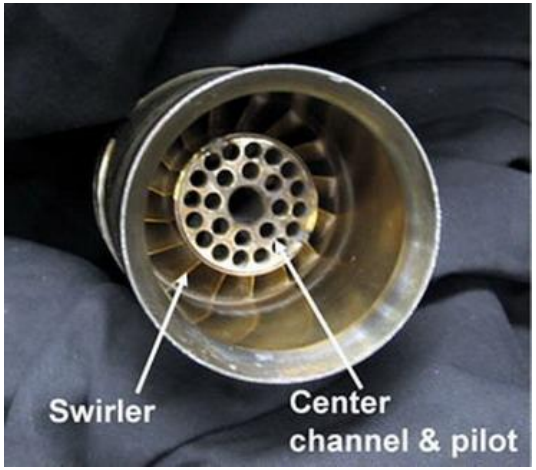
- **Low Swirl Injectors (LSI)**
  - Flame stabilization method
    - ***Recirculation*** region
    - ***Lean Premixed*** flame
  - Advantages
    - Simple & robust
    - Ultra ***low emissions*** (NO_x, CO)
  - Fuel considered: CH_4, H_2

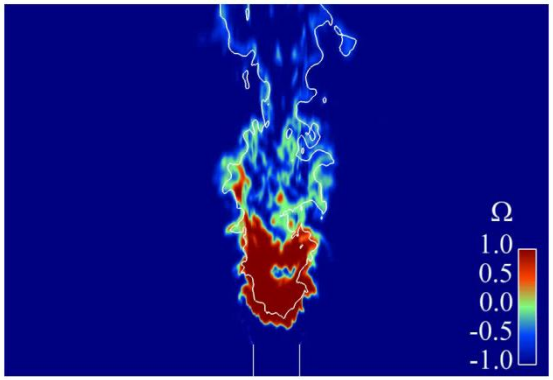
- **Modeling challenges**
  - ***Partially premixed*** combustion
    - Premixed flame
    - Diffusion flame
  - ***Non-unity Lewis*** number effects
    - Differential diffusion
    - Combustion instabilities
    - Noise

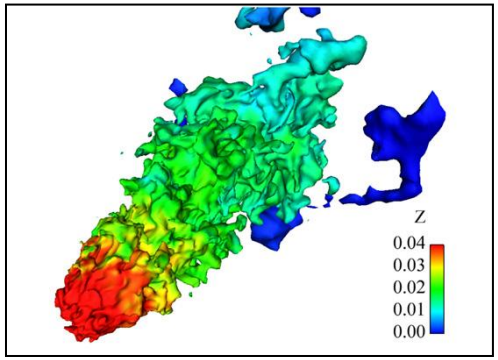


Day *et al.* Comb. Flame **2009**

Previous Work & Limitations

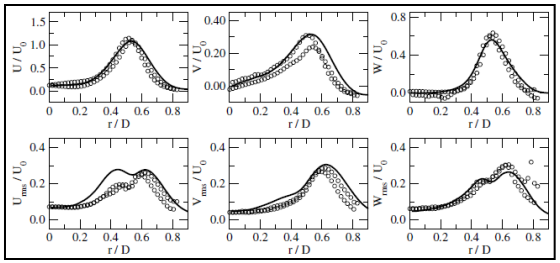






- ***Previous work / modeling***
  - "A dynamic model for the turbulent burning velocity for large eddy simulation of premixed combustion", *Combustion & Flame*, **2008**, E. Knudsen, H. Pitsch
  - "A general flamelet transformation useful for distinguishing between premixed and non-premixed modes of combustion", *Combustion & Flame*, **2009**, E. Knudsen, H. Pitsch

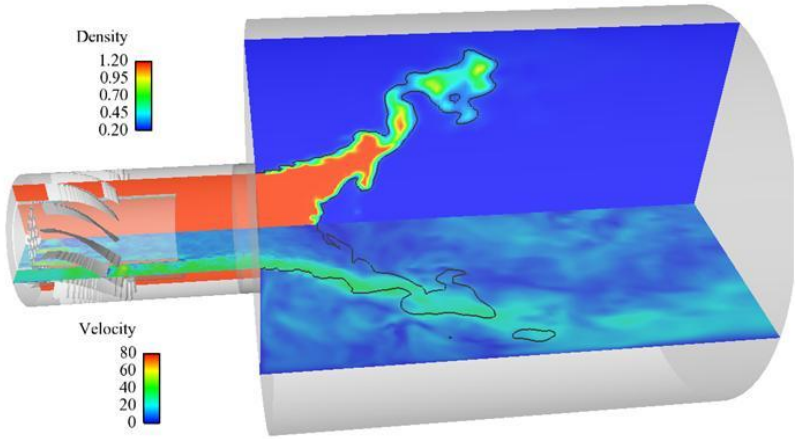
- ***Limitations / next step***
  - Does not include ***differential diffusion***
    - Assumes same diffusivity for all species (Le = 1)
  - Extend the framework to *hydrogen combustion* (Le ≅ 0.3)



Outline

- **Premixed combustion**
  - Modeling approach
  - Validation
  - Application: low swirl burner

- **Non-unity Lewis number effects**
  - Modeling approach
  - Validation
  - Application



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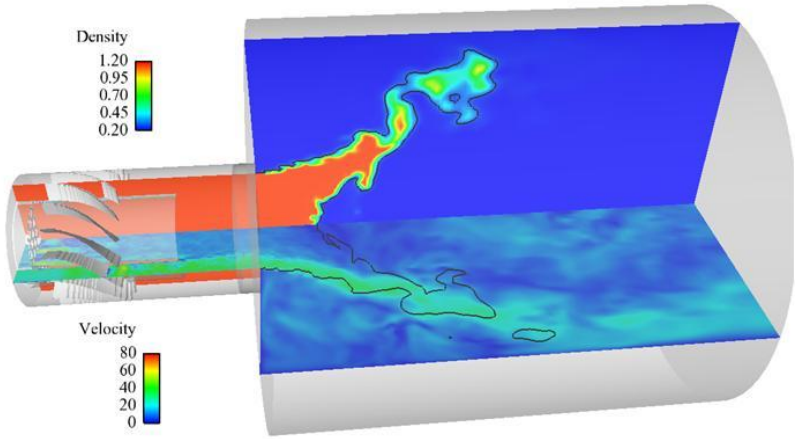
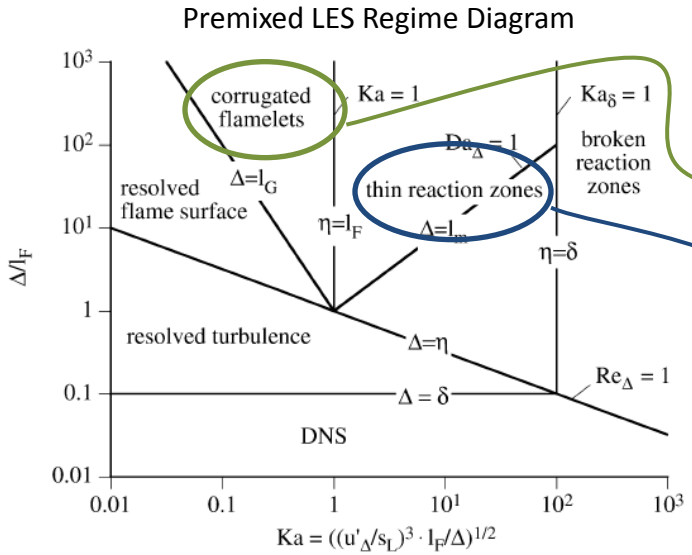
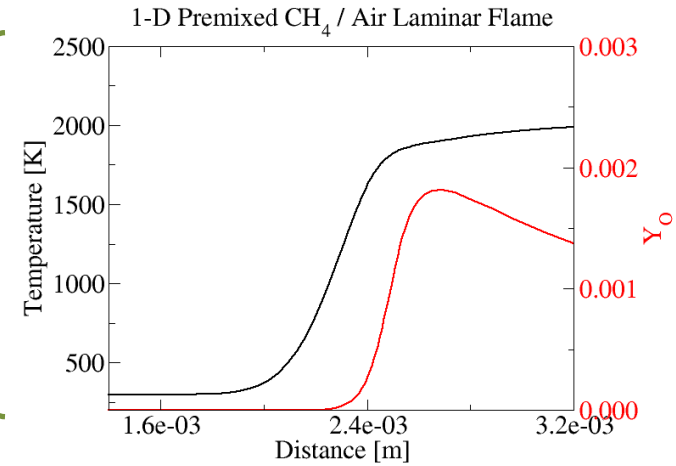
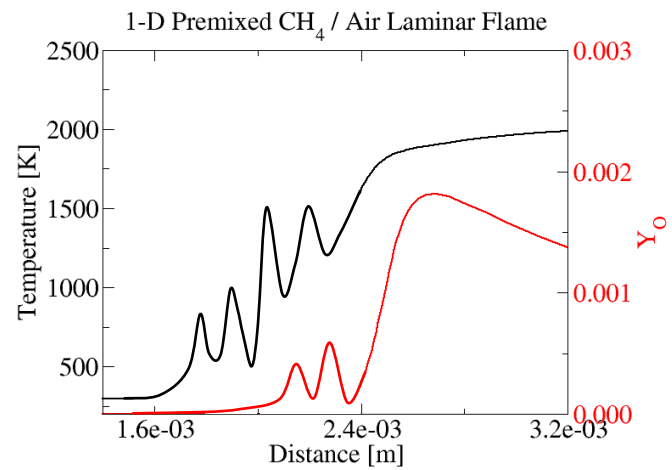


Premixed Combustion







- **Lower Ka #** (milder turbulence)
  - Does not perturb 1-D flame structure
  - Well described by 1-D flamelets
- **Higher Ka #** (intense turbulence)
  - Perturbed flame preheat zone
  - Deviation from 1-D flamelets

Modeling Approach

- **3 transport equations**
  - ***Mixture fraction***

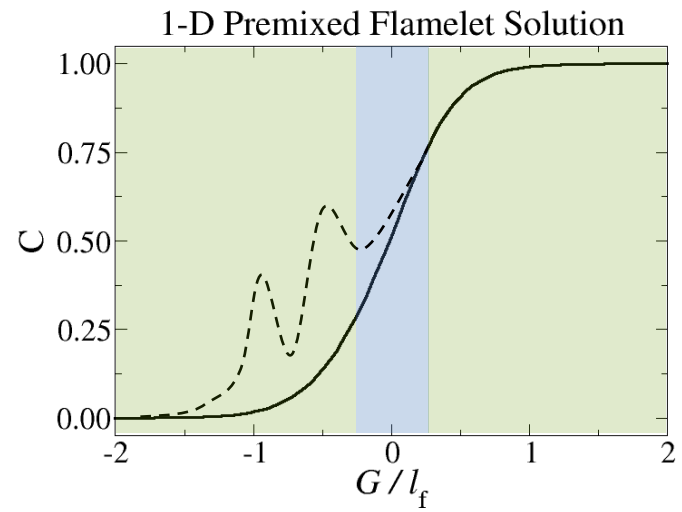
$$\partial_t(\rho Z) + \nabla \cdot (\rho \mathbf{u} Z) - \nabla \cdot (\rho \mathcal{D} \nabla Z) = 0$$

  - ***Progress variable***

$$\partial_t(\rho C) + \nabla \cdot (\rho \mathbf{u} C) - \nabla \cdot (\rho \mathcal{D} \nabla C) = \dot{\omega}_C$$

  - ***Levelset***

$$\frac{\partial \mathcal{G}}{\partial t} + u_j \frac{\partial \mathcal{G}}{\partial x_j} = (D\kappa)_{c0} |\nabla \mathcal{G}| + s_{L,c0} |\nabla \mathcal{G}|,$$



- **Source Terms**
  - Prog. Variable Src. Term: $\boldsymbol{\omega_C}$

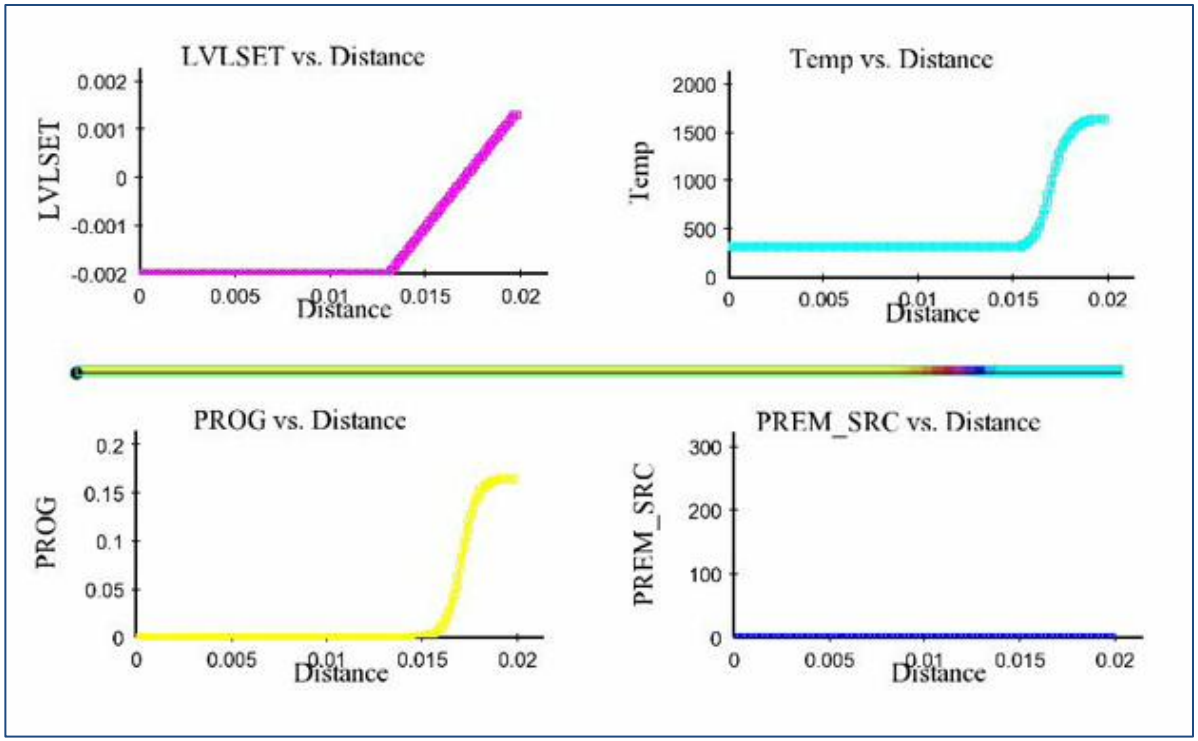
Transported Progress Variable: *C*

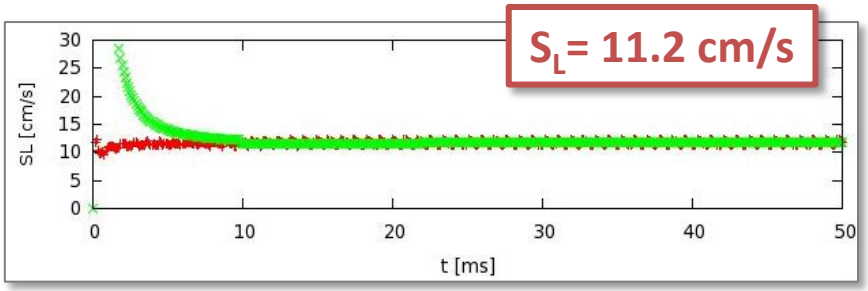
Assume Progress Variable Profile: *C*(G)*

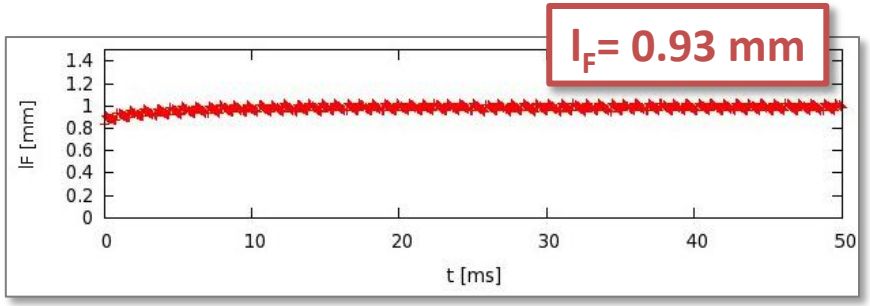
Region of Level Set Influence

Validation – Laminar Flame

- **1D laminar case**
  - CH_4 / Air
  - ϕ=0.59
- **Targets**
  - Comparison with ***detailed chemistry***
  - Burning speed: S_L
  - Flame thickness: l_F



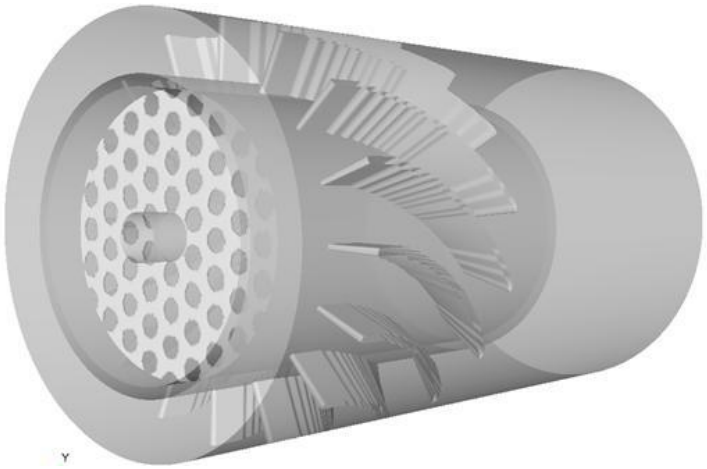


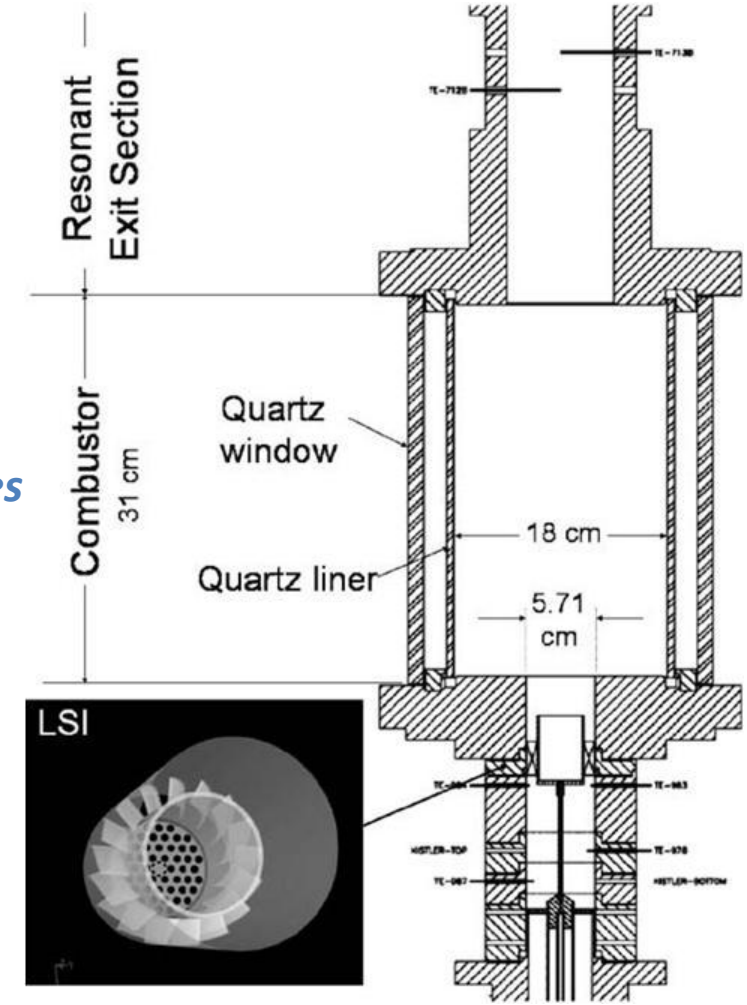


Low Swirl Burner - Geometry

- **Configuration**
  - *Cheng et al.* Proc. Comb. Inst. 32 (2009)
  - Pure ***CH_4*** and pure ***H_2*** flames

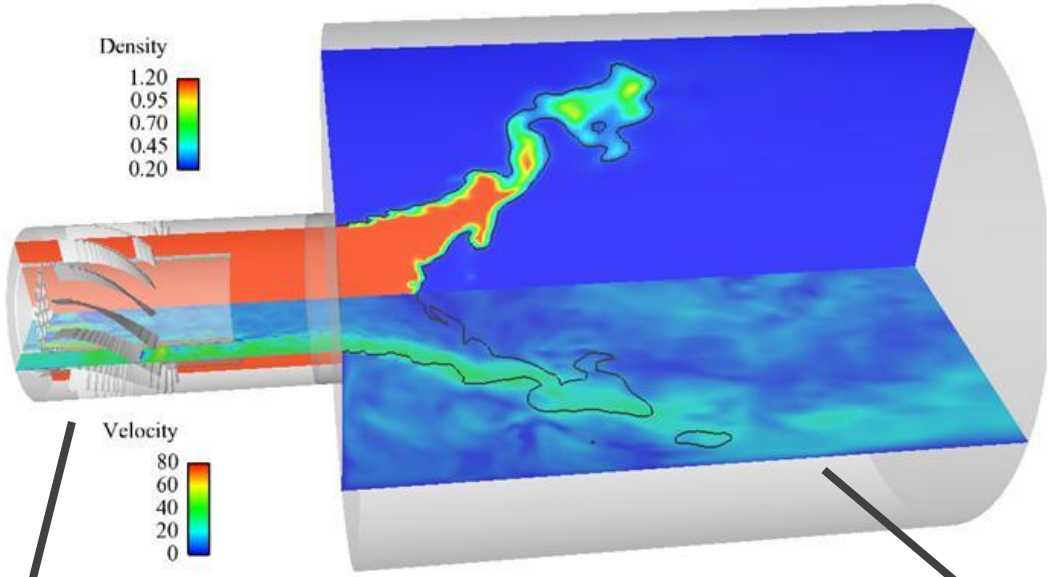
- **Large Eddy Simulation**
  - Structured Code: ***NGA****
  - Swirler described with ***Immersed Boundaries***



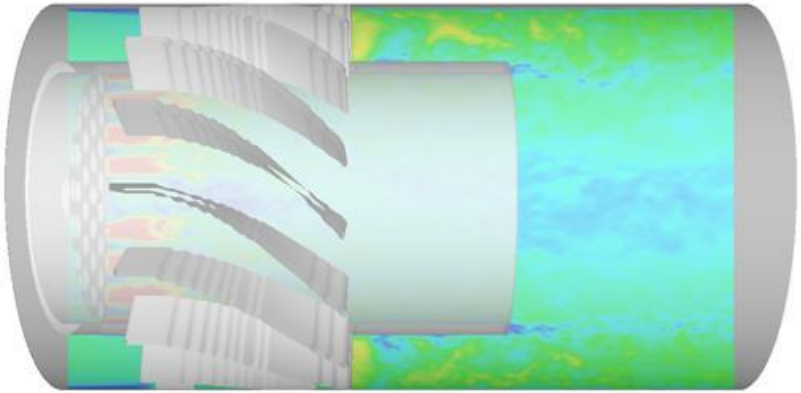


* Desjardins, O., Blanquart, G., Balarac, G., Pitsch, H. *Journal of Computational Physics* (**2008**)

Two Step Approach

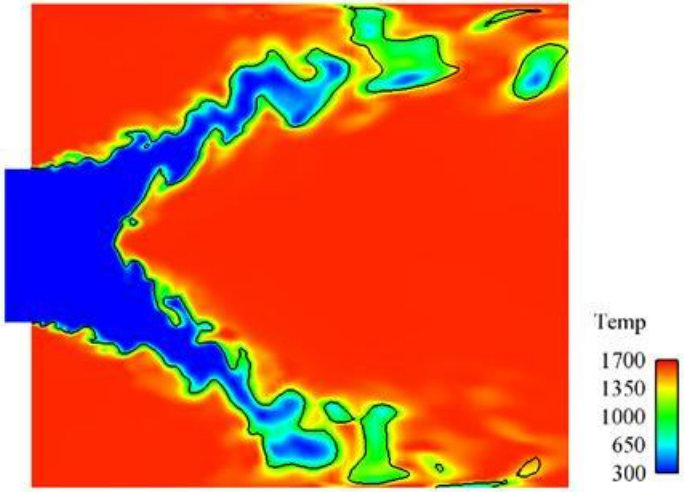


Swirler

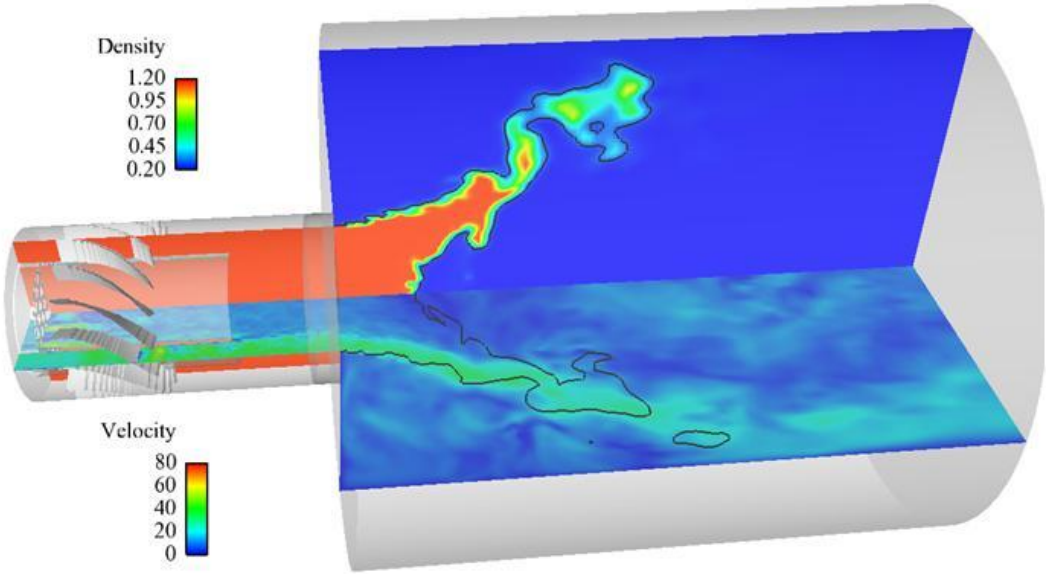


Inflow conditions

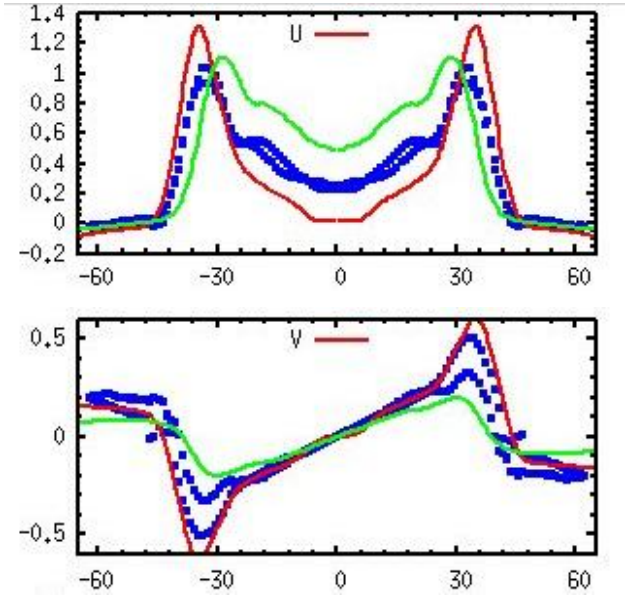
Combustion chamber



Boundary Conditions



- **Effects of boundary conditions**
  - Bulk velocity
    - Small effects
  - Percentage of massflux through center
    - ⇒ *Recirculation region*
    - Strong effect



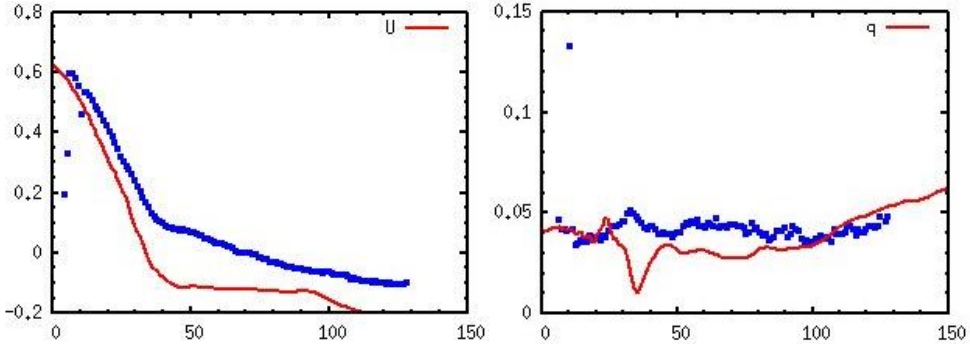
36 % through the center

45 % through the center

Pure Methane Case

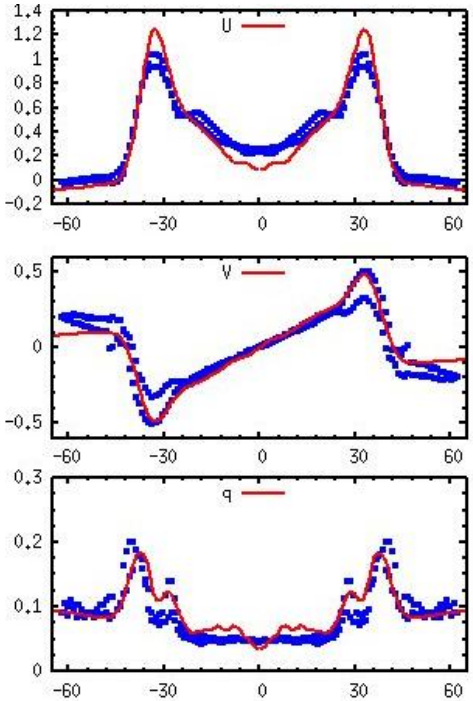
40 % through the center

Along the centerline

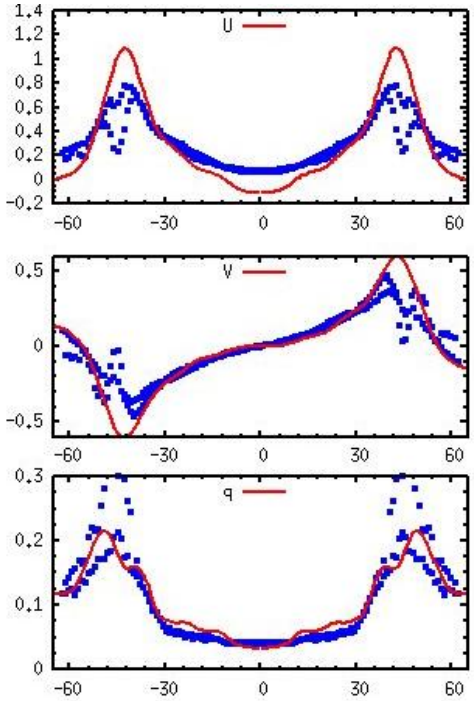


CH_4 / Air
ϕ=0.59

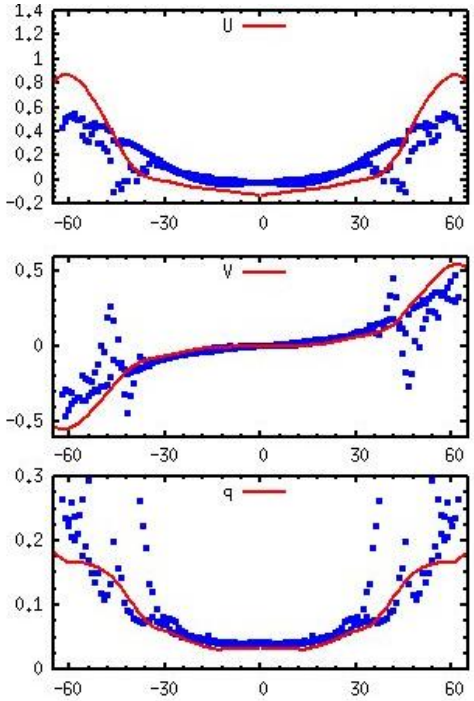
x = 30 mm



x = 50 mm



x = 80 mm



Outline

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- **Non-unity Lewis number effects**
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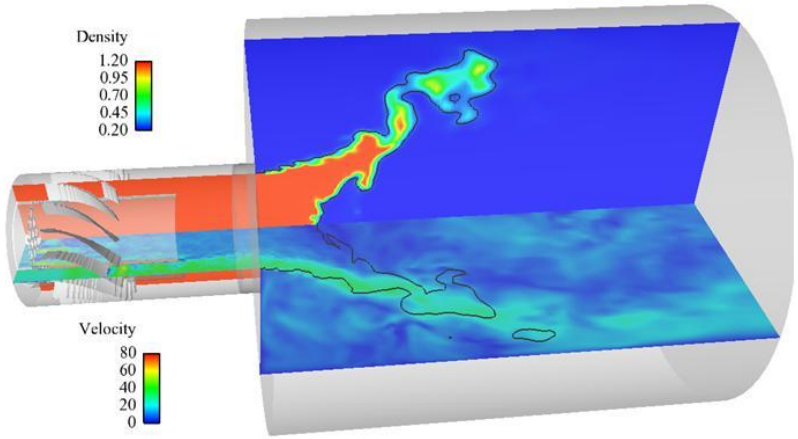


Non-Unity Lewis Number Effects

E. Knudsen, H. Pitsch, *Combustion & Flame*, **2009**

- **Mixture fraction transport equation**

$$\partial_t(\rho Z) + \nabla\cdot(\rho \mathbf{u} Z) - \nabla\cdot(\rho \mathcal{D}\nabla Z) = 0$$

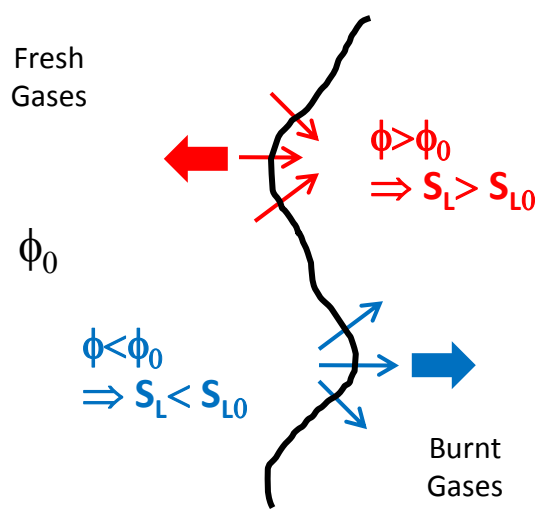
- **Progress variable transport equation**

$$\partial_t(\rho C) + \nabla\cdot(\rho \mathbf{u} C) - \nabla\cdot(\rho \mathcal{D}\nabla C) = \dot{\omega}_C \longrightarrow \tilde{\dot{\omega}}_C = \int_Z\int_C \dot{\omega}_C(Z,C)\tilde{P}(Z,C)\,dZ\,dC$$

- **Levelset transport equation**

$$\frac{\partial \mathcal{G}}{\partial t} + u_j\frac{\partial \mathcal{G}}{\partial x_j} = (D\kappa)_{c0}|\nabla\mathcal{G}| + s_{L,c0}|\nabla\mathcal{G}|, \longrightarrow \frac{\partial \bar{\mathcal{G}}}{\partial t} + \tilde{u}_j\frac{\partial \bar{\mathcal{G}}}{\partial x_j} + \bar{\Gamma}_u = \frac{\rho_u}{\bar{\rho}}\left[(\overline{D\kappa})_{\bar{T},u} + s_{\bar{T},u}\right]|\nabla\bar{\mathcal{G}}|$$

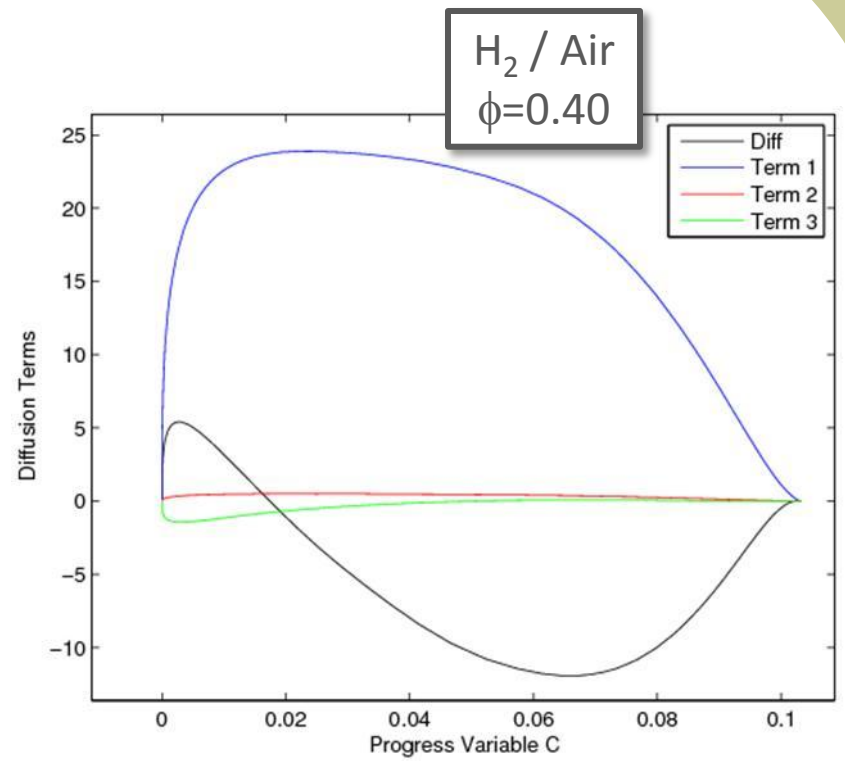
$$s_{\bar{T},c0}|\nabla\bar{\mathcal{G}}| = \overline{s_{L,c0}|\nabla\mathcal{G}|}$$



- **Differential diffusion**
  - Small scales (subgrid)
  - $\Rightarrow$ **Change local f $\Rightarrow$ Change burning speed**
- **Approach 1**
  - Express S_L as a function of curvature
  - Model **subgrid scale curvature**
- **Approach 2**
  - S_L already expressed as a function of f
  - Model **mixture fraction fluctuations** due to curvature

Modeling Approach

- **Modeling assumptions**
  - Lewis number for ***H_2: Le<1***
  - All ***other species unity Lewis*** number
  - Mixture averaged species diffusion



- **Mixture fraction fluctuations**
  - Mixture fraction equation

$$\partial_t(\rho Z)+\nabla.(\rho u Z)+\nabla.j_Z=0$$

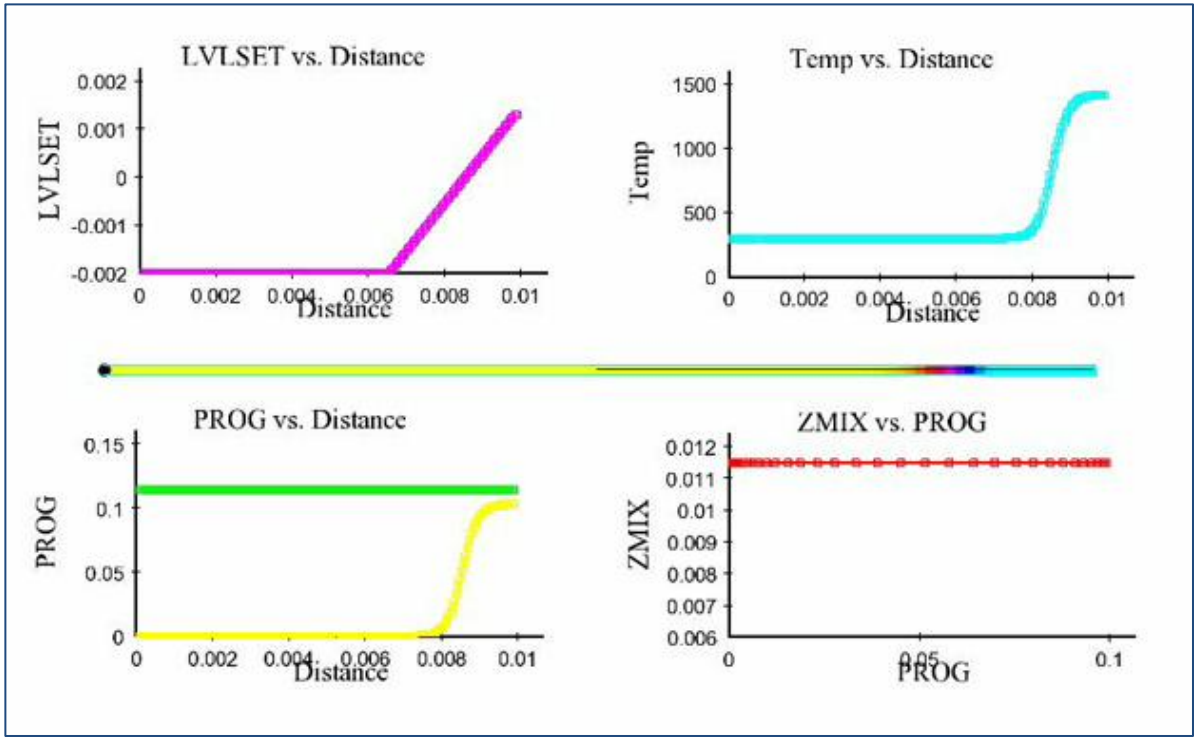
  - Full mixture fraction flux term

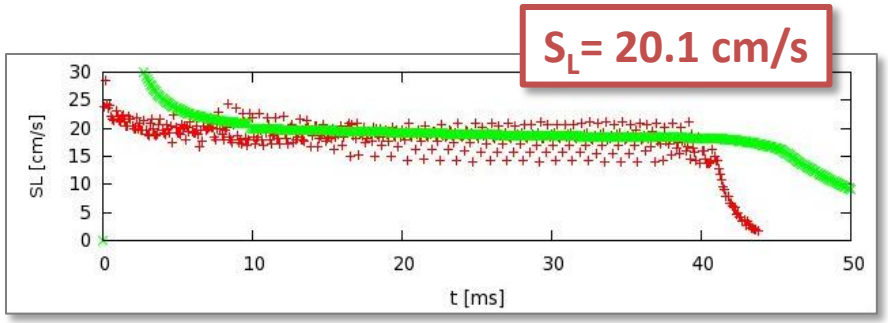
$$j_Z=\rho Z V_Z=-\rho D\nabla Z-\rho D(1-Z_{st})\left(\frac{1}{Le}-1\right)\nabla Y_{H_2}-\rho DZ\left(\frac{1}{Le}-1\right)\nabla Y_{H_2}-\rho D(1-Z)Y_{H_2}\left(\frac{1}{Le}-1\right)\frac{\nabla W}{W}$$

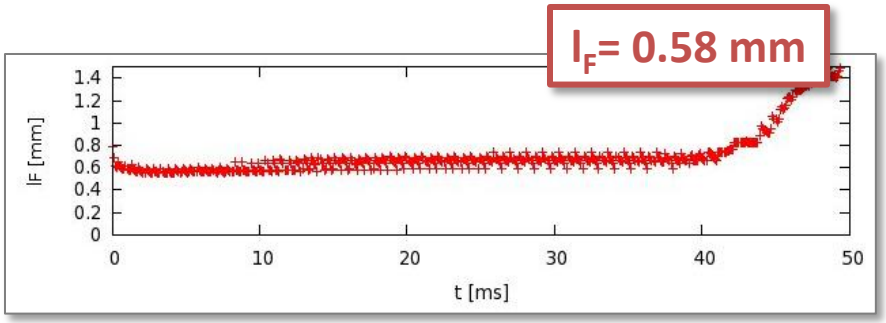
Normal diffusion — ***Term 1*** — ***Term 2*** — ***Differential diffusion*** — ***Term 3*** — ***Molar/mass diffusion***

Validation – Laminar Flame

- **1D laminar case**
  - H_2 / Air
  - ϕ=0.40
- **Targets**
  - Comparison with ***detailed chemistry***
  - Burning speed: S_L
  - Flame thickness: l_F

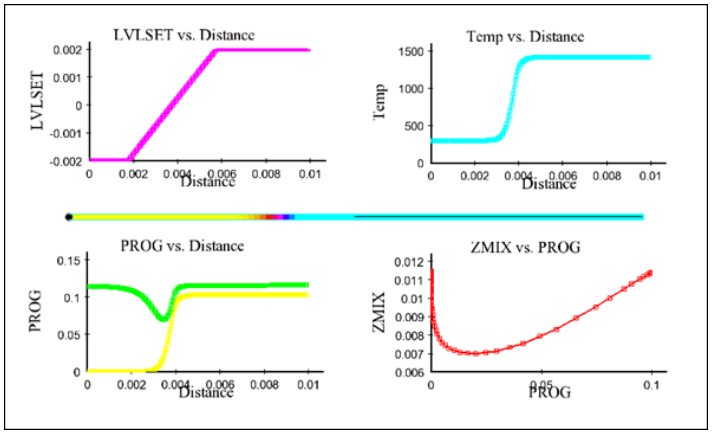


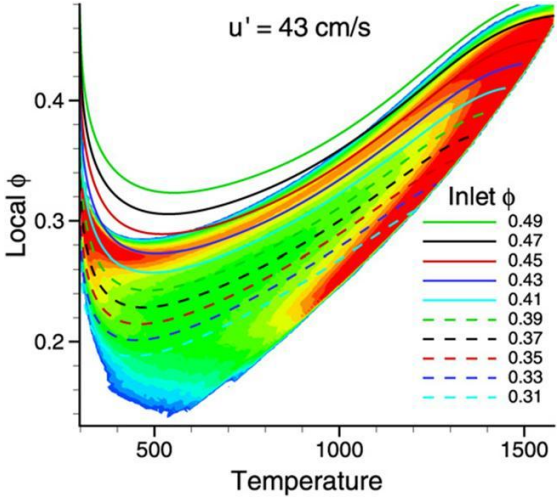




Validation – Laminar Flame

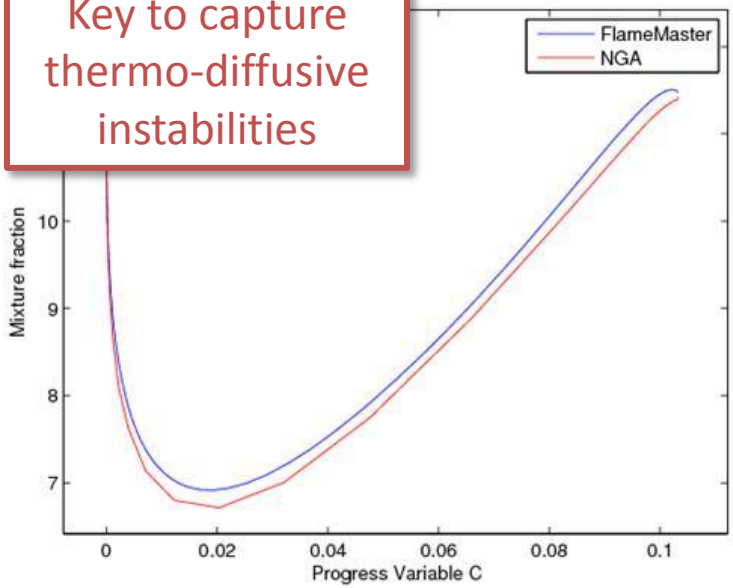
- **1D laminar case**
  - H_2 / Air
  - ϕ=0.40
- **Mixture fraction**
  - ***Not constant***
    - Non-unity number effects
  - Source term
    - Captures ***correlation Z ↔ C***





DNS of Turbulent H_2 flame
Day *et al.*
Comb. Flame **2009**

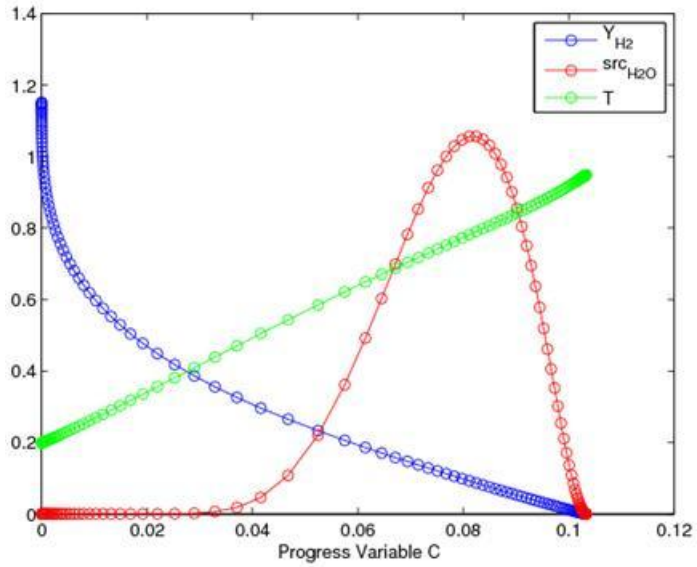
Key to capture thermo-diffusive instabilities



Flamelet Table Creation

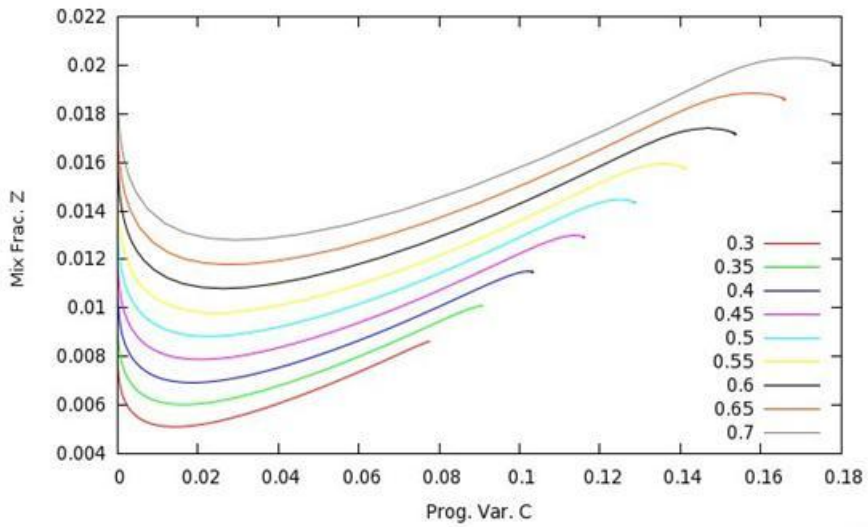
- **Flamelet table**
  - Compute laminar flames
    - Different ***equivalence ratios*** (flamelets)

    $\Rightarrow$ Different Z
  - Mapping
    - 2 table entries: Z & C



- **Mapping difficulties**
  - Fast H_2 diffusion

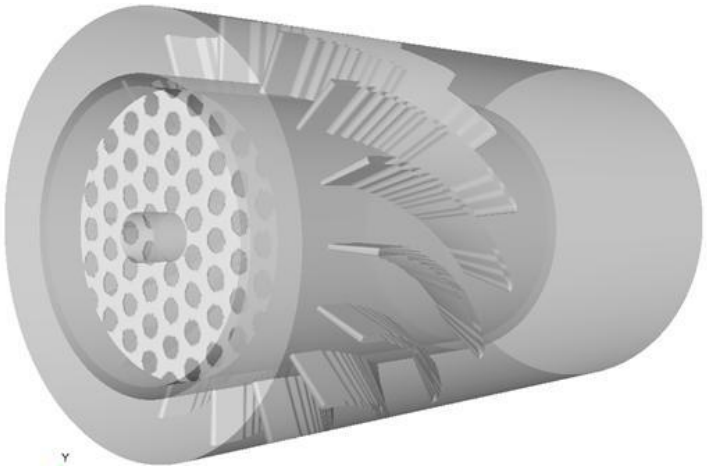
    $\Rightarrow$ ***Steep gradient*** at C=0
  - Need smart discretization

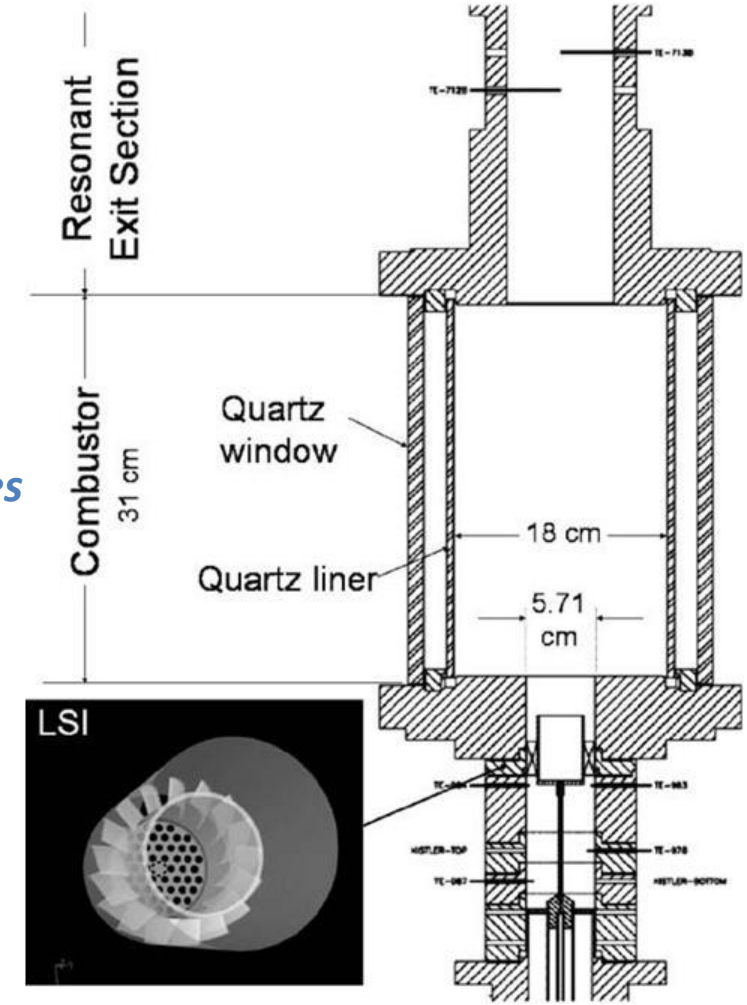


- **Mapping uniqueness**
  - ***No crossing*** of flamelets!

Low Swirl Burner - Geometry

- **Configuration**
  - *Cheng et al.* Proc. Comb. Inst. 32 (2009)
  - Pure ***CH_4*** and pure ***H_2*** flames
- **Large Eddy Simulation**
  - Structured Code: ***NGA****
  - Swirler described with ***Immersed Boundaries***





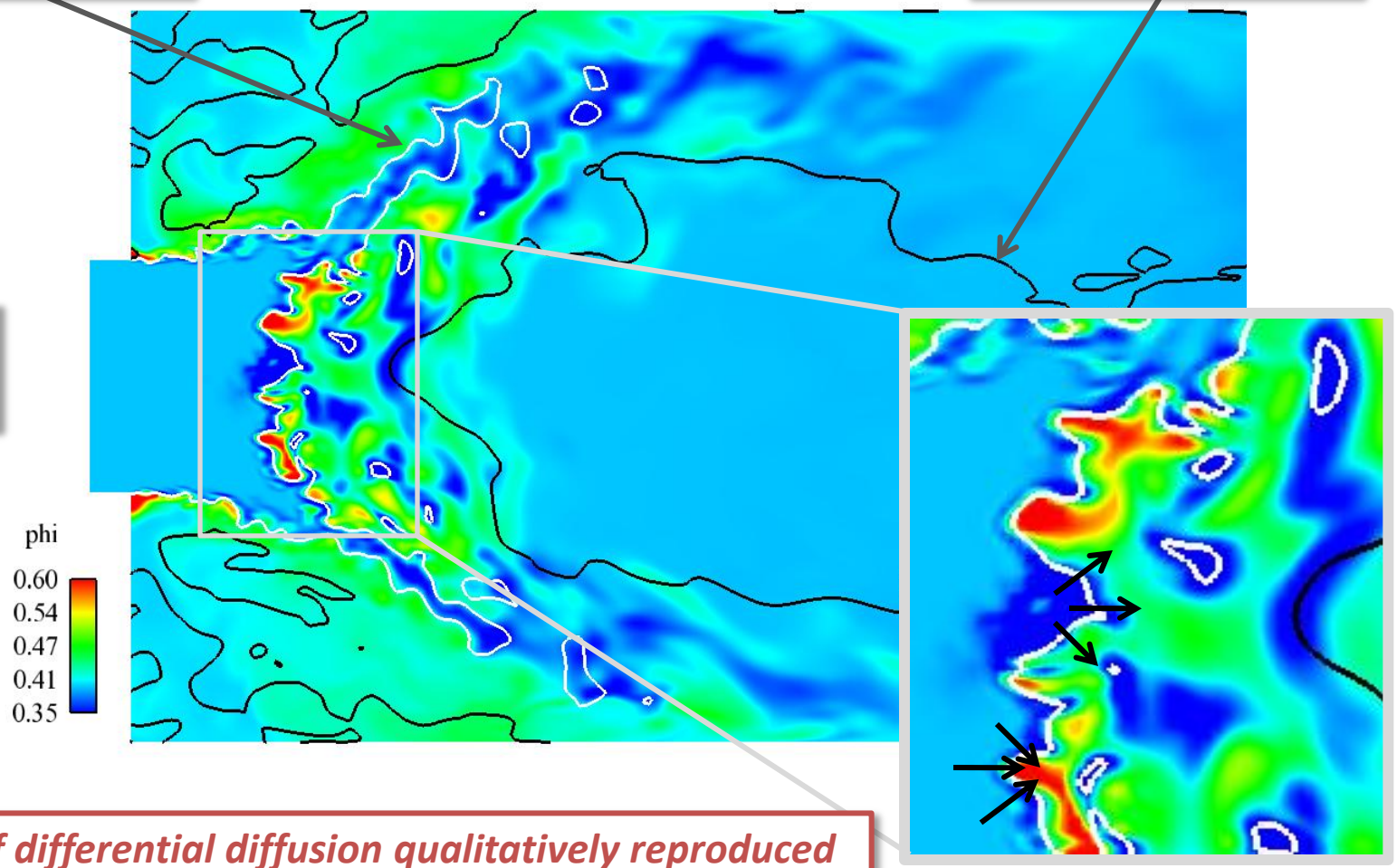
* Desjardins, O., Blanquart, G., Balarac, G., Pitsch, H. *Journal of Computational Physics* (**2008**)

Pure Hydrogen Flame

Isocontour G=0
Flame front

Isocontour U=0
Recirculation region

H_2 / Air
ϕ=0.40



Effects of differential diffusion qualitatively reproduced

Conclusion

- **Model for premixed combustion**
  - Coupled ***levelset*** / ***progress variable*** approach
  - Valid for low / high Ka number
  - ***Validated*** & ***applied*** to low swirl burner

- **Partially premixed combustion**
  - ***Mixture fraction*** equation
  - Regime index

- **Non-unity Lewis number effects**
  - Mixture fraction equation
    - Additional ***source term***
  - ***Tested*** & ***validated*** in laminar flame
  - Application: low swirl burner
    - Reproduce ***local mixture inhomogeneities***