PENNSTATE

Detailed Computational Modeling of Laminar and Turbulent Flames with Soot

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Overview

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   - Laminar diffusion flames
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Motivation for the Study

Combustion and pollutants

- Combustion is at the heart of our modern civilization and meets a large part of our energy needs.
- Combustion produces CO_2, which is a greenhouse gas.
- By-products of combustion pose an immediate risk to human health and wellbeing.
- The major by-products are soot and oxides of nitrogen (NO_x).
- In this work the focus is on numerically modeling soot formation, growth and oxidation in flames.

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  3. Surface growth and oxidation of soot by reaction with the gas-phase species.
  4. Agglomeration of soot particles.

Background

Modeling soot

- Modeling efforts are clearly limited by our understanding of the processes that lead to the formation and growth of soot.
- We can broadly divide the models into three categories:
  1. Empirical soot models
  2. Semi-empirical soot models, eg. two-equation model [Guo et al., 2004] [Leung et al., 1991]
  3. Detailed soot models, eg. the Method of Moments with Interpolative Closure (MOMIC) [Frenklach, 2002]

Background

Laminar diffusion flames

- Diffusion flames are a fundamental flame type.
- The fuel and oxidizer are not *premixed* prior to entering the combustion chamber.
- The effects of differential diffusion are important in these flames.
- Co-flowing laminar diffusion flames are useful to study as they can be used to build and calibrate models.

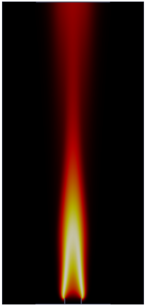


Figure : A laminar diffusion flame

Background

Laminar diffusion flames

- Diffusion is usually modeled using a Fickian model:

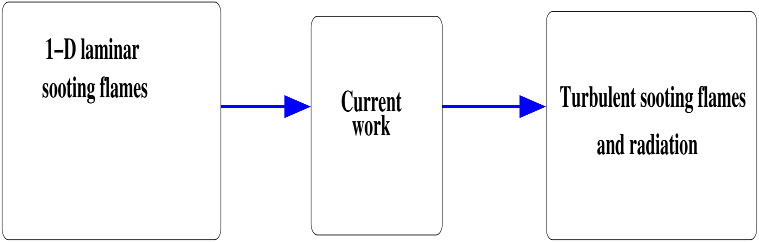
$$V_{\alpha,i} = -\frac{D_\alpha}{Y_\alpha}\frac{\partial Y_\alpha}{\partial x_i}$$

- The diffusivities for different species are different, and energy also diffuses down its own gradient.
- But energy *also* diffuses down the species concentration gradients, as the species themselves carry energy with them.
- This ‘interdiffusion’ flux introduces an additional term in the energy equation for a multicomponent system.

The laminar flame solver

Motivation for the current work

- To develop an open-source code to study sooting laminar diffusion flames, so as to act as a bridge between the 1-D laminar flames and more complex turbulent flames with soot and radiation effects included.



The laminar flame solver

- The solver is based on the open-source CFD code `OpenFOAM-1.7.1` [OpenFOAM, 2010].
- Use of OpenFOAM for laminar flames has been reported in literature [Messig et al., 2013, Cuoci et al., 2013].
- Transport properties are calculated using a mixture-averaged approach [Kee et al., 1986] and differential diffusion effects are taken into account.
- The source terms for chemical kinetics calculations (chemistry) are obtained using the the `cvode` stiff ODE solver from `SUNDIALS` [Hindmarsh and Serban, 2012, Cohen and Hindmarsh, 1995].
- An optically thin radiation model has been included in the flame solver [Guo et al., 2004, Barlow et al., 2001].

Soot model

- A semi-empirical, two-equation soot model [Leung et al., 1991, Guo et al., 2004] has been implemented.
- The soot model is C_2H_2-based, and solves for the soot mass fraction Y_s and the soot number density N_s (particles/kg).
- A detailed soot model, the Method of Moments with Interpolative Closure (`MOMIC`) [Frenklach, 2002] has also been implemented, and is currently being tested.
- Here we solve for the moments of the soot particle distribution function,

$$M_r = \sum_{i=1}^{\infty} m_i^r N_i .$$

- This model accounts for the role of polycyclic aromatic hydrocarbons (PAH).

Turbulent flame solver

- The solver is based on a Reynolds-averaged simulation (RAS) for reacting flows.
- It uses a transported PDF method (tPDF) [Haworth, 2010] to account for turbulence chemistry interactions (TCI).
- The main flow solver is based on `OpenFOAM-2.2.x`.
- Radiation is modeled by the photon Mote-Carlo (PMC) method [Ren and Modest, 2013, Pal, 2010]

Numerical aspects

Laminar flame calculations

- The typical advection-diffusion equation for a scalar ω is

$$\frac{\partial \rho \omega}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j \omega) = \frac{\partial}{\partial x_j}\left(\Gamma_\omega \frac{\partial Y_s}{\partial x_j}\right) + S_\omega$$

- The most expensive part of the solution procedure is to evaluate the source term S_ω, followed by the transport coefficient Γ_ω.
- These two terms can be computed locally, so we can use multiple processors to speed up the calculations.
- We used a domain-decomposition method to assign cells to each processor.

Numerical aspects

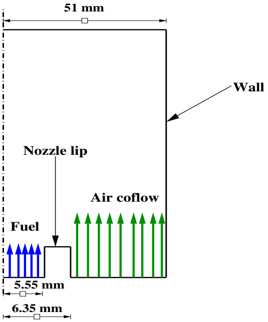
Turbulent flame calculations

- Each CFD cell has a number of notional particles (PDF particles), each at a different state.
- The average for the cell is the average of the states of the particles.
- For calculating the source terms for a cell, they are calculated for each particle in the cell and then averaged over all particles in the cell.
- Load-balancing is ensured by distributing these notional particles to processors so that each processor has a similar number of particles.

C_2H_4-air flame

Computational domain

- Coflowing laminar C_2H_4-air flame [Santoro et al., 1983, Kennedy et al., 1996, D'Anna et al., 2007].
- Non-smoking flame, peak soot $\sim$ 10 ppm.



C_2H_4-air flame

Flow conditions

- The flow conditions are as given below:

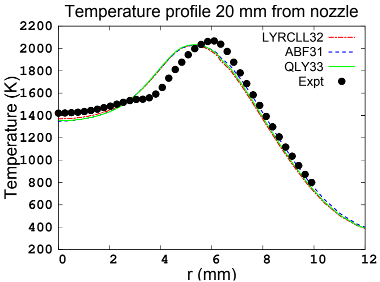
C_2H_4 flow rate cm^3/s	C_2H_4 jet velocity cm/s	Air flow rate cm^3/s	Air velocity cm/s
3.85	3.98	713.3	8.90

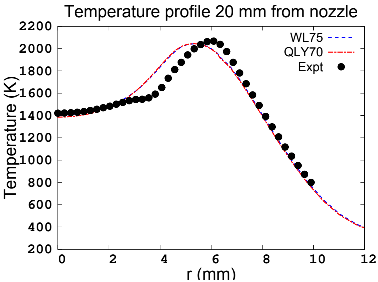
- Five gas-phase mechanisms were used for the two-equation soot model.

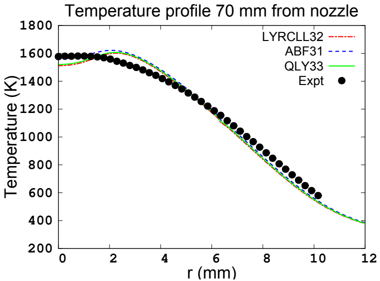
Mechanism	Species	Reactions	Reference
ABF31	31	179	[MECHMOD, 2010]
LYRCLL32	32	206	[Luo et al., 2011]
QLY33	33	205	[Law, 2005]
QLY70	70	463	[Qin et al., 2000]
WL75	75	529	[Wang and Laskin, 1991]

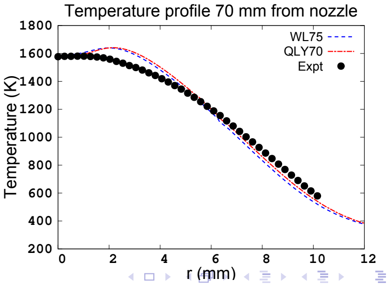
Results: C_2H_4-air flame

Two-equation soot model









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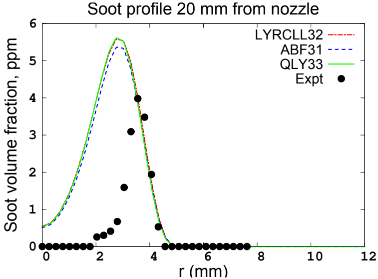

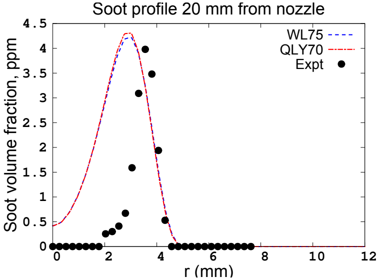

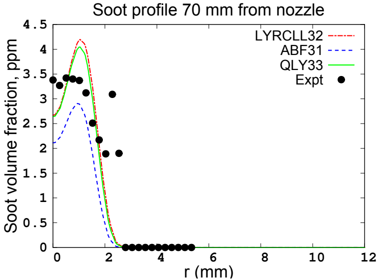

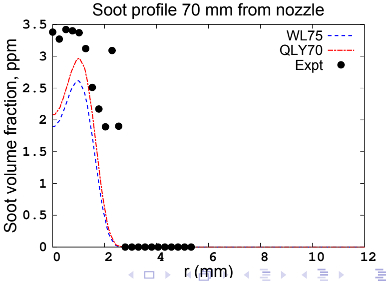

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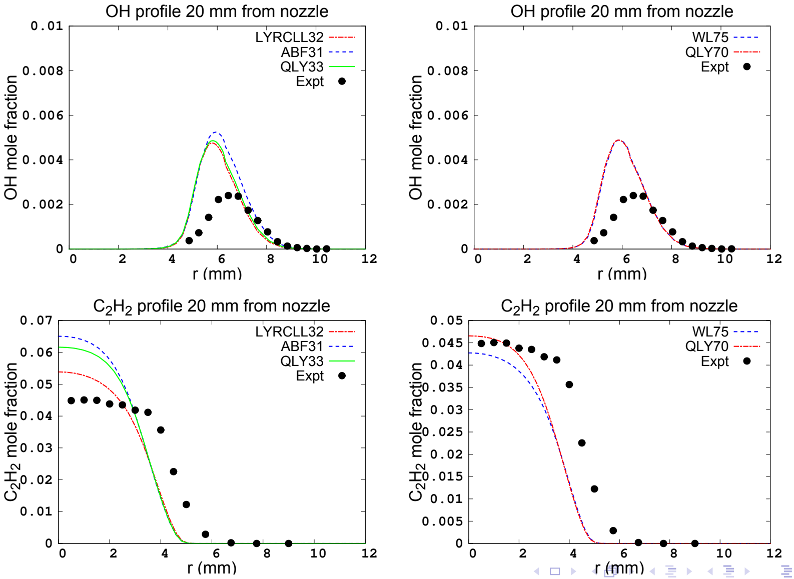
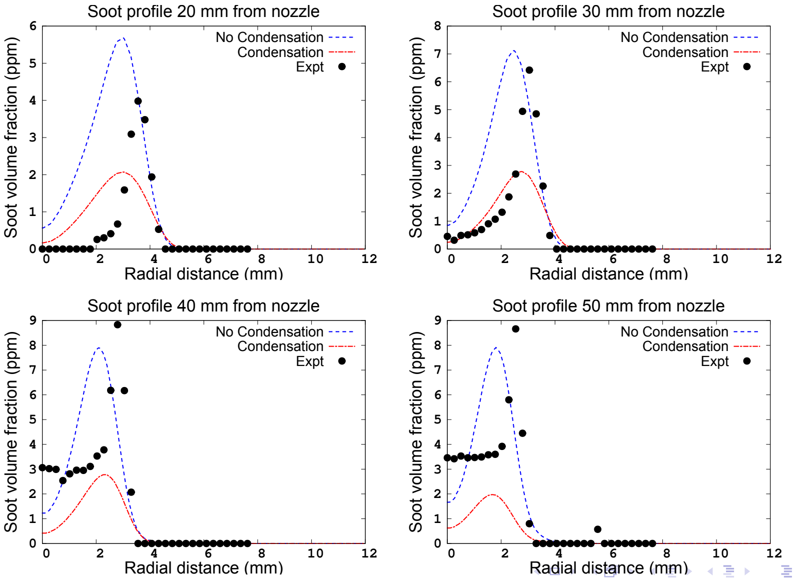


Results: C_2H_4-air flame

- To test the detailed soot model (`MOMIC`), the same flame was run with varying input parameters to the soot model.
- The tests used a 99-species, 533-reactions gas-phase mechanism [Frenklach and Wang, 1997].
- The soot precursor is assumed to be pyrene (A_4, $C_{16}H_{10}$).

Results: C_2H_4-air flame

MOMIC soot model: effect of PAH condensation



Scaling studies

Laminar flame calculations

- A scaling study using the 32-species chemical mechanism was performed.
- The flame solver was run on a mesh of 12400 cells for a fixed walltime using 8, 16, 32, and 64 cores.

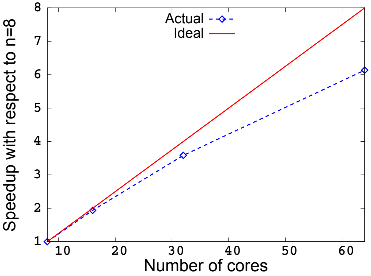


Figure : Scaling study for the laminar axi-symmetric flame

Scaling studies

Turbulent flame calculations

- A scaling study using the 33-species chemical mechanism was performed.
- The flame solver was run on a mesh of 5940 cells for a fixed walltime using 2, 8, 16, 32, 64, and 96 cores.

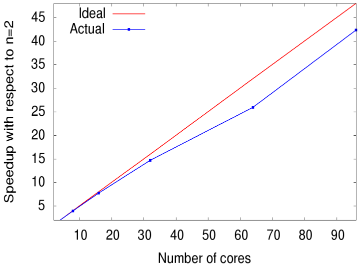


Figure : Scaling study for the turbulent axi-symmetric flame

Conclusions

- An open-source code to study laminar diffusion flames in a coflow configuration has been developed.
- The code for turbulent flames with soot is currently under development.
- The soot volume fraction predictions from the two-equation soot model are comparable to those in other numerical studies [D'Anna et al., 2007, Kennedy et al., 1996] for the same flame configuration.
- Qualitatively the `MOMIC` soot model behaves as expected on varying input parameters, but more work is needed to use the model for this flame.
- Both the laminar and turbulent flame simulations can benefit from the use of parallel computing.

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Thank You

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Questions ?