The Proceedings of the

Second International Sooting Flame (ISF) Workshop 5

Written by: Guillaume Blanquart, Bassam Dally, Seth Dworkin, Klaus-Peter Geigle, Dan Haworth, Venkat Raman and Murray Thomson

Edited by: Murray Thomson

Invited Contributors to the Second Workshop

Randy McKinney, Pratt and Whitney

Organising Committee

Prof Gus Nathan, Prof Heinz Pitsch, Prof Hai Wang, Prof Bassam Dally, Dr Chris Shaddix, Dr Klaus-Peter Geigle and Prof Murray Thomson.

Program Leaders and Co-leaders

Laminar Flames: Prof. Seth Dworkin, Prof. Guillaume Blanquart
Turbulent Flames: Prof Venkat Raman, Prof Bassam Dally.
Pressurised Flames: Prof Dan Haworth, Dr Klaus-Peter Geigle

Laminar Sooting Flames

Presenters: Seth Dworkin / Guillaume Blanquart

Session Chair: Hai Wang

Target Flames

Premixed flames 1	McKenna burner-stabilized flames	Ethylene/Air	ὲ =2.07 and 2.16
Premixed flames 2	McKenna burner-stabilized flames	Ethylene/Air	ὲ =2.34, 2.64 and 2.94
Premixed flames 3	McKenna burner stabilized flames (LII target flames)	Ethylene/Air	ὲ =2.1 and 2.33
Premixed flames 4 (Linked to Pressurized Session)	McKenna burner-stabilised flames (slightly lifted flames)	Ethylene/Air	ὲ =2.3 and 2.5
Premixed flames 5	McKenna burner-stabilized flames (Pure oxygen flames)	Ethylene/O2	ὲ =2.42 and 3.03
Premixed Flames 6	Burner-stabilised, stagnation (BSS) flame	Ethylene/Air	ὲ =2.07
Coflow 1	Santoro Burner data (Smoking/Non-smoking diffusion flames)	Ethylene/Air	a) Non-smoking b) Incipient-smoking c) Smoking
Coflow 2	Santoro Burner Data (Partially premixed non-smoking ethylene flames)	Ethylene/Air/ N_2/Ar	a) ū = Đ, 24, 12, 6, 4 and 3 (C2H4 at 220 cm3/min) b) ū = Đ, 24, 20, 15, 10 and 5 (C2H4 at 231 cm3/min)
Coflow 3	Smooke/Long Burner Data (Non-smoking, diluted with varying levels of nitrogen)	Ethylene/Air	a) 32%, 40%, 60%, 80% at a fuel flow rate of 0.044cm3/s b) 80% at a fuel, flow rate of 0.022cm3/s
Coflow 4	D'Anna Burner Data (Non-smoking flame, co-flowing laminar diffusion ethylene flame)	Ethylene/Air	3.85cm3/second
Coflow 5	De Iuliis Burner Data (Non-smoking, co-flowing diffusion ethylene flame	Ethylene/Air	fuel flow rate of 2.5cm3/second

From presentations of data:

1. A question arose during the presentation of Premixed Flame 2 comparisons: Why was the Faeth configuration (Flame 2) devised? The reason given was that it was a stable, and locally one-dimensional configuration to model.
2. Soot is defined as a PAH dimer in most models, however, in experimental data, soot refers to particles that are often larger than 20 nm. What is the best way to compare numerical results to experimental data given this contrast?
3. It was noted that in flames where soot inception occurs from large PAHs, with five or more rings, that pyrene based inception may lead to early soot formation, and therefore cause spatial inaccuracies.
4. It was noted that for Premixed Flame 3 in particular, but also others, that scattering coefficients need to be better related to particles, but the soot particles donôt all have the same optical properties, so this is challenging.
5. It was noted that nearly all models assume nucleation from small PAHs, while we know that it is much more physically accurate to describe nucleation from larger PAHs.
6. It was noted that sampled soot may often favour mature soot, so how can this be accounted for when trying to match soot predictions and measurements in flame conditions that favour nascent soot.
7. It was noted that thermal diffusion has not been exhaustively explored. Might thermal diffusion of large PAHs have a significant influence on the soot distribution within flames?

From the discussion topics:

1. In some flames, transparent/translucent particles are found near the flame centreline. This may be a clue as to why some models break down in this area. Perhaps there is a soot growth mechanism other than HACA and PAH condensation that leads to these clusters. Polyynes? PAH thermal diffusion? TEM images show that the soot particles in this region have both aliphatic and aromatic content. The HACA mechanism may be incomplete because it requires radicals, such as H, to activate a site for the chemical addition of acetylene, however, in regions devoid of H, growth still occurs. Many models also consider PAH condensation as a growth mechanism though.
2. One concern is the change in soot caused by the TEM measurement process, such as ablation, evaporation, and condensation, distorting the picture of what the soot looks like in the flame, versus what it looks like by the time the TEM image has been acquired.
3. Better distinctions of definition between nascent and mature soot are needed. When does soot transition from being nascent to mature? Is there an intermediate step?
4. One potential area of inquiry relates to the flames studied by the Lille group. They can demonstrate that flames with certain phi contain only inception dominated soot. Are these flames good for development and validation of an inception model? What are the diameters of these particles?

5. It was noted that there may be too many target flames. There is a need for experimental redundancy, and the application of a variety of modelling ideas to one flame. For the laminar diffusion flames, it was generally agreed upon that the 32% Yale flame would be the target flame. It has many advantages; the burner is inexpensive and easily reproducible, soot on the centerline of that flame is hard to model and poorly understood, the flame is completely lifted so the boundary conditions are well-

Specific measurements were discussed that might have the potential to address these issues and others. Ideas included using Rayleigh or Raman close to the nozzle exit, PIV, and full-field temperature measurements.

All model results presented to date for the laminar coflow flames fail to give the correct evolution of soot volume fraction along the centerline, especially at lower pressures. This suggests that something fundamental is missing in the models. Along the centerline, the temperature and concentrations of key radicals are relatively low. However, the extent to which the centerline behavior in this configuration is or is not relevant in a high-pressure turbulent flame is not clear.

Use of species information provided in the data set (target flame 3) for comparison with model results is encouraged.

Other Potential Target Configurations

It was emphasized that we need targets that multiple research groups can and will simulate. Some of the current ñlegacyò configurations were designed to explore the underlying physical processes, rather than specifically as targets for model validation.

It was also noted that the current configurations tend to emphasize in-flame soot formation processes, whereas in practical applications, it is the net soot emission (difference between what is formed and what is oxidized) that is of interest. Perhaps more emphasis should be placed on configurations that would provide insight into oxidation, and that lend themselves to systematic parametric studies to establish emissions trends. On the other hand, taking data far downstream would require more information on the particular burner geometry compared to the present measurements that emphasize upstream processes, and the laboratory burners might not be very representative of practical burners in this respect.

The benefits of alternative target flame configurations were discussed. In particular, it was suggested that the counterflow configuration reduces the uncertainties in inlet conditions that are inherent in coflow laminar diffusion flames, and it allows control over the temperature-time history. The counterflow configuration might help to resolve the issues with soot prediction along the burner centerline that has been found in all simulations to date for the coflow laminar diffusion flames. The relative stability of coflow versus counterflow configuations at high pressure was debated. Both configurations may be needed, as they represent different environments with respect to the orientation of gradients in equivalence ratio and temperature, etc.

For turbulent flames, the concept of using trace amounts of a high-sooting additive in a baseline nonsooting flame was discussed. This idea was also discussed in ISF-1.

General Procedure

It was acknowledged that the contributing groups had spent significant effort into preparing their

Group	Domain	Grid	Numerics
Mueller (Princeton)	~900mm X 250mm (cylindrical)	192 X 96 X 32	2^{nd} order low-Mach solver +BQUICK scalar solver
Koo (UT/Princeton)	750 X 175mm (axisymmetric)	400 X 200	Second-order low-Mach solver
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Appendix I: Turbulent Flames Session Slides

	
	
	
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