The Proceedings of the

Second International Sooting Flame (ISF) Workshop

Sat August 2 - Sun Aug 3 2014

Pleasanton Hilton, Pleasanton, California

Version 2, April 8, 2015

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.

Scientific Advisory Committee

Prof Ömer Gülder, Prof Michael Frenklach, Dr Meredith Colket, Prof Andrea Danna, Prof Henning Bockhorn, Prof Peter Lindstedt, Prof Mitch Smooke and Prof Dan Haworth.

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

Table of Contents

Workshop Aims and Objectives

Aims of the Workshop

- To identify common research priorities in the development and validation of accurate, predictive models of flames with soot and to coordinate research programs to address them.
- To identify and coordinate well-defined target flames that are suitable for model development and validation, spanning a variety of flame types and fuels in each of the Research Programs.
- To establish an archive of the detailed data sets of target flames with defined accuracy; and to provide a forum for the exchange and dissemination of these data.

Objectives of the Second Workshop

- To compare the predictions of different models against measurements for the target flames selected for the Second Workshop in each of the three programs;
- To identify target flames and research priorities for the next workshop based on research outcomes, current capability and current research plans of the participants;
- To coordinate any administrative tasks needed to facilitate the goals and activities of the workshop.

Workshop Programs

The workshop is organised around the following three Research Programs:

- Laminar flames: Chemical Kinetics (PAH, inception, growth and oxidation); Particle dynamics (moment methods, sectional models, coalescence vs. aggregation);
- Turbulent flames: jet flames, bluff body flames, swirl flames, pool fires, influence of scale;
- Pressurised flames and sprays: simplified IC engines, pressurised jet flames, shock tubes;

International Sooting Flame (ISF) Workshop
Program (Final)

Date	Time	Topic	Chair / Presenter
Saturday 2nd	14:00 - 15:45	Registration and coffee	
	15:45 – 16:05	Welcome, History, Structure, Aims, Agenda	Nathan
	16:05 - 16:25	Review of key outcomes from First Workshop	Pitsch
	16:25 – 16:45	Discussion	Pitsch / Nathan
	16:45 – 17:15	Industry Perspective	Saddat Syed (PW) (Chair: Shaddix)
	17:15 – 17:30	Discussion	
	17:30 - 18:00	Coffee	
	18:00 - 20:00	Laminar Target Flames	Dworkin / Blanquart (Chair: Wang)
	20:00 - 22:30	Posters & Informal Dinner	
Sunday 3rd	8:30 - 9:45	Pressurised Target Flames	Haworth / Geigle (Chair: Shaddix)
	9:45-10:15	Coffee Break	
	10:15-11:45	Turbulent Target Flames:	Raman / Dally (Chair: Nathan)
	11:45-12:15	Invited Reflections	Prof D'Anna Prof Desgroux A/Prof Bisetti (Chair: Wang)
	12:15-13:20	Lunch	
	13:20 - 14:20	Discussion: Scientific Questions	Pitsch / Thomson
	14:20 - 15:00	Discussion: Linking 3 programs	Shaddix / Nathan
	15:00 - 15:30	Discussion: Next Target Flames	Pitsch / Wang
	15:30 - 15:40	Feedback on Workshop	Dally / Geigle
	15:40 -15:45	Close	Nathan / Pitsch
	16:00	Buses depart for International Combustion Symposium	

- Note: self service coffee at the back of the venue for Sunday pm

Laminar Sooting Flames

Presenters: Seth Dworkin / Guillaume Blanquart

Session Chair: Hai Wang

Target Flames

Premixed flames 1	McKenna burner-stabilized flames	Ethylene/Air	ϕ =2.07 and 2.16
Premixed flames 2	McKenna burner-stabilized flames	Ethylene/Air	ϕ =2.34, 2.64 and 2.94
Premixed flames 3	McKenna burner stabilized flames (LII target flames)	Ethylene/Air	ϕ =2.1 and 2.33
Premixed flames 4 (Linked to Pressurized Session)	McKenna burner-stabilised flames (slightly lifted flames)	Ethylene/Air	ϕ =2.3 and 2.5
Premixed flames 5	McKenna burner-stabilized flames (Pure oxygen flames)	Ethylene/O2	ϕ =2.42 and 3.03
Premixed Flames 6	Burner-stabilised, stagnation (BSS) flame	Ethylene/Air	ϕ =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) Φ = ∞, 24, 12, 6, 4 and 3 (C2H4 at 220 cm3/min) b) Φ = ∞, 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 don't 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-defined, a variety of experimental datasets already exist for this flame, the dilution ratio can be varied to 40%, 60%, and 80%, for which there is already experimental data, and three groups (CalTech, Yale, Toronto) have already modelled this flame.

Pressurized and Sprays Flames

Presenters: Dan Haworth / Klaus-Peter Geigle

Session Chair: Chris Shaddix

Most of the discussion centered on measurement and simulation issues for the laminar coflow jet diffusion flame target configuration, and on potential alternative target configurations that might help to resolve these issues.

Laminar Coflow Jet Diffusion Flames

The importance of having well-characterized inlet conditions for coflow laminar jet diffusion flame configurations was emphasized. This includes velocity profiles as well as temperature profiles. Configurations with simple, well-defined velocity profiles at the burner exit (e.g., a fully developed parabolic profile, or a plug-flow profile) would be preferred. Simulation domains may need to extend upstream into the burner nozzle, but in any case, well-characterized boundary conditions at some location and precise burner geometry are needed. Experimental datasets should include velocity measurements, especially close to the burner. The question was raised of how accurately one could expect to measure temperature and velocity close to the nozzle in these small burners.

The importance and difficulty of measuring nozzle wall temperatures were discussed. Thermographic phosphors might be one possibility. Simulations that account for coupled wall heat transfer show large differences in nozzle exit temperature and composition profiles. In the absence of reliable wall temperature measurements, it may be that the best that we will be able to do is to perform sensitivity studies using simulations to map out the extremes (e.g., fixed temperature versus adiabatic wall). The possibility of heterogeneous chemical reactions involving the wall was also raised.

It was suggested that the reported measured temperatures may be too high for the KAUST C_2H_4 coflow laminar diffusion flames (Target Flame 3): are they higher than the adiabatic flame temperature, in some cases?

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 "legacy" 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 input for the session. However, for future workshops earlier submission of results (not within 1-2 days before the workshop) is recommended to enable best possible representation of the results of various groups on the workshop.

Given the relatively small number of contributing groups future workshops will include existing model calculations of prior workshops for those target flames maintained.

Turbulent Sooting Flames

Presenters: Venkat Raman / Bassam Dally
Session Chair: Gus Nathan

Introduction

The main focus of the second ISF workshop (with regard to turbulent flames) was the validation exercise involving the hydrogen/ethylene/nitrogen turbulent jet flame from Adelaide. There was strong participation from the soot modeling community, with nearly eight different simulations submitted for comparison. See appendix I for details about this flame.

Summary of outcomes of the discussion:

1. The simulations generally failed to predict the soot levels, often failing by many orders of magnitude. Surprisingly, RANS models did better than LES.
2. The experimental centerline mean temperature profile shows two distinct regions. The initial soot-free region where soot-induced radiation is not important, and the soot-laden environment where radiation losses decrease the temperature and alter the mean temperature profile.
3. Due to the dominant axial convective term, these two regions could be treated sequentially. In other words, predicting the soot-free region is not tightly coupled to the soot-laden region downstream.
4. None of the simulations were able to predict this initial centerline temperature profile. In fact, many of the LES computations showed a lifted flame, which led to a nearly constant centerline temperature until the lift-off height, followed by a steep increase in mean temperature values.
5. Simulations of Wick and Pitsch tried to rectify this lift-off issue by introducing an artificial pilot. But, ensuring attachment was not sufficient to predict the radial spread of the jet. All simulations (except that of El-Asrag) predicted the wrong spread in the radial direction.
6. The RMS of the temperature in the initial soot-free region were reasonable even though the mean temperatures were lower than experiments, indicating that the simulations predict higher levels of turbulence compared to the experiments.

7. There is considerably ambiguity in the inlet velocity boundary condition, since it is difficult to confirm if the experimental data corresponds to a fully developed flow. Nevertheless, simulations that tried to match the experimental profile through inflow-fitting did not provide any improvement in predictions (temperature or otherwise).
8. All variations in RANS turbulence and mixing parameters failed to predict the soot and temperature profiles. Interestingly, a decrease in scalar variance corresponding to enhanced mixing led to higher soot volume fraction values. This attests to the fact that soot source terms occupy a very narrow region in composition space, and any level of fluid unmixedness dramatically reduces the average/filtered source terms.
9. Xuan and Blanquart carried out almost fully-resolved calculations including differential diffusion effects. However, their simulations also failed to show any improvement. However, a similar laminar flame calculation showed that differential diffusion would have a significant impact regardless of the strain rates involved. This discrepancy is yet to be resolved.
10. To see if the issue is with the flame configuration, the experiment of Shaddix and co-workers at Sandia was simulated. It was found that there was some improvement, but due to the lack of additional temperature and velocity measurements, it is difficult to ensure that this is not merely coincidental.
11. It was generally accepted that we should consider the flame series and not focus on a single flame. Subsequent calculations by Koo, Mueller, and Raman showed that this did not improve predictability either.

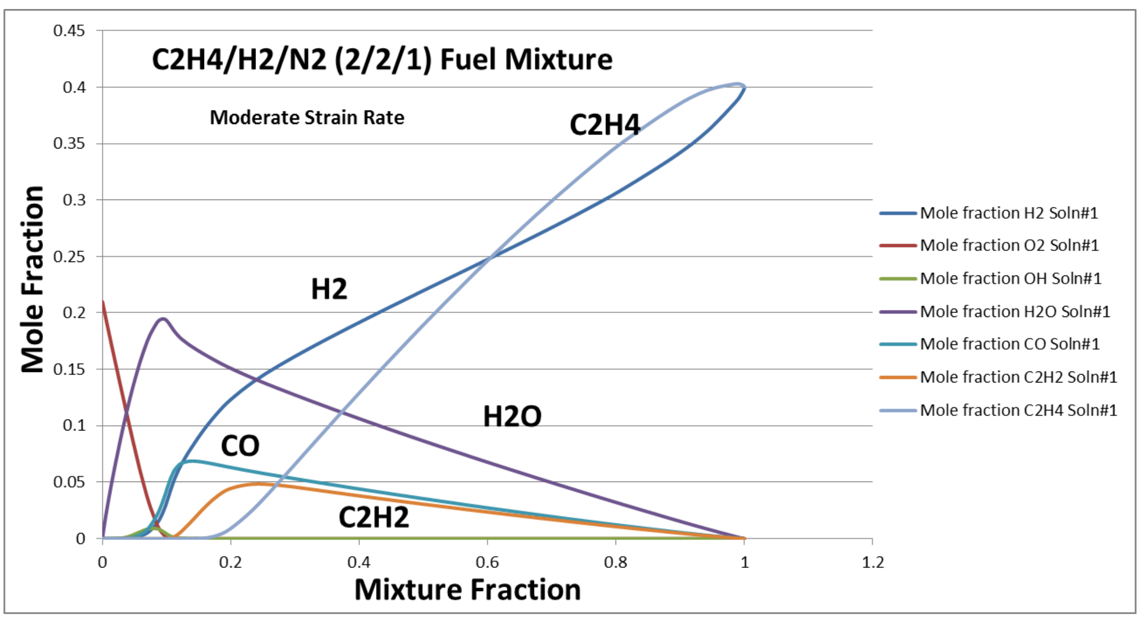


Figure 1: Laminar flame calculation of the fuel mixture showing the effect of differential diffusion at relatively moderate strain rate.

Contributions and Simulation Details

The contributors to this session were:

1. Michael Mueller (Princeton)
2. Heeseok Koo, Venkat Raman, and Michael Mueller (UT/Princeton)
3. Hossam El-Asrag (Ansys Inc.) (RANS and LES)
4. Vish Katta (ISSI, Wright-Patterson AF Base)
5. Achim Wick, Jens Dornieden, Heinz Pitsch (Aachen University)
6. May Yen, John Abraham (Purdue/Adelaide)
7. Yuan Xuan, Guillaume Blanquart (Caltech)
8. Colin Heye, Venkat Raman, and Michael Mueller (UT/Princeton LES)

The different groups performed a variety of computations designed to explore the assumptions and boundary conditions associated with this flame. A summary of the methods used and the simulation details are provided in the next two tables.

Group	Framework	Turbulence model	Gas Chemistry models
Mueller (Princeton)	LES	Dynamic	Based on Narayanaswamy et al. + RFPVA
Koo (UT/Princeton)	RANS	K-e	Based on Narayanaswamy et al. + RFPVA
El-Asrag (Ansys)	1. RANS 2. LES	1. SST-K-omega 2. Dynamic	San-Diego mechanism + flamelet + C-equation
Katta (ISSI)	RANS	K-e	San-Diego mechanism
Yen & Abraham (Purdue/Adelaide)	RANS	K-e	Flamelet + mechanism of Luo et al.
Wick/Dorneiden, Pitsch (RWTH Aachen)	LES	Dynamic	Based on Narayanaswamy et al. + RFPVA
Xuan and Blanquart (Caltech)	High resolution LES	(Dynamic)	Bisetti et al.
Heye (UT/Princeton LES)	LES	Dynamic	Based on Narayanaswamy et al. + RFPVA

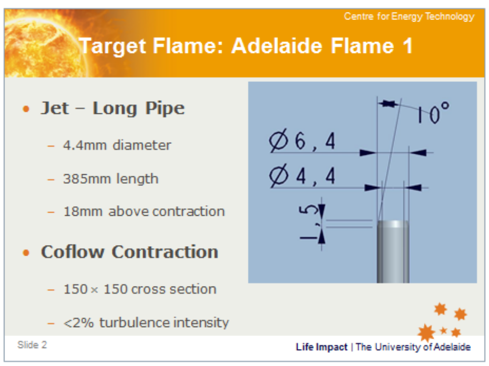
Although there appears to be considerable overlap in terms of the turbulence description, there were subtle variations in the techniques used leading to significant changes in the results.

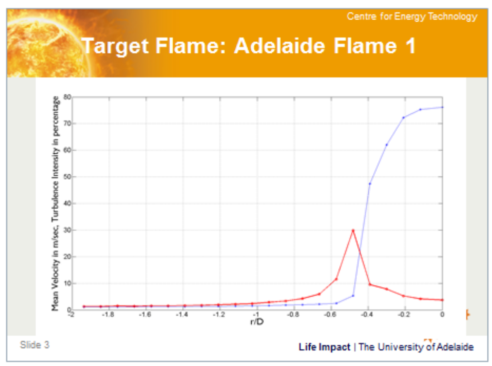
Group	Soot description	Soot-phase models	Turbulence-soot interaction
Mueller (Princeton)	HMOM	Detailed PAH chemistry	Double-delta function subfilter soot PDF
Koo (UT/Princeton)	HMOM	Detailed PAH chemistry	None
El-Asrag (Ansys) (RANS only)	MOM	Acetylene nucleation + Moss-Brookes-Hall two equation model + oxidation	None
Katta (ISSI)	Mass fraction+number density eq.	Acetylene/Benzene nucleation + HACA + oxidation	None
Yen & Abraham (Purdue/Adelaide)	MOM	Appel-Bockhorn-Frenklach model	None
Wick/Dorneiden/Pitsch (RWTH Aachen)	HMOM	Detailed PAH chemistry	Double-delta function subfilter soot PDF
Xuan and Blanquart (Caltech)	None	None	None
Heye (UT/Princeton LES)	None	None	None

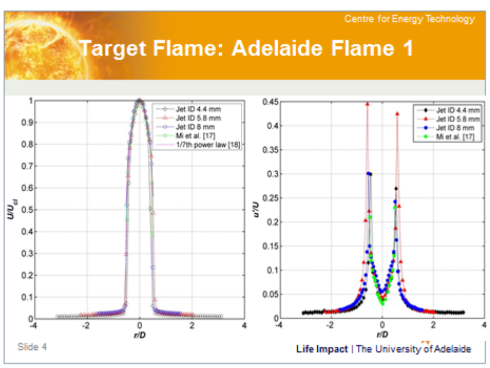
Group	Domain	Grid	Numerics
Mueller (Princeton)	~900mm X 250mm (cylindrical)	192 X 96 X 32	2^{nd} order low-Mach solver +BQUICK scalar solver
Koo (UT/Princeton)	750 X 175mm (axisymmetric)	400 X 200	Second-order low-Mach solver
El-Asrag (Ansys) (RANS only)	800mm X 150mm X 150mm	Hexahedral mesh with 2.6 mill. cells	2^{nd} order low-Mach solver
Katta (ISSI)	1000 mm X 100 mm (axisymmetric)	951 X 151	Nominally second order
Yen & Abraham (Purdue/Adelaide)	1000mm X 260 mm (axisymmetric)	600 X 160	2^{nd} order
Wick/Dorneiden, Pitsch (RWTH Aachen)	1000mm X 250mm (cylindrical)	384 X 192 X64	Double-delta function subfilter soot PDF
Xuan and Blanquart (Caltech)	~32mm X 12mm (cylindrical)	198 X 264 X 64	2^{nd} order low-Mach solver +BQUICK scalar solver
Heye (UT/Princeton LES)	800 X 185 mm (cylndrical) *No inlet block	224 X 112 X 32	2^{nd} order low-Mach solver +QUICK scalar solver

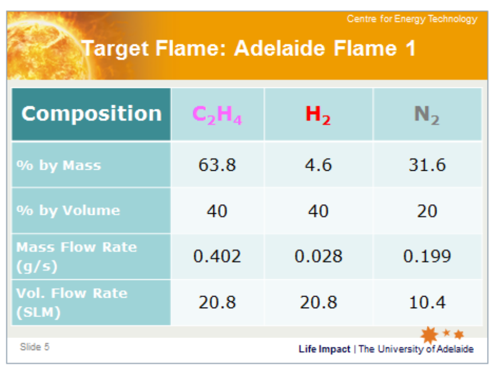
Most of the simulations used and extended pipe upstream to generate realistic inflow conditions. This usually leads to fully developed turbulent pipe flow at the exit, which may not be attainable in the experiment. Since there is no data to confirm this, the boundary conditions are a source of uncertainty.

Appendix I: Turbulent Flames Session Slides

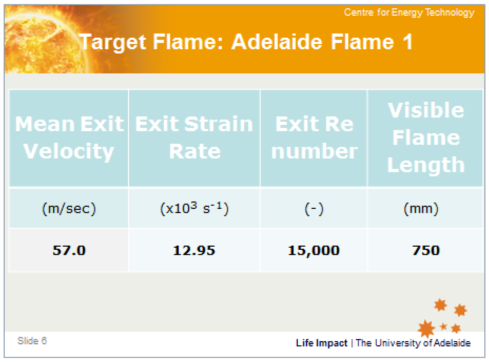


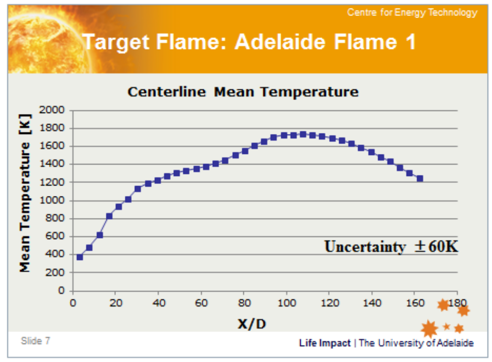


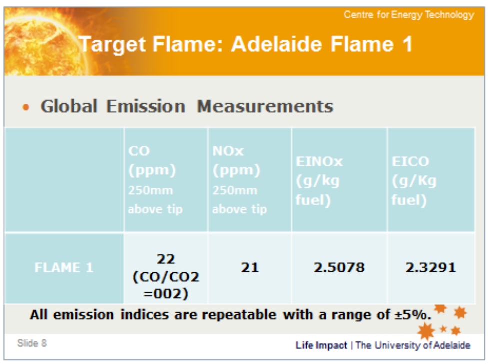


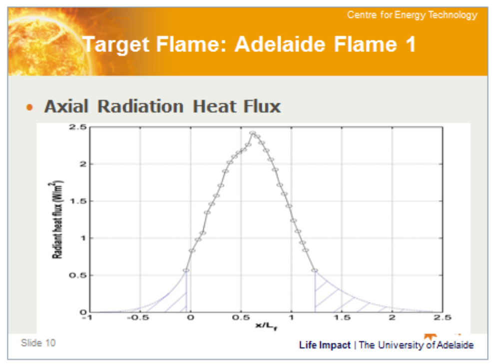


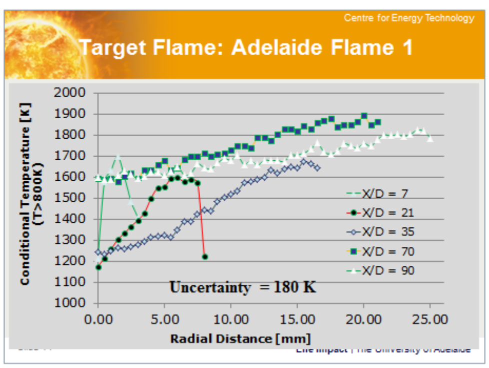
Composition	C_2H_4	H_2	N_2
% by Mass	63.8	4.6	31.6
% by Volume	40	40	20
Mass Flow Rate (g/s)	0.402	0.028	0.199
Vol. Flow Rate (SLM)	20.8	20.8	10.4

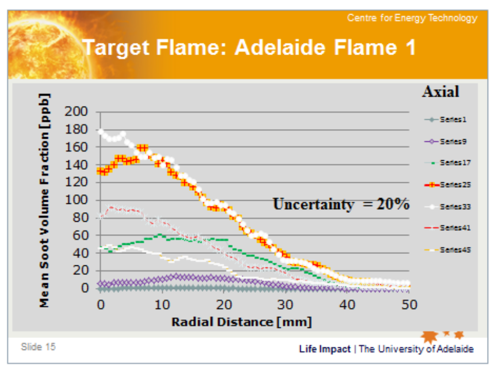


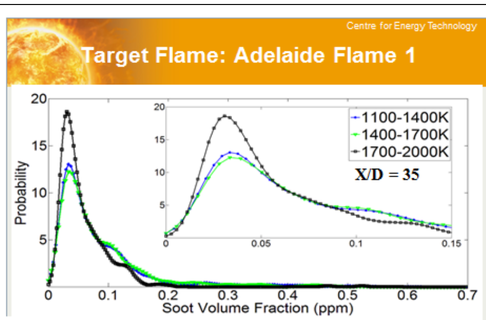












5E08: Simultaneous planar measurements of temperature and soot volume fraction in a turbulent non-premixed jet flame, Mahmoud, Nathan, Medwell, Dally, Alwahabi