Communique from the ISF-6 Workshop

Sixth International Workshop on the Measurement and Computation of Reacting flows with Carbon Nanoparticles

Friday 22 – Saturday 23 July, 2022,
Pinnacle Hotel Harbourfront, Vancouver

Date Issued: 31 August, 2022

Issued by the Joint Committee of the ISF as a synthesis of the key outcomes arising from the deliberations of the ISF-6 Workshop:

1) **Plan to introduce a new program in pyrolysis:** Backed by the 85% broad agreement of the delegates, as measured by the survey, the Joint Committee has agreed to establish a new program in pyrolysis of methane and other fuels. This will build on the ISF's established research programs in combustion-generated soot, to extend our activities into new regimes. This program is driven by the long-term significance of this class of reacting flow, not only as an important and challenging field of research, but also as a regime with numerous applications. It has strong potential to contribute to the global challenge of lowering the cost of the production of hydrogen with near-zero net CO_2 emissions by co-production of carbon products from methane and to the broader field of the synthesis of valuable carbon products. Evidence for the growing significance of this field can be found both in the attached power-point slides of the introductory session (Prof Gus Nathan) and from our invited industrial speaker, Dr Enoch Dames (Monolith Corp). The main components of the ISF's plan are as follows:
    a. **To establish a series of new reactors to investigate pyrolysis,** starting with methane, which will be both well suited to the development and validation of numerical models and be able to operate under a range of conditions of relevance to the various classes of emerging methane pyrolysis technology. These reactors will provide well-controlled input and boundary conditions, while also providing access for measurements employing both optical and extractive sampling, drawing on the experience established by the ISF community. A working group will develop one or more proposed configurations, in consultation with the joint committee, who will then coordinate a process to build multiple units at once (thereby ensuring consistency and lowering cost) with the opportunity for all interested groups to purchase one;
        i. **Action – Hope Michelsen (Boulder) – Convenor; Prof Nick Eaves (Windsor), Prof. Reza Kholghy (Carleton), Prof. Mario Commodo (Naples)[1], Cuong Thi-Kim (Lund) [2]:** To develop one or more recommended configurations for reactors in consultation with the community for review by a meeting of the Joint committee. Roscoe Taylor agreed to be an advisor. **Target date: 28 Oct, 2022.**

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b. **Call for new research contributions** to support the development and validation of models of methane pyrolysis by the joint application of state-of-the-art modelling and experimental activities, undertaken collaboratively to accelerate the establishment of complete data-bases and transparent comparison of models for both atmospheric and pressurized conditions.
    i. **Action: Laminar Flames Program Leaders-** Researchers are invited to contribute research to this field in a coordinated way through the ISF's Program Leaders with the aim to accelerate the sharing of knowledge, data, know-how and capability. **Target: to bring new data sets to ISF-7.**

2) **Exploration of opportunities to also establish programs in fire-related soot research and ammonia-blended flames, as follows:**
    a. **Fire-related soot research:** Given the growing interest in the impact of fires on global warming and the atmosphere, it was agreed to explore the potential of establishing a series of target flames in this field, and/or nominating potential speakers for ISF-7. The proposal should consider:
        i. the realistic potential for the development of the detailed predictive modelling techniques of ISF to make a significant impact on the challenges faced by the fire community;
        ii. A plausible configuration for research that has strong potential to provide well defined input and boundary conditions for model development and validation, whilst also being relevant to the above challenges;
        iii. **Action** - Dr Chiara Saggese; Dr Samuel L. Manzello, REAX Engineering (manzello@reaxengineering.com) and Prof Hope Michelsen to develop a preliminary proposal in consultation with the community for review by a meeting of the Joint committee. **Target date: 28 Oct, 2022.**
    b. **Soot from flames** of **ammonia-blended fuels:** Given the growing interest in the use of ammonia as a potential low-carbon liquid fuel, together with the emergence of some data-sets on the influence of ammonia on sooting characteristics of flames, it was agreed to also explore the potential of establishing a program in this field, and/or nominating potential speakers for ISF-7.
        i. **Action – [Bill Roberts or nominee]** to develop in consultation with the community for review by a meeting of the Joint committee. **Target date: 28 Oct, 2022.**

3) Significant progress has been made since previous workshops: The Joint Committee is pleased to note the ongoing and significant progress both in the establishment of additional data bases and in the increased accuracy of predictive capability in its target flames. In particular, the prediction of the main characteristics of turbulent ethylene flames is now achieving useful engineering accuracy and orders of magnitude better prediction than when the ISF was established. In addition, the prediction of methane flames has also improved by an order of magnitude relative to the situation at the start of the workshop. Nevertheless, some further work is needed to resolve the general trend of predicting the formation and burn-out of the soot too early. More details of this can be found in the attachments of the slides from the presentations (Prof. Michael Mueller, Dr Benedetta Franzelli and Dr Zhiwei Sun).

4) Additional research priorities identified at the workshop. The following additional research priorities were also identified at the workshop:

a. **Establishment of new measurements & new methods to measure particle dimensions:** Research on valuable carbon materials will require the measurement of additional dimensions of the carbon nano-materials to what has typically been reported for soot, notably measurements of surface area and morphology. Other parameters, including C:H ratio, will also be needed. In addition, while such measurements can be performed ex-situ, no in-situ methods are presently available. Hence there is also a need to develop new techniques for the in-situ measurement of these parameters;
b. **Need for further development of reliable models of carbon nano-particles, incorporating additional dimensionality:** New models are similarly needed of the evolution of nano-materials to also incorporate greater dimensionality as described above. A range of models will be needed, including those that are suitable for incorporation into CFD models;
c. **Key questions for laminar flow reactor program:** Some of the key research questions to emerge from the discussion, are as follows:
    i. What drives coalescence?
    ii. What is the influence of high volume-fraction of soot on the reaction pathways?
    iii. What is the role of impurities, including potassium salts?
d. **Need for a framework to allow sharing of models:** It was noted that we need to establish a framework to allow modellers to share codes and associated modelling tools. This is needed to avoid inadvertent omission of details that can influence the comparison of the performance of various models. It was agreed to establish a working group to address this, as follows:
    i. **Action: Prof's Michael Mueller and Reza Kholghy**, with Dr Med Colket and others to be engaged as appropriate]
e. **Need for increased coordination between laminar and turbulent reactor programs:** To meet this need, it was agreed to hold a meeting of the joint committee every 6 months, with the meetings at the 6th and 18th month mark being virtual and the other two face-to-face. ;
    i. **Action: Organising Committee –** to arrange;

5) **Organisation and logistics:** The following points were noted from the discussions and endorsed by the Joint Committee:
    a. **Broad endorsement for the overall structure of the meeting:** ISF-6 delegates endorsed the overall arrangements for the workshop, including the mix of industry and research presentations.
    b. **Timing:** It was agreed to seek to reduce the overlap with the TNF Workshop in future forums. The tentative proposal to achieve this is to run the workshop for ISF-7 on the Saturday and Sunday immediately before the Symposium.
    c. **Posters:** The establishment of the three-minute presentations and prizes to accompany the posters was greatly appreciated, and agreed to be continued. However, it was recommended to plan to hold the dinner in the same room as the posters to facilitate discussion.
    d. **Discussion regarding recording of presentations:** In response to some requests that the meeting be recorded, it was noted that this has not been done for both practical and copy-right reasons. From previous experience, it is very difficult to provide recordings of sufficient quality without professional support, which is expensive. In

addition, the recording of a discussion can introduce many challenges. For example, delegates usually discuss partly-formed ideas or express themselves in ways that they later wish to change, as typical in a workshop style discussion. This may inhibit discussion and/or complicate the process of making recordings available. For these reasons, the Joint Committee will continue to issue a written summary of the outcomes.

e. **Child-care:** It was agreed to plan to arrange child-care in an organised way for future events, preferably in coordination with other workshops and the symposium host.

6) **Prizes and Awards:** The ISF Committees is pleased to have introduced to our sixth meeting a series of prizes for PhD students and early career researchers, both for the best 3-Minute presentation and for the best poster. In so doing, we also wish to thank and acknowledge the following contributors:

   a. **Judging Panel for three minute presentations:**
      i. Prof. Christof Schulz
      ii. Prof. Thomas Dreier,
      iii. Dr. Peng Liu;
      iv. Mr David Sharbaugh
   b. **Judging Panel for Posters:**
      i. Prof. Bassam Dally
      ii. Prof. Michael Mueller,
      iii. Dr Med Colket;
      iv. Prof Alberto Cuoci
   c. **Poster Organizers:**
      i. Dr Benedetta Franzelli,
      ii. Dr Zhiwei Sun

The prize winners are listed below, together with a photograph of the award ceremony.

Prize winners for the Three-Minute presentations from ISF-6. From left to right: **Dr Georgios Kelesidis,** ETH Zurich, for presentation entitled ' *Porosity and crystallinity dynamics of carbon black during internal and surface oxidation***, Mohammad Adib**, Carleton University, for a presentation entitled 'Prediction of mass yield, morphology and composition of soot particles generated by pyrolysis of hydrocarbon', **Prof Thomas Dreier**, University of Duisburg-Essen (Judging Panel), **Professor Christof Schulz**, University of Duisburg-Essen (Judging Panel).

Prize winners for the Best Poster presentations from ISF-6. From Left to right: **Dr Med Colket**, Consultant to United Technologies Research Centre (Judging Panel), Special Commendation Awardee: **H. Maldonado Colman,** Special Commendation Awardee: Dr **Peng Liu,** KAUST, Prize Winner: **Una Trivanovic**, ETH Zurich, for presentation entitled '*High throughput generation of aircraft-like soot'*, **Prof Bassam Dally**, KAUST (Judging Panel).

Members of the Joint Committee

Organising Committee

Prof Gus Nathan, Prof Heinz Pitsch, Prof Bassam Dally, Dr Chris Shaddix,
Dr Klaus-Peter Geigle, Prof Hope Michelsen, Prof Tiziano Faravelli, Prof Michael Mueller.

Scientific Advisory Committee,

Dr Med Colket, Prof Andrea D'Anna, Prof Ömer Gülder, Prof Hai Wang, Prof Bill Roberts,
Prof Peter Lindstedt, Prof Christof Schulz, Prof Henning Bockhorn, Prof Angela Violi,
Prof Murray Thomson, Dr Enoch Dames.

Program Leaders and Co-leaders

Laminar Reactors: Dr Chiara Saggese, Dr George Kelesidis, Dr Reza Kholghy,
Dr Joaquin Camacho.
Turbulent Reactors: Dr Benedetta Franzelli, Dr Zhiwei Sun, Dr Federica Ferrarao.
Past Leaders (ISF-6): Prof Fabrizio Bisetti, Prof Thomas Dreier,
Prof Michael Mueller.