Guidelines for Participation in the Second Workshop Organized by the Gas Phase Phenomena Subgroup of the MaCFP Working Group – April 22, 2021

(see https://github.com/MaCFP/macfp-db/wiki/MaCFP-2021-Modeling-Guidelines)

Introduction

The general objective of the "*IAFSS Working Group on Measurement and Computation of Fire Phenomena*" (abbreviated as the "MaCFP Working Group") is to establish a structured effort in the fire research community to make significant and systematic progress in fire modeling, based on a fundamental understanding of fire phenomena. This is to be achieved as a joint effort between experimentalists and modelers, identifying key research topics of interest as well as knowledge gaps, and thereby establishing a common framework for fire modeling research. The MaCFP Working Group is endorsed and supported by the International Association for Fire Safety Science (IAFSS, see http://iafss.org/macfp/) and is intended as an open, community-wide, international collaboration between fire scientists. It is also intended to be a regular series of workshops. The first MaCFP workshop was held on June 10-11 2017 as a pre-event to the 12th IAFSS Symposium in Lund, Sweden. The proceedings have been published in Fire Safety Journal (A. Brown *et al*., *Fire Safety J.* 101 (2018) 1-17).

Second MaCFP Workshop ("MaCFP-2")

MaCFP-2 will take place on April 22-23, 2021, as a virtual pre-event to the 13th IAFSS Symposium (https://uwaterloo.ca/international-symposium-on-fire-safety-science/). The workshop will feature activities organized by both the Gas Phase Phenomena subgroup (on **Thursday April 22, 2021**) and the Condensed Phase Phenomena subgroup (on **Friday April 23, 2021**). We focus in the following on activities of the Gas Phase Phenomena subgroup.

As previously advertised, the Gas Phase Phenomena subgroup is planning to hold discussions corresponding to the following target experiments:

- **Case 1** (Turbulent buoyant plumes): the Helium plume experiment previously studied at Sandia National Laboratories (T.J. O'Hern, E.J. Weckman, A.L. Gerhart, S.R. Tieszen, R.W. Schefer, *J. Fluid Mech*. 544 (2005) 143-171);
- **Case 3** (Turbulent pool fires with liquid fuel): the methanol pool fire experiments previously studied at the University of Waterloo (**Case 3a**, E.J. Weckman, A.B. Strong, *Combust. Flame* 105 (1996) 245-266) and also currently studied at the National Institute of Standards and Technology (**Case 3b**, S.C. Kim, K.Y. Lee, A. Hamins, *Fire Safety J.* 107 (2019) 44-53);
- **Case 5** (Flame extinction. Flame radiation): the controlled co-flow round ethylene diffusion flame experiment currently studied at FM Global (D. Zeng, P. Chatterjee, Y. Wang, *Proc. Combust. Inst*. 37 (2019) 825-832; N. Ren, D. Zeng, K. Meredith, Y. Wang, S. Dorofeev, *Proc. Combust. Inst*. 37 (2019) 3951-3958; G. Xiong, D. Zeng, P. Panda, Y. Wang, *Proc. 11th US National Combustion Meeting*, Pasadena CA, March

24-27, 2019; X. Ren, D. Zeng, Y. Wang, G. Xiong, G. Agarwal, M. Gollner, *Fire Safety J., available online*).

The MaCFP repository hosted on GitHub (https://github.com/MaCFP) contains all available experimental data corresponding to Cases 1, 3a, 3b, and 5. Note that the repository is continuously updated, and users are expected to consult the repository regularly on possible additions and/or corrections. These data are available to computational groups for CFD model validation. For MaCFP-2, Python-based post-processing tools are available (see https://github.com/MaCFP/macfp-db/wiki/Plotting-Scripts). However, contributors need only to submit comma-delimited (*.csv) files with their computational results together with another comma-delimited configuration file listing the plots to be made (see https://github.com/MaCFP/macfp-db/wiki/Submitting-Computational-Results). An example is provided in the wiki. Please contact Randy McDermott (randy.mcdermott@gmail.com) if you have any questions regarding submission of results or post-processing.

MaCFP-2 will present detailed comparisons between experimental data and computational results obtained by participating modeling groups with the intent to review progress, summarize accomplishments, identify knowledge gaps, and provide guidance with clear objectives for the next workshop. The spirit in which discussions will be conducted is reflected in the Proceedings of the first MaCFP workshop (reference, see above). The results from the discussions during MaCFP-2 are intended to be documented as Proceedings and submitted for publication in the *Fire Safety Journal*.

Interested modeling groups should inform the Gas Phase Phenomena subgroup of the MaCFP Working Group of their plans to participate in MaCFP-2 by contacting the Co-Chairs of the MaCFP Working Group, Bart Merci (bart.merci@ugent.be) and Arnaud Trouvé (atrouve@umd.edu). Approximately one month before the Workshop (*i.e.*, by the end of March 2021), participating modeling groups will be asked to submit an electronic copy of their computational results organized in simple comma-delimited ASCII files. All results will be uploaded on the MaCFP GitHub repository and detailed comparisons between experimental data and computational results will be compiled by the MaCFP organizers in collaboration with experimentalists and modelers.

We present below guidelines for submission of computational data by participating modeling groups.

General Guidelines

An important new feature in MaCFP-2 is the following series of requirements in the submission of computational results:

- We ask that for each simulated target experiment, the submission includes a grid convergence study in which the effect of changing spatial resolution in the flow and combustion solver (as opposed to the radiation solver, discussed next) is quantified;
- Similarly, we ask that for each simulated target experiment, the submission includes an angular convergence study in which the effect of changing angular resolution in the radiation solver is quantified;

- We ask that modeling groups explain their modeling choices for the treatment of the turbulent flow, combustion and radiation transport; we encourage modeling groups to define a baseline model and apply that model to all simulated cases considered by the group; we ask that variations in modeling choices be justified.

We believe that these requirements will improve the quality and depth of the comparisons between results obtained by different modeling groups.

Furthermore, we encourage modeling groups to consider performing fine-grained simulations under the high resolution conditions that are often the preferred choice made by CFD researchers, and also consider performing coarse-grained simulations under the moderate-to-marginal resolution conditions (sometimes called VLES) that are more representative of the choices made by CFD practitioners.

Additional Guidelines for Case 1

Groups interested in simulating Case 1 are invited to consult the presentation made at the first MaCFP workshop (https://iafss.org/wp-content/uploads/MaCFP-Case1.pdf) as well as the presentation published in the Proceedings (https://doi.org/10.1016/j.firesaf.2018.08.009).

Suggested grid resolution: Δx from 1 cm to 20 cm.

Plots of interest include:

- The mean Helium mass fraction as a function of radial position *x*, for different elevations *z*; the *rms* Helium mass fraction as a function of radial position *x*, for different elevations *z*;
- The mean vertical velocity as a function of radial position *x*, for different elevations *z*; the *rms* vertical velocity as a function of radial position *x*, for different elevations *z*;
- The mean radial velocity as a function of radial position *x*, for different elevations *z*; the *rms* radial velocity as a function of radial position *x*, for different elevations *z*.
- A plot quantifying the puffing frequency of the Helium plume;
- Plots showing the centerline variations of the mean Helium mass fraction, the *rms* Helium mass fraction, the mean vertical velocity, the *rms* vertical velocity, as a function of elevation *z*.

The data required to generate these plots should be provided as ASCII files organized in simple comma-delimited format.

Additional Guidelines for Case 3a and Case 3b

Case 3b corresponds to a 30-cm-diameter methanol pool fire studied at NIST and is a configuration that is similar to Case 3a previously studied at the University of Waterloo. Case 3b features a database that includes heat flux measurements. An acceptable approximation is to consider that the configurations in Cases 3a and 3b are identical.

The experimental database developed at NIST and posted on https://github.com/MaCFP also considers a 100-cm-diameter methanol pool fire, a 30-cm-diameter acetone pool fire, a 30-cm-diameter ethanol pool fire, and a 37-cm diameter methane fire. Groups interested in simulating several of these configurations are invited to focus on the 30-cm and 100-cm methanol cases first. Because of time constraints, discussions at the second MaCFP Workshop may be limited to the 30-cm-diameter methanol pool fire configuration (Cases 3a and 3b).

Also, groups interested in simulating Cases 3a and 3b are invited to focus first on simulations with a prescribed liquid evaporation rate (taken as the measured averaged value). Simulations with an evaporation rate that is calculated as a function of the thermal feedback are welcome but should be considered as a second step.

Similarly, groups interested in simulating Cases 3a and 3b are invited to focus first on simulations with a prescribed global radiant fraction (taken as the measured averaged value). Simulations that simulate rather than prescribe the radiant fraction are welcome but should be considered as a second step.

Groups interested in simulating Case 3 are invited to consult the presentation made at the first MaCFP workshop (https://iafss.org/wp-content/uploads/MaCFP-Case3.pdf) as well as the presentation published in the Proceedings (https://doi.org/10.1016/j.firesaf.2018.08.009).

Suggested grid resolution (30 cm pool): Δx from 0.5 cm to 6 cm.

Suggested grid resolution (100 cm pool): Δx from 1 cm to 20 cm.

Suggested angular resolution: N_{Ω} = 50 angles, 100 angles, 200 angles.

Plots of interest include:

- The mean temperature as a function of radial position *r*, for different elevations *z*; the *rms* temperature as a function of radial position *r*, for different elevations *z*;
- The mean vertical velocity as a function of radial position *r*, for different elevations *z*; the *rms* vertical velocity as a function of radial position *r*, for different elevations *z*;
- The mean radial velocity as a function of radial position *r*, for different elevations *z*; the *rms* radial velocity as a function of radial position *r*, for different elevations *z*.
- The correlation between fluctuating vertical velocity and fluctuating temperature as a function of radial position *r*, for different elevations *z*.
- The correlation between fluctuating radial velocity and fluctuating temperature as a function of radial position *r*, for different elevations *z*.
- The correlation between fluctuating vertical velocity and fluctuating radial velocity as a function of radial position *r*, for different elevations *z*.
- A plot showing the time variations of the heat release rate;
- Representative plots showing the instantaneous flame shape (*e.g.*, identified as the 200-kW/m^3 iso-contour of the volumetric heat release rate, or using some other method to be specified);

- A plot quantifying the puffing frequency of the pool fire;
- Plots showing the centerline variations of the mean temperature, the *rms* temperature, the mean vertical velocity, the *rms* vertical velocity, the correlation between fluctuating vertical velocity and fluctuating temperature, the correlation between fluctuating vertical velocity and fluctuating radial velocity, as a function of elevation z.
- Plots showing the radial variations of the total heat flux for gauges oriented horizontally, facing upwards, and located near the plane defined by the burner rim;
- Plots showing the vertical variations of the radiative heat flux for gauges oriented vertically, facing the centerline of the fire, and located at r = 60 cm and r = 83 cm;
- Plots showing the centerline variations of mean mole fractions of species of interest, as a function of elevation z.

The data required to generate these plots should be provided as ASCII files organized in simple comma-delimited format.

Additional Guidelines for Case 5

Case 5 corresponds to a 13.7-cm-diameter, controlled co-flow (a mixture of air and nitrogen), round ethylene diffusion flame experiment currently studied at FM Global. Case 5 includes global measurements at coflow oxygen molar fractions of 20.9%, 19%, 17% and 15%, and detailed measurements at coflow oxygen mole fraction of 20.9%, 16.8% and 15.2%. Note that the current experimental database does not include the oxygen extinction limit of the flame and focuses instead on the change in the flame radiation observed as this limit is approached.

Note that the ethylene mass flow rate was incorrectly specified in the initial MaCFP documentation and that the value has been corrected in January 2021 (the ethylene mass flow rate for all detailed measurements is equal to 0.318 g/s, corresponding to a 15 kW flame).

Groups interested in simulating Cases 5 are invited to predict the changes in flame radiation. Simulations with a prescribed radiant fraction (taken as the measured averaged value) are acceptable as well.

Suggested grid resolution: Δx from 0.5 cm to 2 cm.

Suggested angular resolution: N_{Ω} = 50 angles, 100 angles, 200 angles.

Plots of interest include:

- The mean temperature as a function of radial position r, for different elevations z; the *rms* temperature as a function of radial position r, for different elevations z; the probability density function (PDF) of temperature for different radial positions r and elevations z;
- The mean soot volume fraction as a function of radial position r, for different elevations z; the *rms* soot volume fraction as a function of radial position r, for different elevations z; the probability density function (PDF) of soot volume fraction for different radial

positions *r* and elevations *z* (for comparisons, use the experimental soot data corresponding to Laser Induced Incandescence – LII – measurements);

- A plot showing the time variations of the heat release rate;
- Representative plots showing the instantaneous flame shape (*e.g.*, identified as the 200-kW/m^3 iso-contour of the volumetric heat release rate, or using some other method to be specified);
- A plot showing the variations of the predicted global radiant fraction with the coflow oxygen mole fraction;
- Plots showing the vertical variations of the radiative emission power per unit height of the fire (kW/m) (in numerical simulations, this quantity can be estimated by calculating the average of the radiation source term that appears in the energy equation integrated over each horizontal plane and over time).

Points of contact

- For questions on Case 3a, Beth Weckman (beth.weckman@uwaterloo.ca)
- For questions on Case 3b, Anthony Hamins (anthony.hamins@nist.gov)
- For questions on Case 5, Yi Wang (yi.wang@fmglobal.com)
- For questions on the GitHub MaCFP repository, Randy McDermott (randy.mcdermott@gmail.com)
- For any question, Bart Merci (*Co-Chair*, bart.merci@ugent.be) and Arnaud Trouvé (*Co-Chair*, atrouve@umd.edu)