

Compartment fires: challenges for fire modeling as a tool for a safe design (IAFSS workshop, April 2021)

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Abstract

The use of fire models to support fire protection engineering decisions requires an understanding of model shortcomings and assurance in their predictive robustness. This note is a summary of the online ‘compartment fire’ workshop that was organized prior to the International Association of Fire Safety Science (IAFSS) symposium, hosted online by the University of Waterloo (Canada) in April 2021. The objectives of the Workshop were to identify, discuss and prioritize key compartment fire modeling challenges.

It is recognized that the substantial changes in the built environment and the variety of subsequent fire dynamics problems necessitate significant advances in modelling, particularly with respect to (amongst other aspects) (i) under-ventilated fires (the prediction of soot and CO concentrations, extinction and reignition), (ii) heat transfer and the interaction with structural and non-structural elements, and (iii) the interaction with water-based fire suppression systems. High-quality and well-documented experimental tests play an essential role in fostering model development and validation; a good synergy between experimentalists and modellers is of utmost importance.

1. Introduction and context

Addressing concerns about sustainability, community resilience, functionality, and aesthetics, the built environment is experiencing rapid evolution with respect to several factors affecting compartment fire dynamics. For example, with respect to geometry, there are more and more high-rise buildings as well as buildings with large open spaces. Construction techniques are also strongly evolving along with building materials, e.g., timber construction and prospective steel-timber hybrid buildings [1]. Furthermore, green buildings and alternative fuel types such as hydrogen, batteries and solar panels, are more and more prevalent and should be considered in a comprehensive fire risk assessment. Although the fundamentals of the ‘compartment fire’ framework remain the same, all these changes require a continuous

¹ This publication is intended to capture external perspectives related to NIST standards, measurement, and testing-related efforts. These external perspectives can come from industry, academia, government, and other organizations. This report was prepared as an account of a workshop; it is intended to document external perspectives; and does not represent official NIST positions.

examination and comprehensive understanding of a wide range of fire scenarios and their underlying physical phenomena.

For example, in combustible structures made of timber, there is potential delamination, suggesting the potential for successive flashovers in the same compartment [2]. Another example is air-tight buildings such as passive houses or nuclear power plant facilities. In such compartments, the fire-induced pressure effect is substantial, potentially hindering evacuation in residential buildings [3] or altering the ‘pressure cascade’ set up in nuclear facilities in order to prevent the release of radioactive materials [4]. Furthermore, a significant increase in pressure in residential buildings can even cause structural damage. The problems in large spaces such as hypermarkets (‘very large self-service stores with a wide range of goods’) and open offices is different; heating is localized and the cooling phase might matter for structural calculations which are of importance for firefighting intervention.

Although the myriad of industrial tests, such as fire resistance tests using furnaces², provide a first means of assessment (for example with respect to compartmentation), a more science-based approach is required to best address compartment fire dynamics and fulfill safety requirements with respect to evacuation and tenability (in the pre-flashover stage) as well as structural stability (in the post-flashover stage). It is in this context that compartment fire modelling has become an important approach in analyzing the fire hazards and, potentially, proposing efficient mitigation measures. Significant advances in model development have been achieved in the last decades. Several tools, with different levels of complexity are available, i.e., engineering correlations in spread sheets, zone models and computational fluid dynamics (CFD). Nevertheless, a lot of challenges remain to improve the capabilities and reliability of these models. To this end, a series of questions were posed to workshop participants. Their responses found in the Appendix of this article attempt to gauge the fire science community’s perspectives on challenges hindering a full understanding of compartment fire phenomena.

The workshop aimed at briefly screening the state-of-the-art of compartment fire modelling and identifying the current challenges and knowledge gaps that need development and validation. In these processes, experimental testing is seen by workshop participants to play an important role.

2. Fire science and modeling

In addition to fire protection design, compartment fire modelling is often used in fire risk assessment, fire reconstruction (investigation) and in testing theories as virtual experiments. Therefore, obviously, any new advances in modelling compartment fires for design purposes will benefit the other fields of application of fire modelling. In this section, two main aspects of the physics are discussed: (i) chemistry and combustion modelling and (ii) heat transfer. Additionally, a sub-section is devoted to the interest in coupling fire dynamics tools to other

² This has been the topic of lively discussion during the workshop, supporting the statement mentioned in this note.

tools used in the built environment such as heat ventilation and air conditioning (HVAC) models and building information models (BIMs).

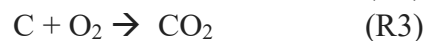
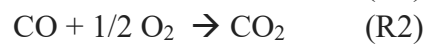
2.1 Fire chemistry and combustion modelling

It is relatively well-documented and demonstrated that current fire models predict relatively well the transport of hot smoke and combustion products in a well-ventilated compartment. However, several challenges remain with respect to fire chemistry.

Regarding soot and carbon monoxide (as well as other products of incomplete combustion), the main approach in well-ventilated conditions consists of considering a global single-step infinitely fast reaction and specifying constant soot and CO yields (i.e., fuel conversion ratios) which mainly depend on the fuel. Additionally, soot and CO production are slow chemistry processes, which depend on the time-temperature history of a packet of gas and the yields are dependent on both fuel type and the scale of the fire. An important limitation at this level is that the fuels involved in fires are generally uncertain. Therefore, predictions using single values of yields as input are not particularly reliable and are certainly not reliable within flames.

The challenge is even more important when the fire becomes under-ventilated. The main approach here consists of remaining within the global single-step infinitely fast reaction framework mentioned above but with an adjustment of the values of the soot and CO yields. This can be done based on the ventilation conditions as characterized by the global equivalence ratio (GER). This approach is not often used because of the difficulty in estimating *a priori* the GER of a specific scenario, and even more so in a dynamic way, i.e., when the fire conditions change from over-ventilated to under-ventilated. As a consequence, the yields are prescribed based solely on specific (and a limited number of) experiments typically made in small flames such as [5].

An alternative to the global single-step reaction approach is to consider multiple chemical reactions such as:



Several options open-up at this level. The first one is to remain within the infinitely fast chemistry framework for all three reactions, in conjunction with the eddy dissipation concept (EDC) model for combustion [6]. This option is particularly attractive because the computational cost remains low, but it has not yet been fully explored. A more advanced approach is to rely on advanced combustion models using finite-rate chemistry in conjunction with, for example, PDF (probability density function)-based combustion models [7], such as the conditional moment closure (CMC) approach [8]. This can be done for the full set of chemical reactions or only for the chemical reactions not involving fuel, because fuel

oxidation is a fast reaction. Several drawbacks are associated with finite-rate chemistry modelling such as the associated computational cost (which can be prohibitive for practical fire dynamics simulations) as well as the stiffness of the numerics. The main advantage is the capability of finite-rate chemistry in handling extinction and reignition phenomena without adding specific sub-models devoted to that. In any case, extinction and, even more so, reignition phenomena remain currently difficult to model. Autoignition itself is not well understood, nor is its experimental determination consistent from one study to another. Many test methods, test results and more recently, calculation methods have been conducted to determine the autoignition temperature (AIT) and the results are dependent on the method and apparatus employed for its determination. Reputable sources using different methods have reported experimental AIT values that vary by about 100 K for the same material. (See for example, Tables 17.1, 18.2 and A.29 in Ref. [9], where the AIT of methane is listed as 540 °C, 600 °C and 632 °C, respectively).

At this point, two modelling '*philosophies*' can be confronted. Do we need to remain within a 'simplified' (yet robust) modelling framework bearing in mind the computational constraints inherent to practical fire dynamics simulations? Or do we invest in more advanced but 'costly' approaches with the hope that the growth in computational resources will be sufficiently fast to render advanced detailed modelling applicable in real (practical) fire scenarios? This is a question which is perhaps not only relevant to fire chemistry and combustion, but to other aspects in fire modelling as well.

In any case, there is a very strong need for high-quality compartment fire studies focusing on chemistry. Also, there are databases for single compartment experiments, but not enough for multiple rooms, multiple floors and within heat ventilation and air conditioning (HVAC) systems. These aspects will be addressed later in this document.

2.2 Heat transfer

2.2.1 Thermal radiation

Thermal radiation is the dominant mode of heat transfer in fires. In most fire-driven flows, soot is the dominant contributor to thermal radiation (in comparison to gaseous species), which justifies (to some extent) the simplified grey gas approach. Nevertheless, the need to potentially address 'new'/'decarbonized' fuels such as hydrogen, calls for consideration of a more detailed treatment of the thermal radiation of gases.

Furthermore, given the uncertainties in local temperature predictions and the fourth power temperature dependence of the emitted radiation, a radiative fraction is typically prescribed. This approach may be viable for over-ventilated fires, but can become a poor estimate for underventilated scenarios. Some important research questions that require further understanding here are (i) is there an added-value in the spectral treatment of radiation, given the added computational cost? (ii) How can path lengths in simulations with a wide range of length scales be effectively treated? and (iii) How can absorption coefficients be accurately estimated? In fact, the second research question provides an answer to the first research

question in that the spectral (or non-gray) method is the main strategy for tackling different path lengths.

2.2.2 Pyrolysis and flame spread

Heat transfer is very important in pyrolysis and flame spread, which are phenomena of interest, particularly in large open plan compartments, involving eventually combustible structures. In general, there is no consensus on the approaches to be used for modeling fire spread at an engineering scale. A first approach is to decouple the gas phase from the solid phase and prescribe an approximate spread rate. In a more predictive approach, the question is how to ensure reasonable spread when predicting pyrolysis at large scales.

2.2.3 Water-based fire suppression systems

Modelling the interaction of water-based fire suppression system remains challenging, especially when it comes to predicting for instance the effect of sprinkler systems on fire growth and spread. Although a lot of interesting and valuable work has been carried out for instance for rack storages, some aspects of the modelling remain not applicable to a wider variety of fire scenarios. It is of interest to further develop ‘wall models’ for heat transfer that can cope with the evaporation of droplets and ‘films’ at solid surfaces (important for flame spread in the presence of water) and the subsequent cooling which slows down pyrolysis and flame spread.

2.3 *Coupling Fire dynamics tools with other tools*

Prior to the discussion on coupling fire dynamics tools with other tools, it is of interest to highlight the benefit in developing hybrid models for fire dynamics, which are models combining field models, i.e., CFD, with zones models (e.g., one zone or two zones). This approach is attractive because detailed field information in the compartment can be used to solve the fire development therein, whilst relying on a less costly method, i.e., zone modelling, for smoke and heat transport transport to adjacent compartments. Let us consider for example a high-rise residential structure with an HVAC network allowing for smoke movement between floors. Significant computational savings could arise if the ‘fire unit’ is modeled with CFD using multiple cores and other spaces are modeled with a zone and/or a network model using one core. Additionally, hybrid 3D-1D coupling is emerging for tunnel fires, in particular because of the strong need to reduce the computational cost in (very) long tunnels. It is thus of interest to further develop this approach for other types of compartment fires such as residential buildings.

Merging fire models with building air quality models such as HVAC models allows integration of important building information (regarding ventilation in this case) in fire safety design. More generally, this is done by coupling fire dynamics modelling to building information models (BIM), which is particularly relevant when considering studies focused on tenability and egress in the early stages of a fire.

The coupling of fire dynamics with structural calculations remains mainly carried out in one way: fire dynamics provides a heat flux mapping onto the structure (and several structural

elements). In this regard, the traveling fire method [10] can be further developed and applied to provide a more realistic exposure.

Although one way coupling may be believed to be an acceptable approach for design purposes, it is of high interest to consider two-way coupling for a more realistic representation of the fire development in research and fire reconstruction (investigation) activities. This is because significant changes at the level of the structure, e.g., window frame expelled from a compartment, may have a substantial impact on the fire dynamics. In this context, it is perhaps of importance to seek a better representation of structures in CFD models. More generally, there is a need for more advanced and user-friendly tools carrying out the coupling between fire dynamics and structural engineering.

3. Design experiments to support compartment fire modeling

Experimental work is of utmost importance in developing reliable fire modelling tools. In this section, the relation between experiments and modelling is discussed before addressing the challenges related to designing experiments for compartment fires. Finally, the need for collaboration between experimentalists and modellers is highlighted through, for instance, the development and maintenance of common and open databases.

3.1 Links between experiments and modeling

Three types of experiments have been identified depending on whether the objective is:

- to validate a model,
- to guide model development, or
- to uncover new fire scenarios (and underlying poorly understood phenomena).

With the objective of validating a model, the physics and the models are mostly well-known and the variables of interest are well-defined. The experiment is thus designed in order to assess the quality of the physical model with respect to several quantities such as amplitudes, trends, and time and space-resolved information over a defined range of parameter space. Aspects of the physics relevant to compartment fires are turbulence, combustion, extinction, pyrolysis, and heat transfer in the gas phase and through solid boundaries. It is very important also to ensure well-controlled boundary conditions and good quality measurements, which must include estimation of measurement uncertainty. A model cannot be validated to higher accuracy than the uncertainty of the data that is used in its evaluation. It is important to carry out repeatability experiments to ensure experimental quality and enable estimation of measurement uncertainty.

With the objective of model development, the physics and the models are partially understood but experiments are needed to (i) deepen our understanding of the physics, (ii) propose correlations and/or (iii) determine model constants. The quantities of interest here are mainly averaged, steady or global information. In compartment fires, several phenomena and aspects of the physics still require a deeper understanding and more reliable models such as combustion in a vitiated environment (including soot production and deposition), combustion

regimes, and pressure effects. Other compartment flow dynamics features are also of interest such as thermal plumes in a stratified environment, ceiling jets, thermal stratification and smoke filling. The number of experiments can be high, depending on the number of input parameters considered. A design of experiments test grid method can be recommended to reduce the number of tests.

In the last type of experiments, the physics and models are very uncertain. Experiments are therefore designed to understand and uncover specific aspects of the physics in order to be able to propose a first modeling approach. The knowledge of some important details in a real event is of importance. The number of tests can be important; the location and type of measurements can be adjusted along the test campaign. The scenarios of interest here involve, for example, complex fire sources (such as cables, electrical cabinets or batteries), complex geometries (e.g., multi-compartments), transient phenomena (such as backdraft), and the interaction with the structure. The process of unburned gas ignition is also a topic of interest.

It is important to note that, regardless of the objective (i.e., model validation, model development or uncovering new aspects of the physics), the question of downscaling may arise. This is particularly true in fire science applications for which real phenomena occur at large-scale, as rendering real-scale experimentation can be costly and, sometimes, dangerous. Downscaling is then a very attractive option which should be used with caution. Full scaling of all physical phenomena occurring in a real (and complex) fire scenario is often not possible. Therefore, partial scaling has to be defined and applied correctly, often requiring some subtlety in the analysis [11].

Finally, it is very important to mention that a close collaboration between experimentalists and modellers fosters the design of high-quality and tailor-made (fit-for-purpose) experiments, which ensures an efficient valorization of the experiments with respect to the research objectives (such as model validation or model development). A fine example of this type of collaboration is the IAFSS working group on Measurement and Computation of Fire Phenomena (MaCFP), which is considering various aspects of solid and gas phase fire physics [12, 13].

3.2 Challenges in designing experiments for compartment fires

Many workshop participants felt that more large scale, high quality data (considering measurement uncertainty) is urgently needed to provide further confidence in modelling compartment fires (see Question #10 in the Appendix). In addition to the importance of high-quality measurements as well as the development of collaborative work between experimentalists and modellers, several other challenges arise when designing experiments for compartment fires.

Depending on the objectives, several scales need to be considered. First, for practical engineering purposes, a sufficiently large scale should be set in order to be as close as possible to real fire events and avoid unrealistic phenomena induced by partial downscaling. If the objective is more science-based, with the intent to focus on one or just a few specific

aspects of the physics, canonical reduced-scale experiments can be carried out. The development of such experiments can be inspired from other research communities, e.g., combustion, heat transfer and thermal radiation. Intermediate-scale experiments can combine advantages of both small and large-scale facilities: easy handling and high measurement quality on one side and close enough to a real fire on the other side. Real-scale experiments are generally expensive. The challenge is how to coordinate the fire research community's efforts to maintain a good stream of realistic large-scale experimental tests, without losing sight of the need to push for smaller well-instrumented tests, which are important for model development.

Regardless of the scale, a lot of effort is required to produce high-quality and comprehensive experimental data for the support of compartment fire modelling. In this regard there are few studies that provide a detailed characterization of the fire-driven flow in terms of (i) the thermal field, (ii) the flow field, and (iii) the concentration distribution of gaseous species and particulates. This is particularly interesting for unsteady phenomena, such as underventilated compartment puffing as documented for example in [14]. Decoupling the fuel mass burning rate from the fire's heat feedback can be accomplished by consideration of gaseous fuels. This approach may be useful to simplify model calculations and can be seen as a first step towards understanding more complex compartment fire physics.

One of the most commonly measured quantities in compartment fire experiments is the temperature. Although using thermocouples is a basic and robust technique, more advanced techniques should be investigated in order to obtain more field and time-resolved information. Temperature measurements are often complemented by video fire analysis (VFA) techniques [15] in order to characterize the flame properties such as its size and dimension (e.g., height, shape). Temperature fields provide important, but limited information on the fire-induced thermal environment. That is why it is very important to measure total and radiative heat fluxes, which allow estimation of heat losses to inert boundaries as well as combustible materials, the latter being particularly important in understanding the pyrolysis (respectively evaporation) processes of solids (respectively liquids). Regarding the flow field, and especially smoke flows, in addition to bidirectional probes, it is of interest to develop and apply more advanced techniques such as particle image velocimetry (PIV). This is challenging given the 'harsh' environment induced by a fire. Few such studies are available in the technical literature.

Measurements of the concentration of species in a compartment fire are particularly important and challenging in a vitiated environment. For example, the knowledge of oxygen and combustion products concentration fields are needed to address (near-)extinction conditions. Also, information related to soot are of interest in order to better understand and predict the radiative transfer within the compartment. Developments are needed in sampling techniques as well as in the development of field measurements with, for example, the planar laser-induced fluorescence (PLIF) technique.

A common issue to all measurement techniques is the development of field measurements or space-resolved techniques in order to respond to the needs expressed by CFD model developers. Such sentiment was expressed by workshop participants as seen in their response to Question 5 in the Appendix.

3.3 Common database to share experimental and simulation data

In addition to the technical challenges highlighted above, it is very important to develop strong capabilities in sharing knowledge within the fire safety science and engineering community. Both large-scale and canonical reduced-scale experiments with advanced measurement techniques are costly and the fire community remains small in comparison to other scientific fields. The perspective of setting a common database platform, containing well-documented experimental and numerical simulation results are of great interest (e.g., the MaCFP platform [12, 13] available at <https://github.com/MaCFP> or the FDS validation repository available at <https://github.com/firemodels/fds/tree/master/Validation>). Such a platform can be used to spread and disseminate knowledge from researchers to practitioners. It is believed that this approach can strongly contribute to improving the background of fire protection engineers and consequently, safety and fire risk assessment.

4. Conclusions

This note presents a very brief state-of-the-art on compartment fire modelling capabilities and hints at several research and development routes to be carried out in the coming decades.

With respect to the physics and chemistry, the prediction of soot and carbon monoxide in under-ventilated fires remains a ‘bottleneck’; more developments are required, particularly for practical engineering calculations. In terms of heat transfer, thermal radiation plays a central role and poses challenges regarding, for instance, the estimation of absorption coefficients and the prediction of the overall (as well as local) thermal radiation from a flame. Also, the coupling between heat transfer and pyrolysis for predictive calculations of flame spread remains very challenging especially at large-scale; simpler approaches with a prescribed flame spread remain of interest. For the interaction of water-based fire suppression systems with fire-driven flows, although significant progress has been achieved in the interaction of water with hot smoke, further is to be done at the level of the flame as well as the fire source (in terms of cooling and subsequent effect on flame spread and fire growth).

All the above developments at the level of fire dynamics can be coupled to other tools such as structural engineering models, BIMs and HVAC models in order to address fire safety in a holistic manner, combining several elements of the built environment. Finally, it is strongly believed that model development must be fully supported by high-quality, well-documented and tailor-made experiments. This can only be achieved by promoting the collaboration between experimentalists and modellers at the planning stages of experimental campaigns. The set-up of open databases and a dedicated ‘task force’ group would be a useful means to address this issue.

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Appendix: Questionnaire to the participants

Questions about the participants

1) Which of the following is your main occupation?:

- PhD student 20/44
- Course work Bachelor / Master student 4/44
- Researcher 8/44
- Fire and emergency services 2/44
- Academic (research and teaching) 6/44
- Industry professional (fire safety engineer) 4/44

2) From what part of the world are you joining us today?

- Europe 29/44
- North America 6/44
- Oceania 6/44
- Asia 3/44

3) What is the main motivation for you to join this workshop?

- I want to learn more about fires in general 12/43
- I want to learn more about the pressing research question for compartment fires 23/43
- I want to criticize (constructively) specific methodologies for modelling compartment fires 1/43
- I had nothing else to do today and I heard Tarek, Jason, Hughes and Talal are nice peeps 1/43

- I am an expert in compartment fires and would like to steer key research priorities 6/43

4) Have you been actively involved in experiments (the user can have multiple choices)?:

- For model validation 32/56
- For model development 7/56
- To study a 'poorly understood' physical phenomenon 13/56
- To demonstrate specific physical phenomena 2/56
- None of the above 2/56

Design of experiments

5) What is most often lacking in the design of experiments (the user must choose 1 answer)?:

- A variety in the type of measurements (flow field, temperature, heat fluxes...) 6/15
- The density (number) of measurements 1/15
- Control on data uncertainty 8/15

Modelling

6) According to you, what is the priority level of advanced PDF-based combustion models for practical engineering calculations (the user must choose 1 answer)?:

- very high 2/48
- high 11/48
- medium 12/48
- low 3/48
- very low 7/48
- I don't know 13 /48

7) According to you, what is the priority level of the spectral treatment of radiation for practical engineering calculations (the user must choose 1 answer)?:

- very high 2/49
- high 15/49
- medium 12/49
- low 7/49
- very low 4/49
- I don't know 9/49

8) When determining the performance of structural elements under fire conditions for large, open-plan compartments, what approach do you consider more adequate for establishing heat exposure?:

- I don't know 14/49
- CFD modelling (e.g., FDS) 12/49
- Localized fire (e.g., Hasemi's model or Alpert's model) 4/49
- Parametric time-temperature curves 6/49
- Zone modelling (e.g., OZone, CFAST, BRANZ, etc.) 6/49
- Compartment Fire Framework (Thomas, Heselden, Law) 4/49
- Standard time-temperature curves 2/49
- Travelling Fire Methodology (e.g., TFM, iTFM, ETFM) 1/49

Applications, challenges and research needs

9) From a fire safety engineering practice point of view, what type of application do you consider more challenging?

- Modelling fire growth in large, open plan compartments with no combustable linings / structures 18/46
- Modelling under-ventilated compartment fires 9/46
- Modelling fire growth in quasi-cubic (small) compartments with combustable linings / structures 17/46
- Modelling air-tight compartments 2/46

10) From a fire safety engineering practice point of view, what is urgently missing to provide further confidence in modelling compartment fires for the design process?

- More large-scale data 5/25
- More fundamental research into unresolved physical phenomena 7/25
- More practical research translating fundamental research into simplified engineering tools 5/25
- More industry training regarding limitations and capabilities in modelling compartment fires 4/25
- More up to date fire engineering guidelines 2/25
- Benchmarking different approaches to model compartment fires 2/25

Feedback

11) Feedback score about the workshop:

- 5 (it was great) 27/51
- 4 (it was good) 20/51
- 3 (it was OK) 4/51
- 2 0/51
- 1 0/51

12) From 1 to 5, how much new you learnt about compartment fires in the workshop?

- 5 (I was illuminated by knowledge in this workshop) 9/50
- 4 (I learnt new interesting ideas and concepts) 19/50
- 3 (I learnt some new concepts I was not aware of) 18/50
- 2 (I learnt minor aspects I was not aware of) 3/50
- 1 (I learnt nothing new) 1/50