

Comments on Simulating Big Post-flashover Room Fires Using Computational Fluid Dynamics

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Abstract

Computational Fluid Dynamics (CFD) fire modelling has been used in fire hazard assessment over 50 years. However, most of the CFD models are not properly validated by large-scale fire tests due to high cost and other environmental difficulties. There were many criticisms on having many adjustable parameters and they will be discussed in this article. Application of CFD in fire modelling should be watched with problems rarely discussed in the literature. Improper uses gave wrong predictions and full-scale burning tests are needed to justify the results. Further, using CFD in big fire investigation has to be very careful with support by appropriate burning tests. There is a long way to go in applying CFD to simulate big room fires.

1. Introduction

Computational Fluid Dynamics (CFD) (or known as Numerical Heat Transfer and Fluid Flow before) has been used [1-5] in fire modelling over the past 50 years. The fire model was used in smoke extraction design and fire hazard assessment in performance-based design (PBD) or Fire Engineering Approach (FEA) in many places [6-8] in the Asia-Oceania region. There were numerous problems from day one because there are many adjustable parameters. Reporting long Available Safe Egress Time (ASET) [9,10] based on CFD predictions without considering smoke toxicity is a good example, giving higher responsibility to safety management staff afterward. Previous approved projects with fire safety provisions deduced from PBD-FEA using CFD results must be reviewed for checking the building use matching with assumptions made in those hazard assessment report. Fire safety provisions have to be upgraded if necessary. Installing additional sprinkler in surveyed airport terminals is a good example. Fire safety management [11] must be inspected at the very least. Recent increase in penalty [12] on safety to HK\$10 million is a good move.

Most of the CFD models are not validated systematically at the moment. Very limited developing works were reported and they were done almost 20 years ago. The reason is high cost and other difficulties such as environmental pollution in conducting large-scale fire tests. The free CFD software Fire Dynamics Simulator FDS [13] is a common design tool on smoke management system. PBD-FEA reports through CFD are always criticized. In Hong Kong, hot smoke tests are required [14,15] in halls of irregular shape or buildings taller than 12 m in order to evaluate the performance of smoke exhaust systems. In fact, many government parties would not consider PBD-FEA if there is no new architecture.

The accuracy of CFD predictions depends on three groups of parameters in physical models [1,16]; numerical parameters such as convergence criteria; and parameters in the simulation including the boundary condition.

Without such clear justification on using CFD in PBD-FEA, it is difficult to be approved by the Authority who has to take safety responsibility. Penalty was very low punishment on violating codes before, but much higher now. That explains why PBD-FEA is avoided in many new projects without innovative architectures. The recent increase of safety punishment to HK\$ 10 million [12] might alert the top management to care more on investing safety. The safety culture [11,18,19] on mainland might be a good practice. Detaining all senior staff managing a hospital in the recent big fire at Beijing [20] should be a good lesson to learn. They must keep appropriate safety management reports, at least, to demonstrate that they are

handling safety seriously. In recent incidents of collapse of concrete [21-23], the government starts to arrest owner and chairman of building's owners' corporation of safety failure.

2. General Concerns

Three-dimensionality and the instability of the flow fields should be included in simulating three-dimensional unstable turbulent flow. Very little validation works had been done, with some good and bad examples reported in the literature [24-28]. Ability of CFD to resolve the flow in the turbulent fire plume only is in doubt. Uncertainty in the ability of CFD to resolve the turbulent exchange flow across the opening is another concern as reported before [5,28].

The common challenges are:

- Air pressure and turbulence parameters are seldom presented, and only the velocity vector patterns and temperature distribution are shown.
- Stability criteria should be monitored [17,29] and reported properly. Grid size
- Grid sensitivity criteria [17,29] are only deduced from temperature and velocity predictions, but not pressure or turbulence parameters.
- There is no justification on fire phenomena by scale-models or full-scale burning tests.

Perhaps CFD is reliable for practical smoke control design only after addressing these concerns. Application of CFD to simulate big room fire storing high amount of combustibles should be careful. Full-scale burning tests on typical scenarios with similar conditions are still necessary for justifying the CFD predictions.

Boundary conditions including bi-directional flow on windows and doors in a building should be specified properly. Extending the computing domain outside was proposed by Galea and associates [30]. There were other examples in using such suggestion [5,31,32].

3. Using CFD in Simulating Big Room Fire

There are general concerns on applying CFD for simulating even small fires in big rooms. A question asked:

How to handle big building fires [3,28]?

There had been CFD simulations of fire in the literature.

CFD investigation of inclined ceiling jets was made to validate the FireFOAM code [33-35] before application in large-scale, rack-storage fire driven sprinkler activation simulations. The study provides a detailed analysis of temperature and velocity characteristics from the simulation results [35]. Predictions were compared against experimental data from the literature for unconfined, smooth ceilings.

FireFOAM is an unsteady solver for buoyancy driven turbulent reacting flows based on a C++ code that employs the Open-FOAM platform [33,34]. The FireFOAM code solves the Navier–Stokes equations using a Favre-filtered fully compressible flow formulation. In addition, transport equations are considered for species mass fractions and sensible enthalpy as in [36]. The diffusivity of different species is assumed to be equal and computed using Pressure-Implicit Split-Operator (PISO) based algorithm [37,38]. The default sub-model for pyrolysis in FireFOAM 2.2.x [33,34] is applied, which is only by a single-step decomposition model.

As reviewed by Ren et al. 2017 [39] was reported on the solid phase pyrolysis. Chaos et al. [40,41] studied fire properties of corrugated cardboard and wood using data from Fire Propagation Apparatus with bench-scale tests [42]. Results on such studies would be difficult to handle for big ministorage fire.

The workshop on Measurement and Computation of Fire Phenomena was held in 2017 [43]. Discrepancies between experimental data and computational results might be attributed to modeling errors. Measurements and modeling of pyrolysis phenomena are very complicated and depend on thermal radiation [44-49].

As reported by Zeinali et al. [50], distribution of mass density through the thickness of medium density fiberboard panels is known to be non-uniform. Material property on flame spread simulations of Single Burning Item corner fire tests. Simulations are performed using FireFOAM 2.2.x [33,34], considering both uniform and non-uniform material density profiles, using model- effective material properties determined from bench-scale fire propagation apparatus.

Applying CFD in fire protection engineering applications, even the flame-to-wall heat fluxes (convection and radiation), which couple the gas-phase combustion with the solid-phase pyrolysis was not estimated properly [51]. For fully developed large-scale fires, radiative heat transfer is a key [52]. Only at the fire development and suppression stages, the fire size is small (at 1 MW), and convection is comparable to radiation. There were challenges as expected. A wall model for convective heat transfer has been developed for under-resolved

engineering applications. Good agreement was found with the measurements at early stage, but again, not fully-developed fire.

There is also another CFD package developed [52-56]. CFD-based pyrolysis studies were discussed [52]. Reaction kinetics suggested to go through molecular dynamics simulation. Non-premixed mixture fraction combustion model was applied to study fire whirls [53] through reaction at flame sheet only. Such approach cannot simulate big fires where flame sheets were difficult to define and simulate. There is still a long way to go before CFD can be used to study complicated combustion involving many types of combustibles in high quantity.

The fire scenario of wooden village buildings in Hunan was investigated by Zhang et. al [57] using CFD based simulation. Temperature, smoke spread, CO concentration and visibility were predicted. The fire was simulated by using a 0.5 m fire source. The boundary conditions were set to match the external environment, with an ambient temperature of 20 °C. The fire simulation time was 1200 s. Fixed and movable fire loads were considered. Fixed fire loads were used for each room including the timber structure, whereas movable fire loads were employed for all the furniture. The doors and windows of the residential houses were kept open throughout the experiment. Wood was modelled separately from furniture. A single-step mixing controlled combustion method was adopted for the simulation. By default, the reaction of fuel and oxygen is infinitely fast and controlled only by mixing. It was claimed that the method can be used to assist fire investigation. However, combustion of wood is complicated as reviewed before [58-65].

4. Importance in Simulating Combustion in Big Room Fires

A big ministorage fire lasting for 108 hours occurred on 21 June 2016 in Hong Kong, which killed two firefighters. Several aspects of this big fire has been reported [29].

Fire investigation should be supported by full-scale burning tests in the fire investigation report, not just by CFD because of storing so much combustibles in limited space. Free CFD software is commonly used and there is no guarantee that the software is appropriate for simulating such big room fires. Problems identified in the application of CFD are well-known. Combustion of burning the stored materials has to be included.

Even burning Poly(methyl methacrylate) (PMMA) with simple kinetics of thermal decomposition [66], there are three stages in the combustion process:

- PMMA decomposes to produce monomer methylmethacrylate (MMA);

- monomer MMA decomposes to generate small gaseous molecules; and
- these small molecules undergo combustion.

Intermediate chemical reactions are very complex with 7 group reactions:

- thermal decomposition;
- thermal oxidative decomposition;
- decomposition of monomer MMA;
- methane combustion;
- methanol combustion;
- formaldehyde combustion; and
- acetylene combustion.

There are thousands of reactions to model. For example, 26 species and 77 elementary reactions in methane combustion. The reaction mechanism of acetylene has 103 elementary reactions and 38 species. As combustion chemistry is too complicated to be included and the CFD studies in PBD-FEA projects are basically on simulating turbulent flow for estimating the possible flow concept of ASET. The fire source is taken as a heat source with specified thermal power [67].

Storage fire is a combustion system [68,69] with many physical and chemical processes. Thermal feedback from the fire to the fuel surface gasifies more fuel vapors to burn in the flame for sustaining the combustion process. Room fires are even more complicated than those fires burning in open air because the heat and smoke generated will be trapped by the walls and ceiling.

Thermal radiative feedback from the enclosure had been identified to be a significant factor in determining the fuel gasification rate. It is the primary cause of instability in growing to a big fire. But the gas temperature next to the ceiling at the onset of instability varies from 450 to 798°C in most cases. There might be some other phenomena, say mixing of the gasified fuel vapors to appropriate ratios.

Further, combustibles with different ignition temperatures were observed to be ignited at roughly the same time under some enclosure fires. The downward thermal radiative heat flux might not increase so fast to ignite combustibles of significantly different ignition temperatures together, though the heat flux itself is increasing rapidly.

In addition to thermal instability of the combustibles due to thermal radiation from the ceiling and the layer, ‘bridge-mixing’ of fuel vapors due to fire-induced indoor aerodynamics might be another possible reason why different combustibles can be ignited simultaneously.

5. Bridge-Mixing

‘Bridge-mixing’ of igniting fuel vapors gasified from different combustibles by thermal radiation during flashover was observed [68]. Combustible items of different ignition temperatures ignited under some mixing conditions. Mixing of gasified fuel vapors by the fire-induced airflow in rooms of different geometry is a key factor in igniting each combustible item. This releases more heat and generates flames to give conditions satisfying the flashover criteria.

The ‘bridge-mixing’ concept is verified by preliminary simultaneous cone calorimetry on different polymer materials with and without mixing of their decomposed products.

The “bridge-mixing” concept [68,69] was proposed on igniting combustibles of different ignition temperatures at the same time in a room fire to give flashover and subsequent burning. The gasified fuel vapors liberated from fuels might mix thoroughly to give a “premixed state” inside the enclosure as in Fig. 1. That depends on whether the airflow induced by the fire could enhance mixing of the fuel vapors from different combustibles. On igniting the gasified fuel mixture to form a flame above the combustibles, thermal feedback might be strong enough to ignite the materials underneath. All solid combustibles are ignited at the same time. The room is suddenly full of flame, which spreads out from all openings, being an indicator of flashover [70-74]. The bridge-mixing concept was verified earlier by bench-scale tests with a cone calorimeter under pilot ignition [68,69].

Based on cone bench-scale tests [68,69] as in Fig. 1 on varying the separation distance of the two plastic cubes, the proposed ‘bridge-mixing’ concept can explain why almost all combustibles were ignited simultaneously during flashover as observed for some scenarios. This should be applied to study combustion process in room fires storing huge amount combustibles as in minisorage areas but with inadequate air due to limited ventilation. In particular, there are hundreds of intermediate chemical reactions, with some key reactions involving short-lived intermediate chemical radicals generating huge heat and stable toxic products such as carbon monoxide.

Putting in firefighting water will suppress many intermediate chemical reactions and give much more toxic gases. Operating positive ventilators would drive in more air to make the

situation much more complicated. Hot fuel gases would be burnt to give out more heat and additional smoke. Cool fuel gas due to water application would mix with the air driven in. The firefighting time can never be safe as surveyed years ago before [75]. That is why the firefighters have to be equipped with personal protective equipment (PPV) which the author has evaluated those portable breathing apparatus in 2007. This supported the Allowed Firefighting Time (AFFT) (Might use Allowed Rescue Time ART [29]) around 30 minutes total, in sending Compartment Fire Attack CFA task force to dangerous fire sites. This is entirely different from the Available Safe Egress Time ASET fire science approach in fire safety management of normal occupants without PPE, but no having mobility difficulties. However, doing this kind of full-scale burning tests requires resources. Those experiments in 2007 spent over HK\$0.8 million (US\$0.1 million) illegal diesel contributed by the Customs Department. Only a small room was burnt, not a ministorage area!

6. Evaluation of CFD Predictions

CFD predictions should be evaluated properly [76]. Longer-term research on the three groups of parameters in the CFD models should be carried out to develop the model, but it would take a long time [77-81].

At the moment, it is only good for designing smoke extraction system. Even so, officers should justify CFD simulations in PBD-FEA project submission, at least on:

- The convergence and stability criteria, turbulent parameters.
- Free boundaries.
- Presentation of predicted pressure and turbulent parameters.
- Comparing with experimental data from several scenarios (out of many up to hundreds of scenarios studied in hazard assessment) full-scale burning tests.
- In-situ field tests to evaluate the system performance on agreed scenario up to 2 MW design fire with hot smoke tests in hall.

It is unknown yet on what to evaluate more in simulating ministorage fires by CFD involving combustion chemistry. However, the above are required as minimum.

7. PPV Operation Simulation

Positive pressure ventilation (PPV) was employed in the firefighting with criticisms [32] that operating PPV led to a more hazardous fire environment rather than improving the visibility or reducing the temperature inside.

Firstly, different views on operating PPV for firefighting and rescue were summarized [32]. Ventilation arrangements including the locations of PPV and exhaust openings in a room should be carefully investigated for better understanding the efficiency of PPV in firefighting.

Secondly, action of operating PPV in a room fire studied by physical scale modelling had been discussed [32]. Temperature changes and fire spread patterns were captured. It is found that the presence of an opposite vent resulted in fire of smaller size and shorter duration.

The CFD study is much more complicated with PPV and easy to be challenged [28,32].

Experts in computer simulation are always joking:

Garbage in, garbage out.

8. Conclusion

Application of CFD in fire modelling should be watched with problems discussed by users but not reported thoroughly in the literature. More experimental works should be done to justify the predictions.

Cutting research funding in the past 30 years limited the development of CFD. Trained fire researchers are working as PBD-FEA engineers to get higher pay.

No doubt, using CFD in fire investigation report has to be very careful and predictions must be supported by appropriate burning tests. Further, some FEA engineers used few fire tests with CFD results to argue code specification. Joking that only HK\$3 million FEA consultancy fee can waive HK\$1 billion fire service installations.

But questions come:

What are the fire scenarios and their consequences?

Who is the Authority to shoulder the responsibility?

What is the cost of Fire Safety Management to keep the designed scenario following FEA report?

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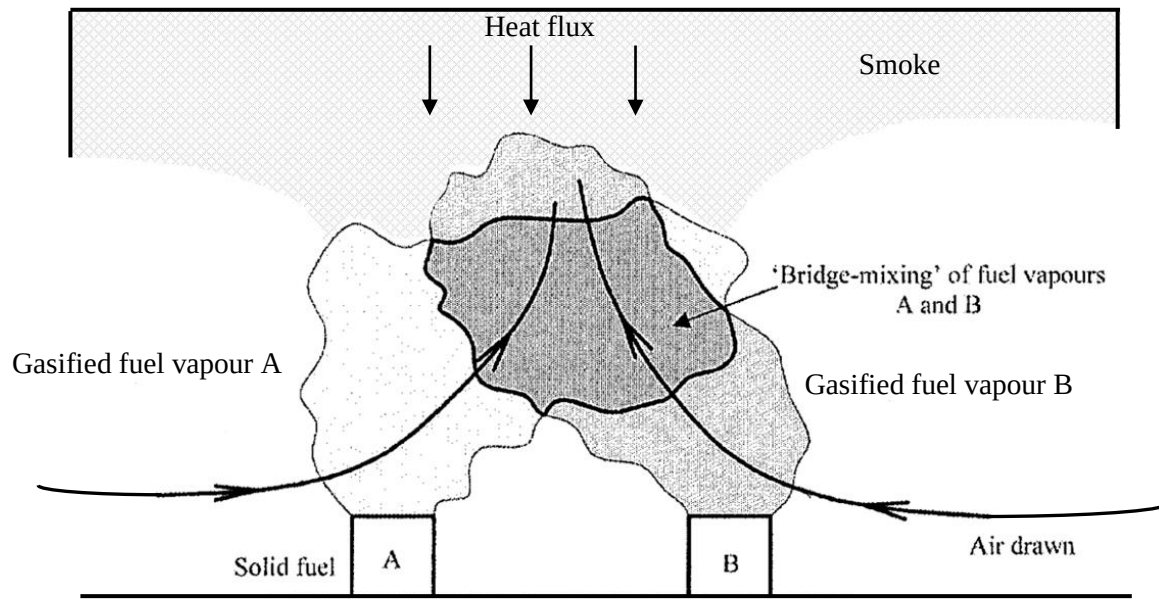
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From Chow & Han (2006)

Fig. 1: Bridge-mixing