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Review

Computational Fluid Dynamics of Compartment Fires: A Review of Methods and Applications

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Abstract: Compartment fires, such as those occurring in buildings and confined spaces, impose modeling challenges due to the complexity of turbulent flows, combustion, and radiative heat transfer. Computational Fluid Dynamics (CFD) has become a vital tool for understanding and predicting fire dynamics in such situations. This review provides an analysis of different available methods and sub-models on the CFD tools which have been applied to compartment fires in the literature, examining current turbulence, combustion, and radiation approaches. Additionally, it identifies challenges and deficiencies in modeling such as combustion, radiation modeling, flame extinction, and ventilation impacts, discussing the balance between accuracy and computational cost. The review also highlights aspects of different sub-models and provides the reader with informative instruction in making the decisions for a more reliable CFD simulation of the compartment fire.

Keywords: compartment fire; CFD modeling; turbulence; combustion; radiation; extinction

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1. Introduction

A compartment fire is defined as a fire which occurs in a closed space or a room in which the fire behavior is mainly dependent on natural physical processes such as combustion, heat transfer, and fluid dynamics. The way they interact with the environment differs from open fires in terms of oxygen restriction, smoke containment, and energy release [1,2].

Computational Fluid Mechanics (CFD) modeling for a compartment fire is defined by the numerical simulation of fire behavior, smoke, heat, and gases within a confined space, such as a room or building. This type of modeling is essential in fire safety engineering for understanding fire dynamics, the real fire scenario, temporal evolution of temperature and other properties in the compartment, evaluating safety measures, and for designing effective fire protection systems [3]. It provides valuable insights into fire behavior and helps to improve fire safety design, which can result in decreasing risks in buildings. For example, from fire protection point of view, predicting the concentration of soot particles using CFD can provide visibility estimation for a person who is trapped in an enclosed space fire and is looking for an exit sign [4].

CFD has been conducted in fire safety science since 1980s [5]. Besides that, there have been always constant attempts to review and improve the CFD methods in fire modeling, starting with Cox in 1997 [6], who reviewed the fire dynamics study tools using the time-averaged approach for the random turbulent fluctuations caused by fluid flow [5], to Beji et al. [7] in 2024, who investigated the challenges in compartment fire modeling.

From a traditional point of view, a compartment fire in its natural mode (i.e., without suppression or control) includes five stages from the first point to the last: ignition, pre-development, flashover, fully developed, and decay [8,9]. However, according to the newer studies [10,11], when the total fuel and burning materials are consumed and HRR drops to zero (i.e., end of the decay phase), an additional stage called the cooling phase starts in which the compartment structure and product gases begin to cool down. This is particularly important when coupling CFD models with structural analysis, fire resistance design, and post-fire assessments. The cooling phase is not considered in fire dynamics as there is no fire, but its heat transfer mechanism, arising from residual heat stored in the compartment structure and product gases, should be accounted for.

A schematic diagram for the temporal evolution of heat release rate in different stages of a compartment fire is illustrated in Figure 1.

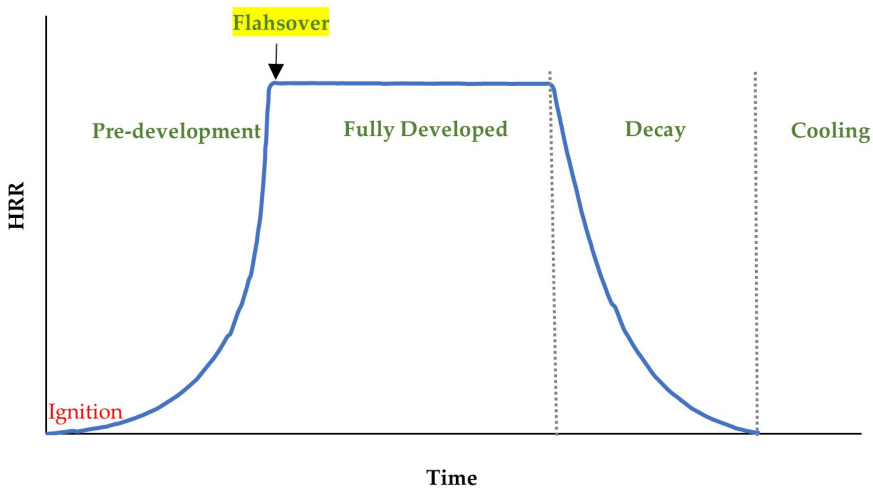

Figure 1. Schematic diagram of heat release rate in different stages. Adopted from Lucherini and Torero [11].

In order to exploit CFD methods in fire modeling, a variety of computer tools have been developed. Among them, FDS (Fire Dynamics Simulator) (developed by the National Institute of Standards and Technology—NIST) [12] based on the Fortan, OpenFOAM (Open Field Operation And Manipulation) (developed by OpenFOAM Foundation) based on the C++, and ISIS (CALIF ISIS-developed by IRSN (Institut de Radioprotection et de Sûreté Nucléaire: Institute for Radiological Protection and Nuclear Safety)) [13] are the tools which are widely used in the numerical simulation of compartment fires. In addition, a specific fire model based on code developed by FM Global [14], called FireFOAM, is used to tackle fire dynamics and combustion modeling.

CFD tools provide an environment to simulate fluid flow and related physical processes (e.g., heat transfer, combustion, etc.) through virtual models, allowing for detailed analysis and predictions without the need for physical experiments. Aside from the required level of expertise to use them, these tools are like machines that need fuel to operate. The initial inputs prepared by the user are considered the fuel. Inputs may include the dimensions, ignition and fire source, fuel type, thermomechanical properties of the materials and boundaries such as compartment walls, duration of the simulation in question, etc.

According to ASTM E 1355 (Standard Guide for Evaluating the Predictive Capability of Deterministic Fire Models) [15] and as cited by [16], fire simulation and modeling can be divided into three categories: blind (priori), specified, and open (posteriori). The difference between these methods is the approach the user takes, the purpose of simulation, and finally, the available data and information, i.e., the required input for the CFD tool. In terms of terminology, blind simulation can be applied to the situation when the user has only limited knowledge of the fire scenario, without any details about geometry, material properties, fire growth, etc. In case of blind simulation, all inputs must be prepared by the user based on the personal impression, and as a result, this scenario can only represent a forecast from the fire behavior. Specified simulation has a different trait, where all required inputs and more details are provided to the user. The most detailed and complete group of simulations is called open. In addition to specified simulation indices, experimental measurements criterion from the first two categories are available in open simulation.

In the specified or open simulation, the inputs to be used in the CFD tool are provided for the user. But how does it work in case of fire simulation? For instance, using measured data in the experiment as the input for the simulation: the mass loss rate (MLR) or heat release rate (HRR) is defined on an obstruction or vent that defines the fire, representing a burner with a controlled amount of fuel [12]. On the other hand, when the fire description is not available, required inputs of the CFD simulation tools (e.g., thermochemical properties of the fuel, thermomechanical properties of the surfaces, etc.) are chosen based on references such as handbooks and standards; blind simulation is conducted. There are some cases in which the modeling is not fully specified/open or blind and is the combination of both modes, i.e., is defined as semi-blind. In other words, when some parameters like geometry details and material properties are specified and known, while other experimental measurements such as MLR or HRR are not. This can result in an output which is not in good agreement with real conditions [17]. In such cases, the predictive ability of the tools comes in handy to predict the HRR (or MLR) using the fuel properties. In such simulations, heat feedback from the flame to the fuel surface determines the burning rate of the fuel [12,18]. According to McGrattan and Floyd [19], when there is no available experimental data for HRR or MLR, the thermal and kinetic properties of the fuel should be specified in the case of simulating free-burning in FDS.

While using CFD tools and methods for simulating fire dynamics such as in a compartment fire, the credibility and reliability of the configured models must be assessed, and it should be determined whether the simulation outputs are authentic. This issue can identify the possible discrepancies between the CFD model and the corresponding real-world scenario and is defined as model validation which will be discussed in following section.

2. Validation in CFD Simulation

A physical aspect and the process of comparing the results from a CFD simulation with experimental measurements and considering the ability of the model ability to behave as in factual circumstances is defined as validation [15,16]. An assessment should be made regarding to what extent the mathematical model accurately predicts the relevant physical facts [16]. The noticeable fact is that validation is assigned to the outputs and results of the simulation using a model for a specific case, according to Roache [20,21] and as cited by Oberkampf and Trucano [22]. Therefore, it cannot be generalized to a CFD tool or code [22].

The Society of Modeling and Simulation (SCS) presented a definition for model validation, confirming that a computer model (e.g., a CFD simulation) demonstrates an adequate level of accuracy aligned with the intended purpose of the model in its own scope of application [23]. Figure 2 shows how a physical incident can be replicated into a model using simulation. Moreover, validation works as a two-way connection between model and reality. While using a simulation, validation can be carried out by comparing it to the real-world scenario, ensuring the credibility of the simulation and model.

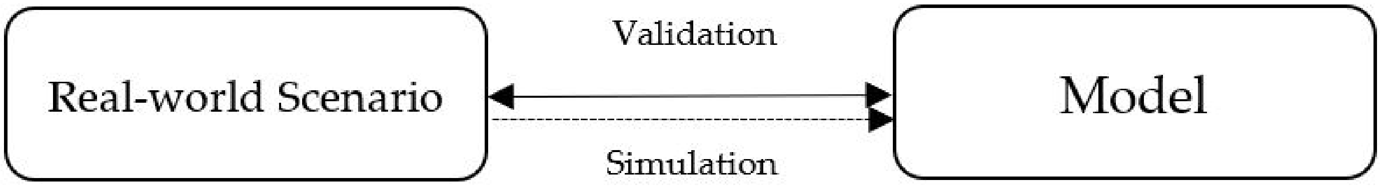

Figure 2. Schematic view of the interaction between the simulation, model, and validation. Adopted from SCS technical report [23].

Currently one of the main concerns in the field of fire modeling using CFD is how far CFD models have been developed to predict and present reliable fire characteristics in a compartment close to real scenario? To answer this question, existing methods available in CFD simulation tools and utilized by various researchers, should be reviewed and their reliability be evaluated. An appropriate fire-based CFD simulation is the result of utilizing adequate sub-models and boundary/initial conditions, not just the CFD code used. The accuracy of the sub-models, as well as the user's skills, determine the success of a CFD simulation [5]. It should be noted that the CFD models can be trusted through validation with experiments. Despite recent development, the reliability of CFD remains limited [2]. In addition, validation of the numerical models is just one side of the broader issue concerning their application and validity. The other key factor is ensuring the appropriateness of user-defined inputs and the correct configuration of the model setup.

3. CFD Simulation in Compartment Fires

As shown in Figure 1, a fire in enclosed spaces contains several stages with different properties. Therefore, it is necessary to simulate all the stages from start to end, while using CFD simulation.

Shen et al. [2] reviewed the CFD modeling used in process safety including compartment fires, jet fires, pool fires, gas diffusion, explosions, etc. Besides that, they also referred to the idea that CFD simulations should be validated only based on the available experimental data. This point, which is mentioned earlier by the authors in the introduction (blind simulation) when there is no experimental measurement available, presents an obstacle in the way of CFD applications. However, CFD simulation is still an accurate and reliable tool to predict the overall behavior of the fire and possible risks, even though it is not validated.

Merci et al. [24] presented the critical role of HRR in CFD simulations of fires in enclosed compartments and outlined the complexities and limitations of current modeling approaches. They proposed that coupling combustion models with radiation models and accounting for extinction and re-ignition behavior in CFD is important for accurately predicting HRR. It was found that accurate prediction of transient phenomena in fires, such as oscillations in pressure and temperature due to variation in HRR, is one of the key challenges. Furthermore, determining HRR becomes complicated by feedback loops involving flame heat transfer, fuel pyrolysis, and compartment boundaries in solid and liquid fuels.

As mentioned earlier, this research is mainly considered as an overview of CFD modeling, and the existing methods used for the case of compartment fires. There have already been some reviews [2,5,7] of the research and methodologies and some challenges in the current path have been presented. While looking for reliable resources, two main categories were highlighted: (1) investigation of different sub-models and the comparison between them and (2) sensitivity analysis. Sensitivity analysis in fire modeling is defined as the influence of the input parameters on the simulation results in CFD tools.

S. Suard et al. [25] conducted a sensitivity analysis for a compartment fire using ISIS. They studied the influence of some input factors on the simulation results. It was shown that the turbulence model constant as well as combustion parameters (e.g., efficiency) had the most impact on simulation outputs (e.g., gas temperature), while the soot absorption coefficient, constant parameters in combustion modeling, and Prandtl number have a low impact on outputs. This can be useful in CFD simulations where no detailed information is provided and some variables must be assumed.

J. Lee et al. [17] investigated compartment with liquid pool fire (dodecane) numerically and compared the semi-blind and open simulation for HRR and ventilation. Pyrolysis and fan curve were used in semi-blind simulation, while the experimental measurements for HRR and ventilation were used in the open simulation. Their results showed that a pyrolysis model in a blind simulation predicts a higher peak value and earlier fire extinction time than experimental data, as shown in Figure 3. There was no significant difference between different methods of ventilation modeling.

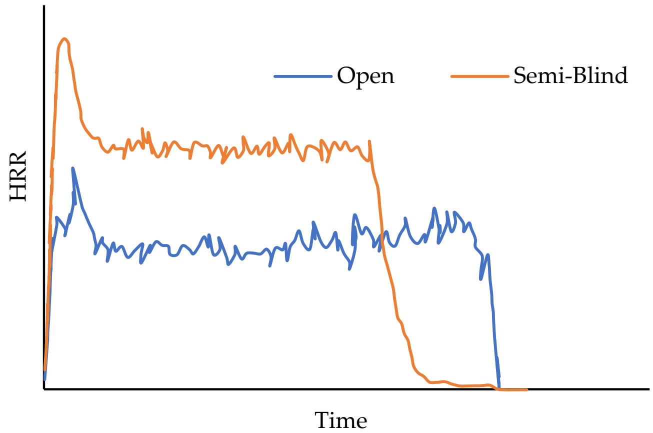

Figure 3. Comparison of HRR prediction over time using different methods: open (experimental measurement of HRR as input-prescribed) and semi-blind (pyrolysis model-predictive method). Adopted from J. Lee et al. [17].

One of the recent reviews on fire modeling by CFD has been conducted by Jennifer X. Wen [5]. She reviewed the achievements in sub-models including combustion, heat transfer, and pyrolysis, while presenting two relevant challenges which modelers and researchers may encounter: (1) upscaling the fire simulation without the need to simplify the sub-models and expanding mesh grid sizes, compared to simulations in smaller scale, and (2) the unavailability of reliable experimental data to validate the CFD simulations.

A numerical simulation of the compartment fire using existing software and tools includes consecutive stages. First, the user needs to specify the geometry and boundaries (simulation domain). At this stage, the mesh grids numbers and sizes are determined. Then, the constraints and behaviors at the boundaries of the system or simulation domain are defined (i.e., boundary conditions). As the next step, proper physical sub-models such as combustion, turbulence, etc., which are needed to simulate the problem are chosen. Numerical simulation of the compartment fires must include the reliable modeling of turbulence, combustion, extinction, pyrolysis, and heat transfer in the gas phase and through solid boundaries [7,26]. Finally, when the simulation is finished, the user should calibrate the CFD results using available experimental measurement data (i.e., validation). Figure 4 shows a flowchart of the pathway for the CFD simulation of a compartment fire.

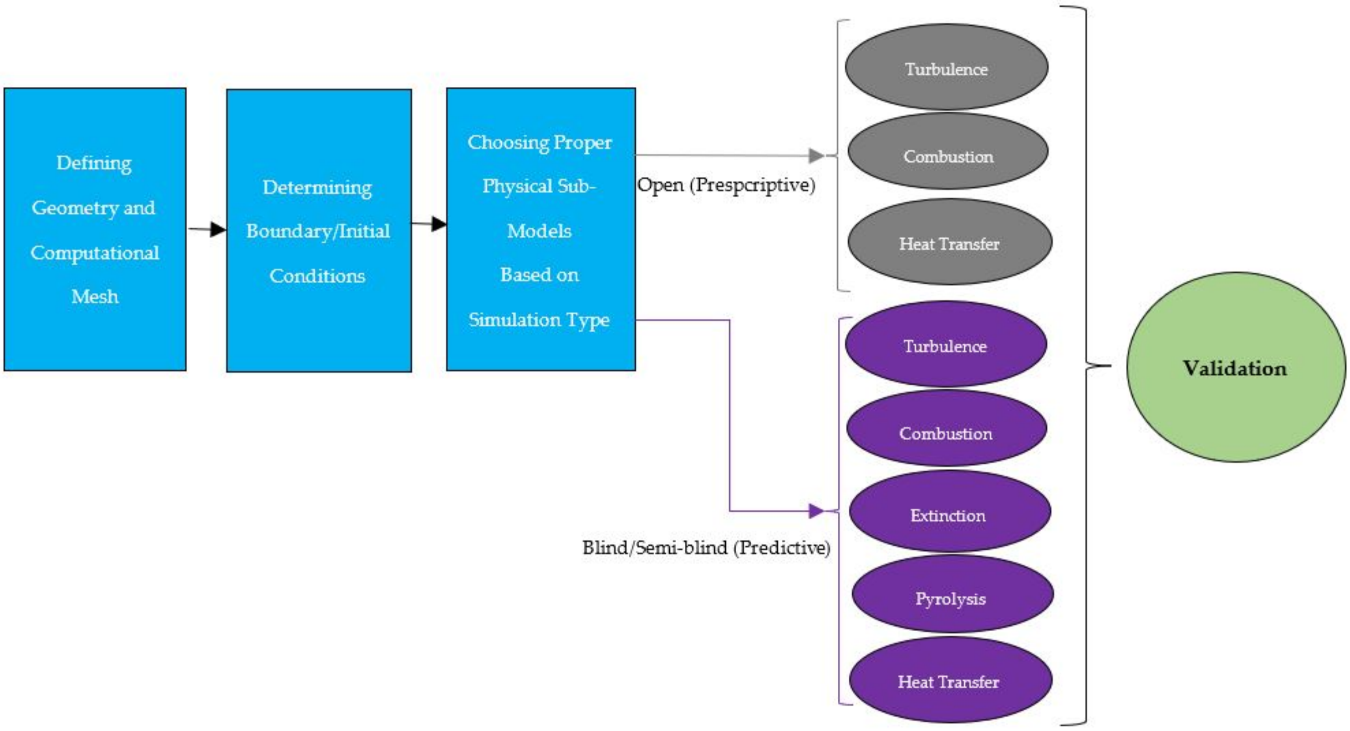

Figure 4. Required steps for CFD simulation of compartment fire.

As illustrated in Figure 4, choosing the required physical sub-models varies based on simulation type: in the case of open simulation, there is no need to model extinction or pyrolysis as they automatically adjust based on the initial inputs (e.g., HRR or MLR).

The methods, sub-models, applications, and some modifications implemented by different researchers, particularly in the case of compartment fires and similar scenarios, will be presented in the following sections.

3.1. Computational Mesh

CFD models divide the room volume into thousands of small cubicles or control volumes. Differential equations are solved for each control volume in space and time, resulting in point-to-point fluctuation in the characterizing variables [27,28]. Therefore, numerical simulation of compartment fires requires discretizing the computational domain into a grid or mesh, where governing equations of fluid dynamics, heat transfer, and combustion are solved numerically. FDS adopts rectilinear volumes (cubic meshes) and uniform meshing [12], while OpenFOAM and ISIS can utilize cubic and unstructured grids such as tetrahedral, polyhedral, and hybrid meshes [29].

Wang et al. [30] studied the effects of extending computational domain on numerical simulation. It was found that the extended domains created more similar results to the real fire scenario. Therefore, in compartments with an opening in the boundary walls, the computation domain should be extended beyond the physical or geometric boundary.

He et al. [31] investigated the effects of extending computational domain and grid size on the numerical simulation of propane fires in an enclosed compartment. Their results indicated that the simulation being limited only to the compartment boundaries influenced the ventilation effect and as a result, affected the predicted HRR. They recommended that the numerical domain should be extended more than half the hydraulic diameter of the door for a fuel-controlled fire, and the full hydraulic diameter for a ventilation-controlled fire.

In a compartment with a vertical opening, the domain should be extended in the perpendicular direction of the opening and in relation to the heat release rate of the fire and the hydraulic diameter of the opening, according to Zhang et al. [32]. In other words, the greater the heat release rate of the fire, the more extended the domain should be.

While [31] and [32] proposed Equation (1) for the domain extension, Lu et al. [33] modified it to cover the HRR dependency on the transition phase between over-ventilated and under-ventilated fire. The optimized value of the domain extension was recommended as Equation (2):

$$Domain\ Extension = \begin{cases} 0.5 \times D_H, & Fuel\ Controlled \\ D_H, & Ventilation\ Controlled \end{cases} \quad (1)$$

$$Domain\ Extension = \begin{cases} 0.6 \times D_H, & 0 < \alpha \leq 0.5 \\ D_H, & \alpha > 0.5 \end{cases} \quad (2)$$

where D_H is the hydraulic diameter of the door and α is the room aspect ratio.

The mesh grid independency check is one of the essential tasks which should be performed in the numerical modeling in order to optimize the simulation time [17]. Quintiere [34] was among the first to use explicit concept of the characteristic fire diameter in compartment fire modeling and described it as Equation (3):

$$D^* = \left(\frac{\dot{Q}}{\rho_\infty c_p T_\infty \sqrt{g}} \right)^{2/5} \quad (3)$$

where $\dot{Q}$ is the maximum heat release rate, g is gravity, and ρ_∞, c_p, and T_∞ are the density, specific heat, and temperature of the ambient air, respectively. The ratio of characteristic fire diameter to the grid size should be more than 10 for reliable results [35].

According to Hietaniemi et al. [36], quoted by Cai and Chow [37], in a numerical simulation of a pool fire, a minimum number of 20 cells are required in the pool diameter to obtain a good prediction of the experimental measurement. However, Maragkos and Merci [38] later recommended having at least 10 cells across the burner as a 'rule of thumb'.

Sahu et al. [39] studied the numerical simulation of pool fires in a compartment and found out that finer mesh grids adjacent to the fire source can improve the temperature predictability of the model.

3.2. Boundary Conditions

Boundary conditions in CFD are essential as they define the behavior of the fluid flow at the boundaries of the simulation domain, which can influence the heat and mass transfer between combustion gases and smoke, compartment walls and openings, and outer space in the case of a compartment fire. Generally, boundary conditions include the following categories:

- Thermal Boundary Conditions: Thermal boundary conditions directly influence heat losses to walls, floors, and ceilings, which in turn affect fire spread, flame temperature, and product gases. For example, a well-insulated boundary can trap heat, causing higher temperatures and more intense fire growth, while highly conductive boundaries may slow fire development by reducing available thermal energy. Accurate representation of these boundary conditions is therefore essential for capturing realistic compartment fire behavior.
- Material and Surface Properties: Material properties directly influence the boundary conditions in CFD simulations by affecting heat flux, temperature profiles, and the fire spread rate. For accurate fire modeling, these properties must be carefully selected and validated based on experimental data to replicate real-world conditions.

- Flow Boundary Conditions: Flow boundary conditions at inlets and outlets such as doors, windows, and vents are essential to define how air enters the compartment and how product gases exit. These boundaries control the oxygen supply, smoke evacuation, and pressure gradients within the compartment, all of which impact the fire dynamics and its growth.
- Burning Rate and Pyrolysis Boundary Conditions: Burning rate and pyrolysis boundary conditions describe how combustible materials are set up to burn, including parameters for pyrolysis and feedback mechanisms (e.g., temperature, and heat flux) affecting fuel release rates. This is critical for accurately modeling the growth phase of compartment fires.
- Initial Condition: Initial condition describes how the initial setup, like ambient temperatures and initial pressures, affects boundary conditions over time, influencing fire spread predictions.

The modelers must ensure they are using proper and reliable boundary conditions on all the surfaces which define the simulation area. For example, in the case of an open simulation of pool fires with available experimental data, measured MLR or HRR are prescribed as boundary conditions on the fire surface (e.g., pool fire) for the simulations [25]. In another example, ventilation or wind effect can be defined as boundary conditions on a wall, window, etc. [17]

A boundary condition can either be defined explicitly as a separate and direct input, such as a prescribed temperature, velocity, heat flux, etc., or in an implicit way where the boundary condition is applied as part of the overall solution of the equations. While each CFD code has its own way of specifying boundary conditions, the overall procedure is similar. Interested readers are encouraged to refer to CFD tools manual for further information about how boundary conditions are defined in different situations [12,40,41].

3.3. Physical Models

3.3.1. Turbulence Modeling

Turbulence in fire dynamics is generally described as unsteady, chaotic, complex, swirling, and disordered motion of the fluid which causes velocity and temperature to fluctuate rapidly [42,43]. This phenomenon is responsible for fire spread and flame shape in the compartment. While small or early-stage fires may initially exhibit laminar characteristics, as the fire grows in size and intensity, it quickly transitions into a turbulent regime due to increased flow velocities, buoyancy, and interactions with the enclosure walls and openings. As shown in Figure 1, compartment fires have two unsteady phases (i.e., from ignition to pre-development, and from decay to the cooling phase), one unsteady transition (flashover), and one steady phase (fully developed).

In terms of CFD, different schemes are applied to estimate and model the turbulent flows behavior, differing in reliability, accuracy, and computational cost: Reynolds-Averaged Navier–Stokes (RANS) [44], LES [45], Direct Numerical Simulation (DNS). A combination of these methods is used in some cases such as in Detached Eddy Simulation (DES) by Spalart et al. [46], and Very Large Eddy Simulation (VLES) by Speziale [47]. The difference between these methods is based on the way they handle turbulence and the range of turbulent scales they resolve. In other words, their resolutions to turbulence and its modeling are different. Resolution in turbulence modes shows the level of detail modeling for turbulence eddies in each method. It means that in DNS, the Navier–Stokes equations are solved without any turbulence modeling, and it captures all scales of turbulence. On the other hand, in LES, the larger turbulent eddies are resolved directly, while the smaller sub-grid scale (SGS) eddies are modeled. The Navier–Stokes equations are time-averaged, and turbulence is modeled using empirical or semi-empirical turbulence models (e.g., k-ε and k-ω models) in RANS. This can be further explained as follows:

- RANS sees the flow properties (e.g., velocity, pressure, etc.) as the composition of mean and fluctuating components and solves the Navier–Stokes equations in a time-averaged manner. As a result, turbulence is modeled using transport equations.
- LES resolves large turbulent eddies (which carry most of the turbulent energy) in the flow while modeling the smaller scales (turbulent eddies at the scales are smaller than the grid size, i.e., sub-grid scale). The method that is used to model sub-grid scale eddies will be presented in following section called sub-grid scale modeling.
- The DNS method resolves all scales of turbulence without any modeling, solving the Navier–Stokes equations directly and completely. It requires extremely fine computational grids and small time-steps to capture the whole range of turbulent scales.
- DES is based on benefiting from LES modeling while keeping the advantages of RANS mode where LES is computationally expensive. The main idea of DES is to use RANS adjacent to the surfaces (such as walls) to neglect the need for fine mesh resolution (as in LES) and switch to LES in other regions where larger scale eddies are present and resolving them is computationally feasible.
- VLES is a flexible approach in turbulence modeling and has been designed to cover a wide range of turbulence modeling modes. It adapts its operation based on the grid resolution and required turbulence details: VLES works in RANS mode and most of the turbulent motions are not resolved when the grid size is very coarse. Finer grids can move it to a transitional approach between RANS and LES and more of the turbulence spectrum is resolved. VLES becomes pure LES when the grids are finer than the previous mode. And finally, if the computational grids are fine enough to resolve all turbulent scales, VLES works as DNS. This was first introduced by Speziale [47] and improved by Han et al. [48,49].

In addition to the approaches mentioned, wall-modeled large-eddy simulation (WMLES) [50] is another strategy which uses an explicit separate wall model near the walls while the flow far from the walls is resolved using LES. Furthermore, simple very large eddy simulation (SVLES), available on FDS [12], is a more simplified version of VLES which is designed to handle coarser grids compared to VLES and relies on resolving the large-scale turbulent structure and modeling the smaller scales regarding to the coarser grids' size.

The computational cost and accuracy of each turbulence modeling approach in CFD depend on the resolution of turbulence scales and level of detail that need to be modeled or resolved. It indicates the time required to model the same reference problem and the validity of CFD modeling compared to a real scenario, respectively. Grid resolution is a relative criterion and is highly dependent on the considered geometry. For example, in a standard ISO 9705 compartment fire test, fine grid size can be in the range of 5 cm [51], while it can be coarse in another case with a lower HRR.

DNS and LES are capable of handling both steady and unsteady flow regimes, although the time-averaging process in RANS filters out the unsteady, fluctuating component of the flow. This means that RANS cannot directly capture transient or unsteady flow features. It is especially important in the case of a compartment fire (as is shown in Figures 1 and 3) that the compartment fire has a steady fluid flow and transition behavior between different stages. Therefore, RANS is not a perfect choice for the CFD modeling of a compartment fire.

Due to the required number of mesh grids and computational cost, there are turbulence ranges in which the models are more applicable: RANS can be used for high Reynolds number flows (e.g., $Re > 10^3$) because it does not require fine grids and is computationally efficient. LES is more appropriate to use in high Reynolds number flows where large-scale turbulence structures are dominant, but the computational cost increases with higher Reynolds numbers (e.g., $10^7 > Re > 10^4$). DNS is limited to very low Reynolds numbers (e.g., $Re < 10^4$), since an extremely fine grid is required for resolving all turbulent scales. DES behaves like LES and is more for high Reynolds flows (e.g., $Re > 10^5$) where both attached and separated flow regions exist. VLES can be applied across different Reynolds number ranges because it adapts to the local grid resolution, allowing for varying levels of turbulence modeling. According to Chow and Yin [52], quoted by Safarzadeh et al. [53], LES provides detailed turbulence effects and is more widely used in fire modeling compared to RANS. It should be noted that DNS needs very fine mesh grids as well as computing time, which make it more difficult and less possible, especially when it comes to larger scales. In a typical fire in an enclosed room, the Reynolds number is around 10^5, resulting in the 10^{13} required cells to simulate the fire and smoke movement [54]. This can eliminate or at least limit the DNS use in CFD modeling of compartment fires.

Therefore, it is better to focus on the application of LES or hybrid methods for CFD simulation of compartment fires (neglecting pure RANS because of unsteady nature of compartment fire and DNS because of high computational costs and detailed resolution).

A comparative analysis between different turbulence schemes in CFD is presented in Table 1, providing an overview of the advantages and disadvantages of a simulation of a compartment fire.

Table 1. Comparative analysis of different turbulence modes in CFD.

Method	Turbulence Approach	Turbulence Modeling	Grid Resolution Requirement	Pros	Cons
RANS	Models all turbulent scales	Uses transport equations for turbulence	Relatively coarse grids	Low computational cost	Unable to capture unsteady/transient flow such as in compartment fires
LES	Resolves the large eddies, models sub-grid scales	Sub-grid scale models	Finer than RANS, coarser than DNS	Captures transient and large-scale turbulent structures accurately	Requires a fine grid near walls (such as for compartment fires): increases computational cost
DNS	Resolves all turbulent scales	No model needed	Extremely fine grids	Most reliable method	Very high computational cost and resources
DES	RANS near walls and LES away from walls	A combination of RANS models and LES sub-grid models	Coarser near the walls and finer in other regions	Balanced computational cost and accuracy between RANS and LES	Accuracy depends on grid resolution and transition between RANS and LES (determining switching criteria between RANS and LES)
VLES	Based on grid resolution, wide spectrum from RANS to DNS	Adapts with grid resolution, either modeled in coarse grids or resolved in fine grids	From course to very fine, depends on the application	Adaptive approach, flexible for different case	May require local refinement strategies (e.g., adaptive mesh refinement).

Sub-Grid Scale (SGS) Modeling

As mentioned in the discussion regarding turbulence modeling, excluding RANS and DNS due to the limits, the LES approach (and other hybrid methods) tends to be more appropriate in the CFD simulation of a compartment fire. It resolves the large-scale turbulent structures directly while modeling the smaller sub-grid scale (SGS) structures that cannot be captured by the computational grid. The SGS models play an important role in LES by representing the effect of these unresolved scales on the resolved flow. Different SGS models have been developed to simulate this influence with different levels of complexity and accuracy and are used in CFD tools. Constant Smagorinsky, Deardorff, Dynamic Smagorinsky, WALE, Vreman, K equation, and Dynamic K equation are presented by different authors [45,55–60] and used by CFD tools based on their design. For example, Smagorinsky models dissipative processes that occur on length scales smaller than those resolved by the user-defined grid. One of the earliest and simplest SGS models used in LES which introduced the concept of SGS turbulent kinetic energy, was Deardorff. To overcome the Smagorinsky limits especially near the walls, Nicoud and Ducros [57] developed a new model called WALE (Wall-Adapting Local Eddy-Viscosity) which depends on both the strain rate and the rate of rotation of the velocity gradients, providing better wall-bounded flow behavior. Moreover, in dynamic Smagorinsky, the basic idea is that the model adjusts the turbulence viscosity coefficient based on local flow properties at each point in the domain, improving flexibility and accuracy, while it is a pre-defined fixed value (typically between 0.1 and 0.2) in Constant Smagorinsky [12]. Vreman [58] is a more recent SGS model, designed to improve the treatment of SGS in complex flows, especially where the assumption of isotropic turbulence may fail. Vreman can be considered a more efficient method than Dynamic Smagorinsky and more accurate than Constant Smagorinsky [12]. K equation and Dynamic K equation were built based on the traditional Smagorinsky model by introducing a transport equation for the SGS kinetic energy, making it more flexible and capable of better representing complex flow dynamics. In general, K equation models aim to improve the estimation of turbulence in LES by using a transport equation for the sub-grid kinetic energy, rather than relying on a constant (e.g., constant Smagorinsky) or formula (e.g., Dynamic Smagorinsky) for the eddy viscosity.

The Constant Smagorinsky, Deardorff, and K equation sub models consider fixed coefficients in their formulation (i.e., depends on the modeler choice: For example, 0.2 and 0.1 in FDS and 0.094 in OpenFOAM default setting, respectively [12,61]). Besides that, Constant Smagorinsky and Deardorff are not capable of handling the buoyant flows, near-wall turbulence, and anisotropy, which lead to inaccuracies in predicting fire behavior, smoke spread, and heat transfer [55]. Similarly, WALE and Vreman both use the fixed coefficient (i.e., 0.6 and 0.07 in FDS default setting, respectively [57,58,62]) but the WALE model inherently adjusts the SGS eddy viscosity to vanish near solid walls without needing additional wall-damping functions [62]. This means that by approaching a wall, the eddy viscosity is automatically reduced to zero in response to the no-slip condition (where velocity must be zero at the wall), ensuring that small-scale eddies near the wall are properly resolved. The same situation is applicable for Vreman, where the model effectively limits the eddy viscosity to prevent over-damping of turbulence in near-wall flows [63]. K equation sub-models provide a more refined and accurate approximation of the SGS turbulence effects in regions with strong turbulence gradients, such as near walls [64], which make them appropriate to be used in the case of a compartment fire.

Comparing the different LES sub models reveals the more appropriate choices to use in the compartment fire simulation. Dynamic Smagorinsky, WALE, and Vreman are more accurate in the case of a compartment fire as they can adapt well to the near-wall flows that are dominant in confined spaces. While the Constant Smagorinsky and Deardorff methods can be used in compartment fires, they may not be able to capture the near wall effects or transient behavior accurately. In practice, choosing between models depends on the specific flow characteristics and the available computational resources. If near-wall accuracy is needed, WALE or Vreman might be preferred. Although, if dynamic adaptation to local flow conditions is important, the Dynamic Smagorinsky model is a better option, despite its higher computational cost compared to WALE and Vreman.

From a grid sensitivity point of view, Dynamic Smagorinsky is highly sensitive to grid resolution, whereas the WALE and Vreman models are moderately sensitive but more robust on coarser grids. The Constant Smagorinsky model, while also grid-sensitive, is the most basic and less sensitive overall.

Table 2 ([12,41,57–59,62]) categorizes the different SGS models which are available in different CFD tools and summarizes the comparison between them, presenting their weak points with regard to compartment fire features.

Table 2. Comparison of different SGS models.

SGS Model	CFD Tool	Weakness
Constant Smagorinsky	• FDS • OpenFOAM • ISIS	• Fixed Coefficient • Over-predicts dissipation in regions where turbulence is low (e.g., near walls) and under-predicts dissipation in highly turbulent areas (e.g., fire plume)
Deardorff	• FDS	• Fixed Coefficient • Over-predicts dissipation in regions where turbulence is low (e.g., near walls)
Dynamic Smagorinsky	• FDS • OpenFOAM • ISIS	• Challenges in wall-bounded flows, where the eddy viscosity needs to approach zero at the wall: sometimes fail to properly capture this behavior without additional wall models or corrections.
WALE	• FDS • OpenFOAM • ISIS	• Fixed Coefficient • May struggle in strongly anisotropic flows away from walls (e.g., Large Open Compartment Fire)
Vreman	• FDS • ISIS	• Fixed Coefficient • Although in a compartment fire, the hot gases create strong buoyancy-driven flows, it does not inherently incorporate buoyancy effects
K equation	• OpenFOAM	• Fixed Coefficient • Assumes isotropic turbulence, which may not be suitable for compartment fires characterized by complex, anisotropic flows due to heat release and wall effects
Dynamic K equation	• OpenFOAM	• Model may not be able to adapt itself to sudden changes in turbulence characteristics such as the ignition/pre-development stage in compartment fires

3.3.2. Pyrolysis

Since a flame is categorized in the gas phase, liquid and solid fuels must be converted to the gaseous form in the first stage, in case of combustion [8]. This thermal decomposition process, in which materials break down into smaller molecules when exposed to high temperatures in the absence of oxygen or other oxidizing agents, is called pyrolysis. In other words, pyrolysis helps us to understand how materials break down in a fire and release flammable gases. The process typically produces three main products:

- Gases: Volatile compounds like hydrogen, methane, carbon monoxide, and other light hydrocarbons.
- Liquids: Condensable products such as tar, oil, or other heavy hydrocarbons.
- Solid Residue: Char or ash.

The main aim of pyrolysis modeling is to determine the mass decomposition of the fuel or the rate of flammable gases produced which can determine main fire characteristics such as HRR. Pyrolysis modeling is fundamentally based on the Arrhenius equation (i.e., finite rate chemistry).

As mentioned before, when no experimental data for HRR or MLR is available, modelers should use the predictive capability of the simulation tools to identify the fire characteristics (which is known as free burning without any further constraint). In such cases, the pyrolysis sub-model is utilized. There are two distinct cases in which pyrolysis can be utilized, combustible solid fuels such as wood, polymers, etc., and liquid fuels (e.g., pool fire), which will be explained in separated categories.

- Solid Fuels

Pyrolysis for solid fuels involves heat transfer into them, leading to the breakdown of their molecular structure and the release of volatile gases, liquids, and char. In this case, simulations should consider conduction, convection, and radiation within and around the solid, as well as the diffusion of product gases. FDS uses single or multi-step Arrhenius models, OpenFOAM can adopt multi-step reactions, variable activation energies, or empirical laws defined by modeler, and ISIS uses a single-step Arrhenius model for pyrolysis of solid materials.

Kim [65] used a detailed pyrolysis model in wood fires, considering cellulose, active cellulose, hemicellulose, lignin, char, ash, moisture, and air as the wood components. Using FDS, they compared the results for three different methods: prescribing an experimental measurement of HRR as the input, and predictive pyrolysis models with and without the burn-away option (used to simulate the combustion and removal of solid materials as they burn and are consumed during a fire) [12]. As illustrated in Figure 5, the prescribed HRR was only able to reproduce the initial stage of the fire. The predictive pyrolysis model resulted in a delayed ignition and initial phase compared to the experimental measurement. However, the detailed pyrolysis model which was used could replicate the overall HRR curve. Besides that, the burn away option of FDS was not able to improve the HRR significantly as it caused the HRR curve to have some fluctuations since removing burned cells in the wood cribs exposed the unburned cell with an ambient temperature to the combustion gases with high temperature.

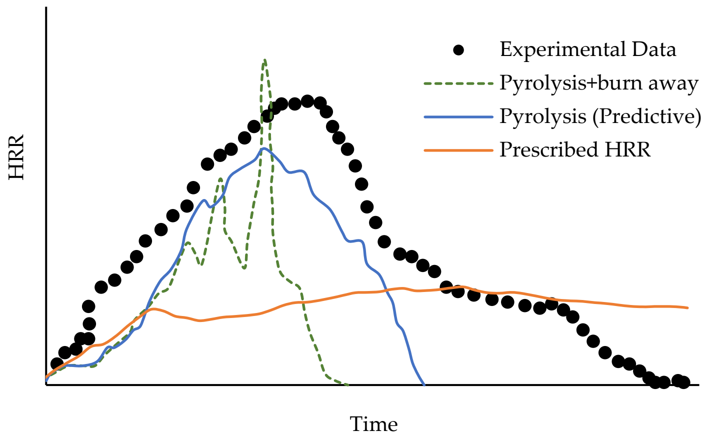

Figure 5. Comparison of different methods in predicting HRR of wood cribs. Adopted from Kim [65].

Yuan and Zhang [66] used a pyrolysis kinetics model of the PUF (polyurethane foam) slab in numerical modeling of a compartment fire, assuming that PUF is converted directly to the gaseous fuel ($C_{6.3}H_{7.1}NO_{2.1}$). They realized that by adopting the thermal decomposition of the PUF and the space within which the fire spread, the MLR of the solid fuel can be calculated and there is no need to prescribe the HRR in CFD modeling.

Considering multiple pyrolysis gases obtained from experimental tests for the non-charring solid fuel polymethyl methacrylate (PMMA) and importing them in a modified version of FireFOAM, Ding et al. [67] validated their model against experimental data. The pyrolysis reaction occurred in a way that PMMA was converted to gas without any charring residue. Pyrolysis gases included the following: MMA, C_2H_4, CO_2, CH_3OH, and CO.

Ding et al. [68] developed a new model for pyrolysis of wet wood in FireFOAM. Their innovation was adopting a simple one-step nth-order Arrhenius expression for dry wood pyrolysis with a moisture drying reaction (i.e., conversion of moisture to vapor, as well as wood to char and Pyrolysate). After the model had been validated using the corresponding experimental data, the mass fluxes of water vapor and pyrolysate were examined in relation to the thickness of wet wood, considering various external radiation heat fluxes.

Markus et al. [69] studied the thermal pyrolysis model for simulating flame spread along the PMMA slabs in FDS. Compared to the finite rate pyrolysis model (Arrhenius model), the thermal pyrolysis model was not able to accurately replicate the experimental trend of the total HRR. To overcome this drawback, prescribed MLR should be increased, enabling the thermal pyrolysis model to produce more accurate HRR according to experimental measurements.

- Liquid Fuels

A fire induced by liquid fuels is generally known as pool fire and is defined by the turbulent diffusion of a flame above a liquid fuel which causes a volatile reaction of liquid evaporation [2,12]. The volatiles are the result of pyrolysis in liquid fuels and depend on the fuel properties, temperature, radiative heat feedback, boiling temperature of the liquid fuel, etc.

FDS, OpenFOAM, and ISIS differ significantly in their approach to model liquid fuel pyrolysis. FDS includes built-in evaporation models for liquid fuels, employing single or multi-step Arrhenius kinetics using parameters like boiling temperature and latent heat of vaporization. However, according to FDS User's Guide [12], it is clearly stated that the pyrolysis model of evaporating liquid fuels in FDS is recommended for research use only, due to the strong dependence of the evaporation rate on mesh grid. OpenFOAM, on the other hand, requires custom implementation, offering unparalleled flexibility for modelling complex evaporation dynamics, multi-step reactions, or user-defined empirical laws. ISIS employs the Clausius–Clapeyron equation for evaporation, defined as Equation (4):

$$X_f = exp\left[-\frac{h_v W_f}{R}\left(\frac{1}{T_s} - \frac{1}{T_b}\right)\right] \quad (4)$$

where X_f is the evaporating liquid mass fraction of the fuel, h_v is the latent heat of vaporization (J/mol), W_f is molar mass of the fuel (kg/mol), R is universal gas constant (8.314 J/(mol·K)), T_s is surface temperature of the liquid fuel (K), and T_b is the boiling temperature of the liquid fuel.

An early use of LES in simulating a pool fire was conducted by Hostikka et al. [70] and they showed that the burning rate depends on the pool size. Hong et al. [71] proposed a modified natural convection correlation instead of the forced convection approach (used in FDS v6.7.5) to simulate the heat and mass transfer for liquid pool fires. The main idea was to depend on a Grashof number (a dimensionless number that characterizes the relative strength of buoyancy forces to viscous forces in fluid flow, particularly in natural convection scenarios) instead of a Reynolds number (indicates whether the flow is laminar or turbulent based on the balance between inertial forces and viscous forces) as the governing parameter in heat transfer through the pool fire. It was shown that although the burning rates were similar in both cases, the fuel surface temperature was predicted more accurately in the natural convection approach.

In other work, [72], they adopted the natural convection correlation for estimating the evaporation rate and the Nusselt number for the heat transfer calculations. They realized that the forced convection approach is not capable of modeling the flame extinction. In addition, assuming a low value for the auto-ignition temperature of the fuel (such as -273 K in FDS as default) can predict the burning rate but not the extinction accurately. Therefore, considering the actual auto ignition temperature is necessary.

The capability of the FDS v6.7.0 in predictive simulation of a liquid pool fire using pyrolysis sub-models was studied by Stewart et al. [73]. Their work on different fuel types showed that a default FDS combustion model (infinitely fast combustion) using fast ignition and burning is sufficient to replicate the experimental measurements in the ignition and fire growth phases for the fuels with low boiling temperature (as illustrated in Figure 6 (left)), while this method is not applicable for the fuels with higher boiling temperature (as illustrated in Figure 6 (right)). In these cases, considering a hot point in the simulation to start the burning process is helpful. As a conclusion, fast chemistry over-predicts the development rate of fire.

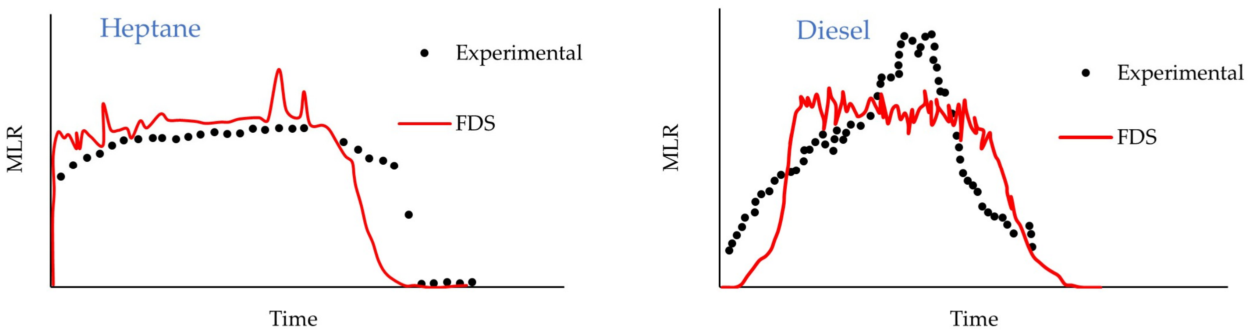

Figure 6. Comparison of measured and predicted mass loss rates for fuel with lower boiling temperature. Heptane (**left**)—higher boiling temperature. Diesel (**right**). Adopted from Stewart et al. [73].

3.3.3. Combustion and Kinetics

As mentioned earlier in Section 3.3.1, compartment **fires** are predominantly **turbulent**. Therefore, combustion modeling can be challenging, especially when it comes to studying the turbulence effects, and pushes the researcher toward introducing different methods in combustion modeling [74]. Since combustion involves processes that include chemical reactions (i.e., fuel oxidation) and physical interaction (e.g., heat transfer, fluid dynamics, etc.), both of these aspects must be considered. Combustion can be modeled using either single-step or multi-steps kinetics, depending on the level of detail required and the computational resources available. Moreover, the rate for these kinetics to be formed can be divided into two categories.

- Infinite rate chemistry: it is assumed that fuel and oxygen can interact with each other instantly and the only limiting criteria is mixing [12], eliminating the influence of chemical kinetics.
- Finite-rate chemistry: consider the actual chemical reaction rates and their dependency on temperature, pressure, and concentration of reactants.

A variety of sub-models have been developed by researchers; the infinitely fast chemistry (IFC) combustion model [75] assumes that the combustion is mixing-controlled and combustion occurs instantly as soon as fuel and oxidizer mix (local equilibrium assumption).

Eddy break-up (EBU) was first introduced by Spalding [76], assuming that chemical reaction rate is controlled by the turbulent eddy break-up rate and only considering fuel and oxidizer in determining the reaction rate; even though chemistry itself is infinitely fast in EBU, turbulence controls the reaction rate. Then, Magnussen and Hjertage [77] modified the EBU and presented the Eddy Dissipation Model (EDM). Similarly to EBU, the EDM combustion model is mixing-controlled, with infinitely fast kinetics, but it also accounts for products in the reaction rate.

In terms of kinetics reaction, EBU, EDM, and IFC are only compatible with one/two-step kinetics [53], resulting in them not considering all species. To overcome this barrier, implementing flamelet models helps to simulate all species using more detailed mechanisms. According to Yuen et al. [78] and cited by Safarzadeh et al. [53], flamelet models simplify complex turbulent combustion by treating small-scale reaction zones as if they behaved like laminar flames, i.e., a flame which is viewed in multi dimensions can be modeled through a number of one dimensional flames [79].

Two different approaches for flamelet models have been presented, namely the laminar flamelet model with infinite rate and Flamelet-Generated Manifolds (FGM) [79,80] with finite rate.

In the development of finite rate models, Magnussen [81] extended the EDM for finite rate chemistry and presented the eddy dissipation concept (EDC). Other models such as probability density function (PDF) by Pobe [82] and volumetric heat source (VHS) by Petit and Dulong [83] handle turbulence–chemistry interactions differently. PDF focuses on direct solutions for the probability distributions of key variables such as species concentrations, temperature, and velocity instead of the mean values [84]. VHS is a simple combustion model which calculates the total heat release in each volume due to combustion. It simplifies the process by calculating the rate of energy release based on reaction rates without modeling the detailed turbulence–chemistry interactions [85].

Existing combustion models can predict the combustion products in a well-ventilated compartment [7]. For example, FDS proposes mixing controlled and finite-rate combustion approaches [12]. According to Beji et al. [7], in a well-ventilated compartment fire, a single-step infinitely fast reaction with defined initial inputs for soot and CO yield is applicable. Although, since the fuel decomposition is not certain, assuming single input yields does not predict the combustion characteristics precisely [7].

Comparing the EDC combustion model with standard EDM in a methanol pool fire, Maragkos et al. [86] revealed that EDM could not predict the flame temperature, even with major justification of the EDM coefficients compared to EDC.

In a similar work, Heidarinejad et al. [87] compared the EDM and IFC for simulating a pool fire in FireFOAM and the results indicated that the latter over-predicts the velocity and temperature and the former can simulate the combustion more accurately due to its adoption of the time characteristic of turbulence and diffusion. EDM is the better choice in predicting velocity with OneEqEddy SGS model, and IFC is more reliable when using the Smagorinsky approach.

Safarzadeh et al. [53] used the FGM combustion model and compared the simulation results with IFC and EDM. Although IFC and EDM provided more accurate temperature predictions, FGM was more precise in simulating different species. Moreover, it was recommended to include radiation effect in FGM to improve the results. Authors studied the FGM ability in compartment and pool fire simulations and investigated the effects of considering radiative heat transfer [88]. It was shown that combustion–radiation coupling enhanced model accuracy in a pool fire scenario. Compartment fire modeling was not influenced much by radiation coupling, although the results showed better agreement with experimental data. In addition, IFC and EDM are not able to model the extinction, while FGM is.

Huang et al. [75] simulated an enclosed clean room fire using three different combustion models, namely VHS, EBU, and presumed probability density function (prePDF), in which a PDF is used to consider turbulence chemistry interaction. Their results demonstrated that prePDF was the best choice, while VHS was the worst in the case of temperature prediction for large fires. Considering computation time, EBU had the longest one and VHS had the shortest.

A comparative study on fast chemistry-based combustion models for pool fires was conducted by Razeghi et al. [89]. Among IFC, EDM, EDC, and steady laminar flamelet model (SLFM), SLFM was more capable of predicting the mean turbulent kinetic energy, while EDM predicted the mean vertical velocity of the flow more accurately.

Jeri At Thabari et al. [90] used two EDC models (1981 and 2005) with infinitely fast and finite-rate chemistry (1, 2, and 6 steps combustion) to simulate pool fires. The results showed that infinitely fast chemistry was less grid sensitive, since the reaction rates in finite-rate chemistry depend non-linearly on the resolved quantities such as mass fraction and temperature. In addition, EDC 1981 produced lower reaction rates and temperature compared to EDC 2005; the reason for this being that unburnt fuel tends to exit the domain, which reduced the heat release rate. Six steps predicted the temperature more accurately than the two-step reaction mechanism. However, more detailed mechanisms caused more fuel to be escaped, resulting in lower HRR. However, six-step mechanism predicted species and flame temperature more precisely.

Regarding the importance of kinetics in fire modeling, Peters and Rogg [91] presented the detailed kinetics for combustion, consisting of 112 reaction steps and 37 species which can enhance the model performance in predicting temperature and species. Furthermore, A.C.Y. Yuen et al. [92] developed a computation code and studied the comparison between detailed and multi-step chemical kinetics for combustion in compartment fires with different ventilation modes. Their results showed that multi-step kinetics over-predict CO_2 and CO concentration. Although in well-ventilated compartment fire, CO_2 and CO concentration were predicted reasonably, they were over-predicted in under-ventilated fires using detailed kinematics.

3.3.4. Heat Transfer: Radiation Transport

The thermal interaction between fuel, product gases, smoke, ambient air, and the compartment solid boundaries (or any kind of media), is known as heat transfer. Besides the thermal energy movement and the temperature distribution in the compartment, heat transfer is crucial in pyrolysis [7]. One of the heat transfer modes which can affect the combustion and fluid dynamics in the compartment fire is thermal radiation [7,93,94]. Although other heat transfer modes, including conduction and convection, have their own level of importance in CFD simulation of compartment fire, radiation is the governing mechanism of heat transfer in fires [38]. Therefore, only numerical modeling of radiative heat transfer is discussed in this study.

A sensitivity analysis for heat transfer in compartment fire by Beshir et al. [95] indicated that conductivity and emissivity are important factors for thermally thick walls, while for thermally thin walls, emissivity is key. Thermally thick and thermally thin are two definitions in heat transfer science which describe how temperature is distributed across the material thickness when exposed to a heat source: thermally thick shows the significant temperature gradient, while thermally thin has a relatively uniform temperature. Centeno et al. [96] illustrated that in the compartments with thermally thin walls, heat loss through walls is the determining factor in fire dynamics inside the compartment, whereas it is the induced pressure (such as the one caused by outside wind) in thermally thick walls. Wen et al. [97] conducted a CFD study investigating the effect of radiation on flamelet calculation in a compartment fire. They found that including radiation in the model can improve the accuracy of soot concentration and temperature prediction. However, the prediction of CO_2, H_2O, and CO is not very sensitive to radiation model presence.

Heat transfer in the form of electromagnetic radiation through a media (fuel, product gases, smoke, soot particles, walls, etc.) is described as the Radiative Transfer Equation (RTE) and it includes the following:

- Emission—radiation emitted by the media itself;
- Absorption—radiation absorbed by media and reducing the intensity of radiation passing through it;
- Scattering—radiation deflected by particles in the media, changing its direction without being absorbed.

In other words, the RTE predicts the effect of how much radiative heat reaches a surface or moves through a fluid based on the material properties and surrounding conditions. Regarding the importance of radiative heat transfer, it should be noted that radiation has a considerable influence on kinetics and flame structure, as it can affect the temperature distribution [97]. Liu and Rogg [98] illustrated that radiative heat loss may result in the temperature decreasing by 100 K in laminar flames.

According to Lockwood and Shah [99], quoted by Zhang et al. [100], the mathematical definition of the radiation transport equation is defined as Equation (5):

$$\frac{dI}{dS} = -(k_{\alpha} + k_{sca})I + k_{\alpha}E_g + \frac{k_{sca}}{4\pi}\int_{4\pi} P(\Omega, \Omega')I(\Omega')d\Omega' \quad (5)$$

where $\frac{dI}{dS}$ represents the rate of change in radiative intensity I along the path S. It shows how the radiation intensity changes as it moves through the media. k_{α} is the absorption coefficient, k_{sca} is the soot scattering coefficient, and $(k_{\alpha} + k_{sca})I$ is the radiation intensity loss due to absorption and scattering in the media. $k_{\alpha}E_g$ is the emission term, where E_g represents the blackbody emissive power at the local temperature of the media $\left(E_g = \sigma T_g^4, \sigma = 5.67 \times 10^{-8}\left(\frac{W}{m^2K^4}\right)\right)$. The last term describes the scattering term, representing how radiation is redistributed. P (Ω, Ω') is the phase function, which describes how radiation from direction Ω' is scattered into the direction Ω. The integral over all solid angle 4π accounts for scattering contributions from all directions in the direction of interest.

Radiation heat transfer is challenging in numerical modeling as this type of energy moves at light velocity, compared to gas or sound velocity [43]. Moreover, this type of heat transfer is computationally expensive and between 50 and 70% of simulation time in LES modeling of combustion is assigned to that [101]. However, there is an option in CFD tools to neglect solving RTE (e.g., "No Radiation Transport" in FDS and "noRadiation" in OpenFOAM) which may result in almost 20% less CPU time [12,102].

Different methods in CFD have been developed and are used based on the modeler choice and conditions, being responsible for solving the RTE:

- P1 [103,104]: This is the simplest method which simplifies the RTE by assuming that radiation is isotropic and diffusive in nature, making it computationally efficient and easy to implement. It approximates RTE based on the spherical harmonics method. It assumes isotropic radiation and works well for optically thick media (such as smoke and flames in fires). P1 is less accurate in optically thin media (to overpredict radiative fluxes from localized heat sources or sinks in optically thin media [104]) but is suitable for optically thick cases, such as fires with heavy smoke. Optically thin media and walls exposed to uncertain boundary conditions may result in the inaccuracy of the P1 method [94]. P1 considers scattering without any additional computational cost [104].
- Discrete Ordinates Method (DOM) [105]: This is is a finite volume method which solves the RTE by dividing the angular space into several discrete directions and solving for each direction. DOM can model anisotropic radiation and complex geometries, although it requires higher computational resources compared to P1, especially when

fine angular resolution is needed. Furthermore, in optically thin regions, errors arise because DOM does not inherently treat scattering accurately and can produce ray effects where artificial patterns of radiation appear.

- Discrete Transfer Ray-Tracing Method (DTRM) [99]: This method traces rays from heat sources to surfaces, calculating radiation directly along these paths. DTRM assumes negligible scattering and is less accurate in optically thick media or for environments with strong scattering effects such as soot. In flows where fire is dominant (such as compartment fire), soot is the determining factor rather than product gases in thermal radiation [7]. Therefore, DTRM is not a good choice in a CFD simulation of a compartment fire.
- S2S Model (opaque Solid): This is a technique to simulate radiative heat transfer between surfaces in systems where the media between the surfaces is non-participating (i.e., it does not absorb, emit, or scatter radiation). This model simplifies radiative heat transfer by only considering radiation exchange between solid surfaces. The S2S model cannot account for the effects of soot, smoke, or combustion gases on radiation, which limits its application. But, in case of compartment fire, it can be used for the radiation model of solid surfaces such as walls, ceilings, floors, furnishing, and objects inside the compartment.

Choosing the RTE model can significantly impact the accuracy and computational efficiency of the CFD simulation. In a compartment fire, radiation from the flames, smoke, and hot gases significantly affect heat transfer and make participating media (soot, product gases, etc.) important factors in modeling. As mentioned, P1 can be considered as an appropriate method for optically thick conditions like smoke-filled compartments, but it may struggle with flame radiation and near-wall effects (optically thin conditions). DOM can handle directional radiation effects and participating media (i.e., soot and gases), although at higher computational cost. DTRM offers directional accuracy like DOM, but it is simpler and less computationally demanding. It is effective in smaller, less complex compartments with minimal scattering and participating media. However, it assumes constant intensity along each ray, which can limit its accuracy in highly dynamic environments, such as those with significant soot or flame radiation. S2S is applicable for compartment boundaries and must be used with another model to include the radiation effect of gases and soot.

FDS uses the finite volume method (DOM-based approach) to solve RTE, P1 and finite volume DOM are available in ISIS, while OpenFOAM can adopt P1, DOM, DTRM, and S2S methods. Besides No Radiation Transport, FDS provides three more approaches for the RTE: optically thin, optically thick with specified radiative fraction, and optically thick with predicted radiative fraction (not specified). The optically thin and optically thick approaches for radiation modeling in FDS were compared by Maragkos and Merci [38] in an open atmosphere free-burning. Their results showed that the optically thin method was more accurate in terms of predicting flame temperature, velocity, and radiative heat flux. But for an enclosed fire, according to [12], the optically thin approach is not appropriate due to its neglect of the re-absorption of thermal radiation by gases in the confined space. Therefore, in CFD simulation of a compartment fire using FDS, the optically thick option is more accurate. However, predicting radiative fraction instead of prescribing required the well-resolved temperature field and absorption coefficient to be calculated directly, as well as fine mesh grids such as in DNS. As a proper method in LES, optically thick with specified radiative fraction can be a better choice for compartment fires, which is a prescriptive method and needs the user to specify the radiative fraction of the fuel. This parameter illustrates the portion of fire energy which is emitted by radiation. The radiative fraction for more common fuels is presented in [12], adopted from *SFPE Handbook of Fire Protection Engineering* [43]. However, the pre-defined values for radiative fraction are typically based on ideal conditions such as complete combustion and a well-ventilated compartment and are not appropriate for under-ventilated fire scenarios, for example. Under-ventilated conditions often lead to incomplete combustion, resulting in a higher proportion of unburned fuel and increased soot production, and changes the radiative properties compared to well-ventilated conditions. It should be noted that considering radiative fraction to be fixed equal to the prescribed value is not always accurate, resulting in over-prediction of the radiative heat flux at the fuel surface [106]. Since the fuel vapor and product gases are accumulated and reduce the radiation, however, this approach can account for soot radiation and is helpful to simplify CFD simulation in a compartment fire [38]. Table 3 presents a summary of different methods for radiation modeling which are available in different CFD tools, presenting their advantages and disadvantages.

Table 3. Comparison of different radiation modeling methods.

Model	CFD Tool	Pros	Cons
P1	• OpenFOAM • ISIS	Computationally efficient Works well in optically thick media	Less accurate for non-homogeneous media Assumes isotropic radiation
DOM	• FDS • OpenFOAM • ISIS	Handles complex geometries More accurate than P1 in some cases	Computationally expensive Can introduce ray effects (false directional patterns)
DTRM	• OpenFOAM	Handles complex geometries Accurate for optically thin media Works well with complex geometries	Computationally expensive Does not inherently include scattering effects
S2S	• OpenFOAM	Efficient for surface-to-surface radiation	Does not account for gas-phase radiation and soot absorption or scattering

As mentioned in Equation (5), k_α is the absorption coefficient (for product gases and solid particles such as soot) and needs to be specified for solving RTE. However, the absorption coefficient is not considered in the optically thin approach as it is assumed that the energy emitted by the fire is not absorbed by the surrounding gases or particles (e.g., soot) to a significant extent. k_α is a critical parameter that quantifies how much radiation is absorbed by a participating medium (such as gases or particles). Several radiative gas property models are available for specifying or approximating the absorption coefficient in CFD [107–111]:

1. Line-by-Line (LBL): This method considers the actual spectral lines of radiatively active gases, resolving absorption coefficients at very high spectral resolution. LBL is used when high accuracy is required. It is the most accurate model for radiative transfer because it considers every spectral line. Due to the intensive computational requirements of resolving individual absorption lines across the entire spectrum, it is not widely implemented in CFD tools like FDS or OpenFOAM.
2. Spectral Band Models: These models divide the spectrum of gas radiation into discrete spectral bands:
    - Narrow Band Models (NBM): These models divide the spectrum into small narrow bands and treat radiative properties as varying within each band. They offer a more manageable approximation compared to LBL but still retain some spectral detail.
    - Statistical Narrow Band (SNB): This incorporates statistical methods to represent spectral lines within each narrow band. It is the most accurate model to replicate the LBL method, especially in high temperature gases.

- Wide Band Model (WBM): This is a simplified version of SNB. It categorizes the radiation spectrum into wider bands rather than treating individual spectral lines. Each band represents a broader wavelength range, where the absorption and emission properties are relatively similar. In other words, the model assumes that within each band, the gas properties, such as absorption coefficients, are constant or vary in a predictable manner. It can result in significantly less computational cost compared to NBM. WBM offers good accuracy, especially for gases like CO_2 and H_2O which have strong and wide absorption bands. This model is available on FDS (Box Model) [12] and OpenFOAM (WideBandAbsorptionEmission) [112].

3. Global Models: These models, including the Gray Gas and Weighted-Sum-of-Gray-Gases (WSGG) models, simplify the radiative transfer by treating the gas as absorbing/emitting uniformly across all wavelengths (or a few representative gray gases with different absorption coefficients). They are commonly available in CFD tools such as FDS, OpenFOAM, and FireFOAM.
   - Gray Gas Model: To reduce the required computation time for solving RTE, gases are often assumed to be gray. It helps the RTE to be solved more efficiently by treating the gas as having uniform radiative properties and eliminates the need for detailed spectral calculations (i.e., no spectral variation is considered), which involves resolving the radiative transfer across a wide range of wavelengths. By treating the gas as gray, the simulation ignores the fine structure of how different wavelengths are absorbed and emitted by gases like CO_2 and H_2O, which are computationally expensive to resolve [94]. This can decrease the accuracy of the simulation in the case of oxyfuel combustion (i.e., more concentrated CO_2 and H_2O in the product gases) and optically thin flames [62] (i.e., soot yield is lower than CO_2 and H_2O yield).
   - WSGG Model [111]: This model improves the gray gas approximation by dividing the radiation spectrum into a sum of gray gases with different absorption coefficients, each weighted by temperature and concentration. When dealing with mixtures of gases such as CO_2, H_2O, and soot, the absorption spectra can overlap. The WSGG model may not handle these interactions effectively, leading to reduced accuracy when modeling multi-gas combustion environments. For similar conditions, the computational cost of WSGG was shown to be around 3.5 times that of the Gray Gas Model [38].

Choosing the appropriate radiative heat transfer model depends on the balance between computational cost and accuracy. While LBL provides the highest spectral accuracy by resolving individual absorption lines of gases and NBM offers improved spectral resolution compared to WBM, the computational cost for LBL and NBM makes them less ideal for practical fire simulations where the simulation time is a major concern and detailed spectral resolution is unnecessary. Gray Gas or WSGG models are more appropriate due to the lower computational cost and reasonable accuracy; they are commonly used in tools like FDS and are effective at handling large-scale, under-ventilated, or sooty environments such as fires in confined spaces. If more spectral details are needed without going to the complexity of NBM or LBL models, Wide Band models are efficient.

In a natural compartment fire without any control, firefighting, or suppression system, at the end of fully developed phase where available fuel and oxygen have been consumed and they become limited, the fire begins to lose intensity, marking the start of the decay phase. During the decay phase in the compartment, flames become smaller, and temperatures gradually decrease. The fire continues to diminish until it reaches extinction, which is discussed in the next section.

3.3.5. Extinction

When either the local concentration of the fuel or oxygen, or the local temperature is too low to sustain the combustion process (reducing the heat feedback to the fuel source), thermal quenching happens which is known as extinction [113]. Modeling the extinction in fire and flame is always challenging [114]. Especially as it is not totally clear in compartment fires as it is caused by various factors including the concentration of the existing oxygen, critical flame temperature, radiative heat feedback to the fuel, etc. [115–119].

According to Maragkos et al. [120], CFD tools used for simulations of compartment fire consider one of the following elements:

- A critical flame temperature (CFT) (a constant value in the range of 1450–1780 K) which does not consider the effects of turbulence [121];
- A critical Damkohler number to model flame extinction, which is defined as Equation (6).

$$Da = \frac{\tau_{mixing}}{\tau_{chemical}} \tag{6}$$

where τ_{mixing} is the characteristic time of the mixing between fuel and air and $\tau_{chemical}$ is the characteristic chemical time. Extinction is expected to happen for low *Da* values [114].

FDS provides two different extinction models, both considering the CFT concept. In the first model, flames cannot sustain combustion if insufficient thermal energy is available to maintain the chemical reactions. In other words, the flame is assumed to extinguish if the gas temperature drops below CFT; if the temperature is more than 600 °C, the flame does not extinguish as long as the oxygen concentration is not zero. On the other hand, the second model does not only rely on CFT, but also considers the availability of fuel and oxygen to ensure that the temperature will be higher than CFT [62]. Figure 7 illustrates the range of extinction or flammability for different modeling approaches in FDS.

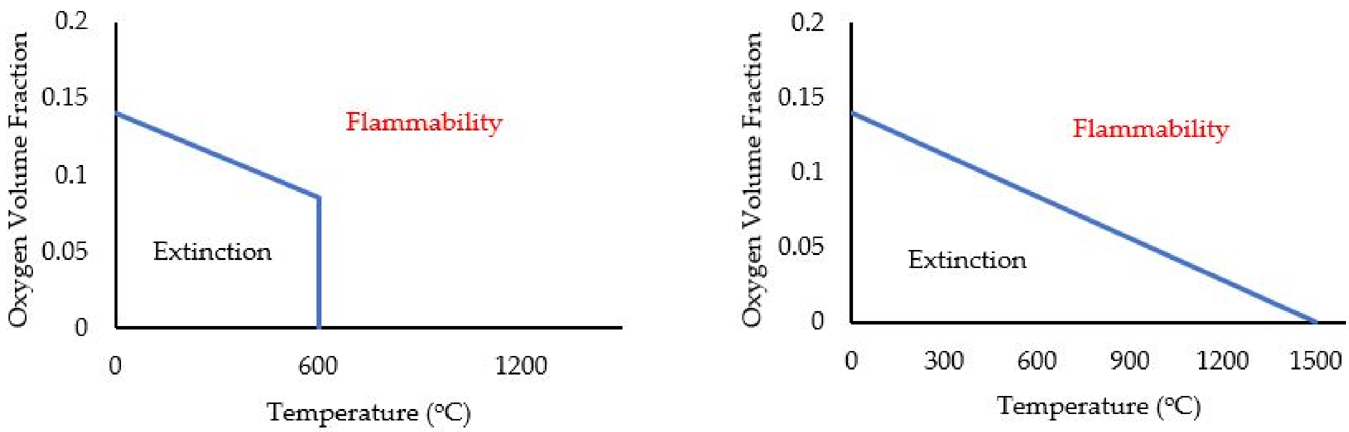

Figure 7. Schematic diagram of extinction criteria in FDS based on CFT and oxygen concentration. Extinction Model 1 (**left**) and Extinction Model 2 (**right**). Adopted from FDS User Guide [62].

ISIS also utilizes the second extinction model like FDS (right hand side in Figure 7) [41]. In OpenFOAM, extinction is typically handled within combustion solvers through sub-models for turbulence–chemistry interaction, combustion, and heat transfer. These sub-models evaluate the conditions under which fires disappear, focusing on parameters such as temperature and oxygen concentration.

Using a Damkohler number as a flame extinction criterion (instead of the approach that compare the LES-filtered temperature with a critical ignition temperature to determine whether the fire is extinguished or re-ignites [114,122]) in compartment fire was the main objective of Vilfayeau et al.'s [114] study. They used the global combustion equation (GR1) for the combustion modeling, while defining two more reactions in which fuel being converted to non-burning fuel and re-ignition of the non-burning fuel occurs. Flammability or the extinction of the fuel (flame) is specified based on whether the Damkohler number is greater or smaller than the critical value, respectively. A critical Damkohler number close to one is the criteria for the extinction regardless of other thermal or aerodynamics effects, according to Vilfayeau et al. [114].

It should be noted that considering extinction within the capability of combustion models mentioned in Section 3.3.2, and according to [113,123,124], quoted by Safarzadeh et al. [88], IFC and EDM are not able to model the extinction while FGM is, making FGM as a good choice for compartment fire modeling.

4. Discussion and Conclusions

Reviewing available sub-models and CFD methods for numerical simulations of compartment fires provides an appropriate framework and procedure for future studies. However, to the best of authors' knowledge, there is no exact algorithm for choosing the best sub-models in the case of a compartment fire and it totally depends on the specific situation, available computing resources, required accuracy and precision, purpose of study, etc. CFD and its applications in fire simulation are complicated operations and need a high level of expertise to implement effectively. This study provides an overview of available CFD methods for simulating different stages of fire, with a particular focus on fires occurring in enclosed spaces. It serves as a fundamental resource for CFD users interested in compartment fire modeling, helping them identify the most appropriate sub-models and tools for their specific needs.

Focusing on CFD modeling aspects such as computational mesh and boundary conditions, as well as physical features including turbulence, pyrolysis, combustion, radiative heat transfer, and extinction, different available sub-models in CFD modeling of the compartment fire have been presented. Moreover, by reviewing relevant conducted studies, their reliability and applications have been investigated. The advantages or disadvantages of different methods have been presented in the current study.

Nowadays, one of the main reasons for CFD modeling is to reduce the number of experimental tests due to their cost and corresponding risks. Meanwhile, the necessity of reliable test results to achieve more physical details and material properties, as well as the requisiteness of calibration tools for CFD models, pushes researchers to conduct experimental tests parallel to numerical simulation. It should be noted that predictive simulations of compartment fires needs more attention as they still have limits, especially in cases when either there is no available experimental measurement, or they are not able to cover all the simulation aspects, e.g., when fire development needs to be modeled in the blind or semi-blind modes, as they were shown to be incapable of replicating initial and extinction stages in compartment fire. In addition, more experimental tests for obtaining the thermochemical properties of materials such as fuels can enhance CFD accuracy when it comes to predictive (i.e., semi-blind or blind) simulation. In other words, conducting more precise tests on fuel combustion will provide more details about their behavior and decomposition which is helpful in combustion modeling and pyrolysis; an example being initial inputs for yield of CO, CO_2, and soot, or radiative fraction of the fuels in CFD tools such as FDS in under-ventilated conditions which differs from well-ventilated conditions. Although there are some reference values available for standard conditions such as well-ventilated, modelers should rely on their own knowledge and trial/error methods to achieve credible simulation in other conditions like under-ventilated compartment fires.

Regarding the importance of radiative heat transfer modeling, it should be noted that a compartment fire typically possess both regions: optically thin in areas with low concentrations of radiative species (such as soot or combustion gases like CO_2 and H_2O) or in areas where the path length is short like near the openings, and optically thick close to the flames or in smoky areas, where soot and other product species are dense. Therefore, choosing a proper method to solve the RTE and predicting the absorption coefficient may be challenging. In many cases, the model choice involves compromises that may limit the precision of radiation predictions, particularly for flame extinction, where small errors in radiative heat transfer can have significant effects.

A reliable CFD simulation of the compartment fire must create a similar temporal evolution of the HRR and, as a result, reliable fire characteristics may provide other properties such as temperature and species concentration. According to the evaluation of combustion sub-models and available literature, one of the existing gaps in predictive modeling is to replicate the fire behavior in the extinction phase. Extinction in compartment fires often occurs in turbulent conditions, where the interaction between turbulence and chemical reactions plays a crucial role. Although combustion models like IFC and EDM can predict HRR, temperature, and species concentration, they lack the detailed reaction rate dependencies and thermodynamic sensitivity needed to predict extinction, which are critical factors in compartment fires. Finite-rate combustion models such as EDC and FGM, couple turbulence and finite-rate chemical kinetics, which make them sensitive to temperature and species concentration (essential parameters in simulating extinction).

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