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Comparison of detailed soot formation models for sooty and non-sooty flames in an under-ventilated ISO room

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ABSTRACT

In fire simulations, it is essential to include detailed chemical kinetics for the description of the combustion process where intermediate chemical products are formed through a series of elementary reactions. A novel in-house fire field model based on Large Eddy Simulations (LES) approach incorporating fully coupled subgrid-scale (SGS) turbulence, combustion, soot formation and radiation models for the interactive and non-linear nature of the turbulent reacting flow in compartment fire phenomena has been developed in this article. It uniquely embraces the detailed reaction mechanisms for the chemical processes involved during combustion. Since the modelling of hydrocarbons by-products are enabled when considering the full chemical profile, the formation of soot particles can be related to the concentration of main incipient such as acetylene, which provides an appropriate representation of nucleation, surface growth processes. The significance of the improvement of soot particles modelling had been numerically investigated applying three different two-equations semi-empirical soot models: (i) Moss model (simplified model taken the fuel as the soot precursor); (ii) Moss-Brookes model (considers acetylene as the soot precursor) and (iii) Moss-Brookes-Hall model (considers acetylene, benzene ring and phenyl radical as the soot precursors). Comprehensive temperature and soot measurements from fire tests in a full-scale ISO compartment constructed purposely with a small opening gap to create the under-ventilated fire condition with which the effect of soot particles generation would be more significant. The computed results were compared with measured results for validation of the implemented soot models.

1. Introduction

Benefit by invention of digital computers and the development in code languages (i.e. FORTRAN, C, C++, etc.), pioneering works on field models, also known as computational fluid dynamics (CFD) models for fire safety studies were proposed by Ku et al. [1], Hasemi [2], Yang and Chang (i.e. UNDSAFE-I model) [3] during the late 1970s. Later on, Cox et al. [4] and Simcox et al. [5] utilised fire field models to investigate the King Cross Fire in the London Underground Station, which was a tragic fire disaster which caused 31 deaths in 18 Nov 1987. Also, Chow and Wong developed the UNDSAFE model [6] to studied the smoke filling processes in atrium fires. Markatos et al. [7] proposed the JASMINE model to investigate the smoke movement in a long fire test hall. Owing to the limited processing power for computer, all these models have so far adopted a simplified approach in representing the fire as spatially distributed heat sources – the volumetric heat source approach.

In order to improve the modelling of the combustion chemistry, the PHOENICS model suggested by Yang [8] adopted a non-premixed conserved scalar combustion model based on mixture fraction reported by Peters [9]. Comparison of CFD models, incorporating combustion and radiative exchange, by Lewis et al. [10] demonstrated the importance that such representations can have on the flow field development. They also showed that the volumetric heat source approach failed to reproduce the two-layer structure prevalent in enclosure fires as seen through Steckler et al. [11] room fire experiments. For an accurate heat transfer and fluid flow predictions, the inclusions of combustion and radiation models are indispensable.

The aforementioned earlier fire field models, have not considered the formation of soot in fire. Nevertheless, soot particles play an important role in radiative heat transfer especially for the absorption coefficient. On the basis of the soot model developed by Leung et al. [12] which accounts the effect of soot formation and oxidation processes, Wen et al. [13] demonstrated in their

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analysis of fire in a large compartment space that soot radiation has a significant impact on the flow and thermal characteristics. Moreover, the numerical study reported by Yeoh et al. [14] showed that the incorporation of combustion, soot and radiation models improved the temperature field prediction in single and multi-compartment(s) fires.

Recently, detailed chemistry combustion simulations have been applied in a wide range of chemical science and engineering studies [15–19]. Most of them are small-scale simulations focus on fuel air combustion kinetics and the flame within a chamber. Nonetheless, owing to high computational burden for larger-scale simulation, there are limited compartment fire simulation studies that utilised detailed chemistry. Numerical simulations was performed by Wen et al. [20] using laminar flamelet model with the consideration of detailed reaction mechanisms provided by Peters [21], which consists of 112 reactions steps and 37 species. It was demonstrated that the inclusion of detailed kinetics significantly improves the temperature, chemical species and soot particles predictions.

On the other hand, the ability of the CFD models to predict intermediate combustion products are also key in the modelling of soot particles. There are several key fundamental steps involved in the process soot formation as shown in Fig. 1, which includes soot particle inception, coagulation, surface growth, fragmentation and oxidation as suggested by Dworkin et al. [22]. Throughout the process, millions of agglomerate soot particles are generated from the base hydrocarbons atoms incipient, involving a gas-solid phase transition. As a result, soot agglomerates consist of a wide range of particle size owing to the random and non-linear features. The major chemical processes and formation kinetics for soot generation was comprehensively reviewed by Bockhorn [23]. He suggested that the initiation of the soot formation process is via the inception or nucleation of particles. In this phase, the aromatic rings such as cyclic benzene $c-C_6H_6$ and phyenyl $c-C_6H_5$ are formed by linear hydrocarbons including C_2H_2, C_3H_x, C_4H_x, etc. The second phase is referred as coagulation, where aromatic rings and other hydrocarbon intermediate species gradually grow into two-dimensional poly-aromatic hydrocarbons (PAH). Subsequently, the smallest identifiable three-dimensional solid phase soot particle incipient is formatted by the continued growth of PAH. Once a primary soot particle is created, it coagulates with other molecules which led to growth in its surface area. On the contrary, oxidation occurs at the surface of the soot particle, in which the interface layer reacts with the oxidant causing a decrease in particle size. In essence, the final size of a soot particle is mainly determined by soot particle surface growth and oxidation phases. Therefore, an appropriate soot model should describe the change in number and size of soot particles within space and time addressing all the aforementioned formation processes.

Numerical simulations have been performed on a full-scale ISO room fire test carried out by Opert et al. [25] using a large eddy simulation (LES) based computation code. This code was designed to simulate the temporal turbulent reacting fire behaviour for in-house situations [26,27]. Previously, the code was associated with the detailed chemical kinetics with encouraging intermediate combustion products predictions [24]. The previous established fire field model will be exploited and developed to include more comprehensive physical and chemical descriptions of the complex fire behaviour and its involvement to the surrounding fluid with the following advancing features: (i) the incorporation of detailed reaction mechanisms for the representation of the chemical processes in combustion, (ii) intermediate species modelling which provides the field concentration predictions for significant chemical by-products including carbon monoxide CO and hydrogen H_2, (iii) a soot formation model coupled with the detailed chemical combustion kinetics where the nucleation and surface growth processes are governed by the computed acetylene benzene and phyenyl concentrations, (iv) and finally the influence soot production to the heat release rate (HRR) and temperature field predictions for both sooty and non-sooty flame conditions within an under-ventilated ISO compartment room.

2. Fire field model

2.1. Governing equations

In this study, a three-dimensional in-house fire field model had been utilised. The code was written in FORTRAN using the LES

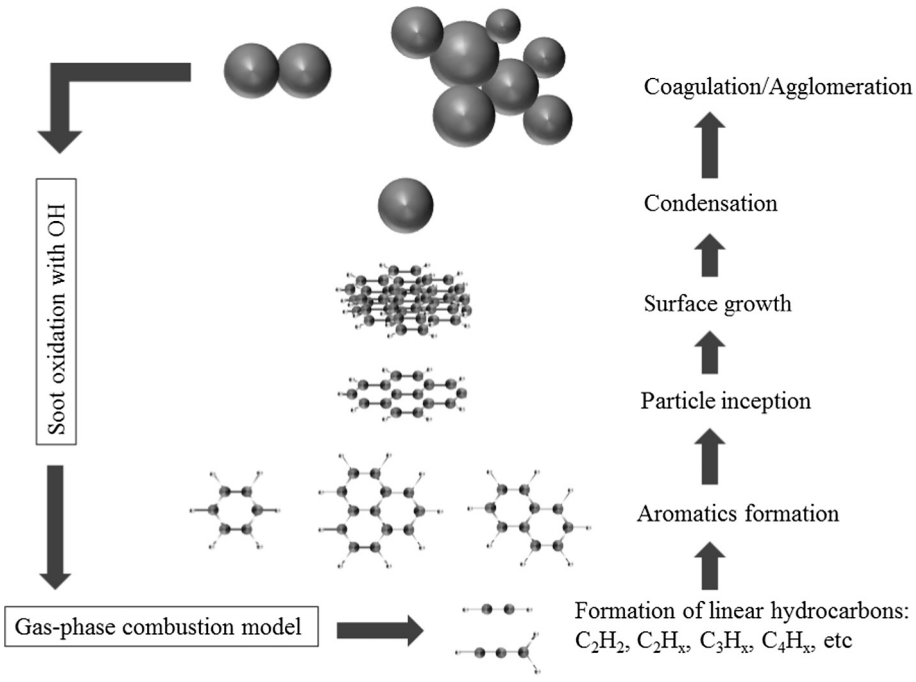

Fig. 1. Illustration of the soot particle generation and reduction processes extracted from Yuen et al. [24].