



Importance of detailed chemical kinetics on combustion and soot modelling of ventilated and under-ventilated fires in compartment



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ABSTRACT

A novel in-house computation code based on large eddy simulations (LES) incorporating fully coupled subgrid-scale (SGS) turbulence, combustion, soot and radiation models for turbulent reacting flows in compartment fires has been developed. It uniquely embraces the detailed reaction mechanisms for the chemical processes involved during combustion, which provides a comprehensive description of the fuel oxidation processes. Furthermore, it gives a more complete representation of the generation of intermediate chemical by-products including toxic gases such as carbon monoxide and irritant gases such as soot. Since the modelling of hydrocarbons by-products are enabled when considering the full chemical profile, the formation of soot particles is correlated to the concentration of main soot incipient acetylene, which provides an appropriate representation of nucleation, surface growth processes. The LES code has been validated with experimental fire tests results for both ventilated and under-ventilated fires in compartment for confirmation of its robustness. The importance of incorporating the detailed reaction mechanisms in compartment fire simulations has been confirmed by comparing with experiments. For under-ventilated fires in compartment, the chemical kinetics become increasingly important since the combustion efficiency drops significantly involving generation of intermediate chemical species. It is discovered that species concentrations especially CO₂ and CO are more accurately predicted by the detailed scheme comparing to the multi-step scheme, since the formation of hydrocarbons and nitrogen oxides are considered. In general, the simulation incorporating detailed kinetics showed an averaged improvement of 9.2% and 81.7% in the prediction of CO₂/CO ratio and volume fraction of soot respectively. This also improves the replication of the flame structure as the fire is chemically-driven within the combustion zone.

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1. Introduction

In the past, fire protection systems have been designed based on prescriptive codes and requirements which have been proven to be effective and adequate for traditional building developments. Nevertheless, prescriptive approach often fails to provide satisfactory and safe fire engineering designs and systems for modern buildings [1], where fire scenarios can be far more complicated by the possible involvement of a wide variety of combustible items and interactions of compartment surfaces with fire. Fire phenomena in compartment involve chemical and physical processes which are non-linear and interactive in nature. It is crucial to better inform the fire engineers for effective and safe fire engineering designs for these complex and mega constructions and infrastructures.

With the rapid advancement of computational technology, the application of numerical approaches in fire simulations has become more popular and generally accepted by fire researchers and engineers especially in performance-based fire engineering approaches and designs [2]. In particularly, field models were found to be major success due to its wide scope of applications and detail considerations of fire dynamics [3–8].

In fire simulations, one of the most critical challenges is the incorporation of detail chemical description for the combustion process, where intermediate chemical products are formed through a series of elementary reactions. The importance of chemical kinetics in fire simulation was addressed by the work of Xue et al. [9]. Three combustion models: volumetric heat source model (VHM), eddy break-up model and Presumed Probability Density Function (PrePDF) model, were examined by comparing with experimental data for medium and large-scale room fires [10,11]. Although the flow patterns were predicted satisfactorily, it was

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discovered that the field predictions by the three combustion models were not consistent over different locations in the enclosure. This was due to the fact that these models were limited in the consideration of chemistry or relative kinetics of the parent fuel. Therefore, it is necessary to apply a comprehensive reaction scheme that fully describes the oxidation processes of the parent fuel and the formation processes of major intermediate chemical by-products. Recently, detailed chemistry combustion simulations have been applied in a wide range of chemical science and engineering studies [12–16]. 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. [17] using laminar flamelet model with the consideration of detailed reaction mechanisms provided by Peters [18], 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.

In addition to the careful consideration of detailed combustion kinetics, it is also important to account for the multiple chemical and physical processes occurring during the formation of soot particles in compartment fires. There are several key fundamental steps of soot particle generation or reduction as shown in Fig. 1, which includes inception, coagulation, surface growth, condensation and oxidation as suggested by Dworkin et al. [19]. 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 initiation of the soot formation process is via the inception or nucleation of particles [20]. In this phase, the aromatic rings such

as cyclic benzene $c-C_6H_6$ and phenyl $c-C_6H_5$ are formed by linear hydrocarbons including C_2H_x , C_3H_x , C_4H_x , etc. For non-premixed diffusion flames, it is suggested by Lindstedt [21] that the chemical reaction rates for nucleation and surface growth can be correlated by the concentration of acetylene C_2H_2 , which can be predicted by detailed chemistry combustion modelling. 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. Owing to the fact that the main soot incipient for the particulate nucleation and surface growth is C_2H_2 , as well as other higher order hydrocarbons, and also the reduction of soot particles is caused by soot oxidation with OH, it is necessary to incorporate detailed chemical kinetics in the gas-phase combustion model to couple with the soot formation procedures.

In this article, numerical simulations have been performed on a reduced-scale compartment fire test carried out by Bundy et al. [22] 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 [23,24]. Recently, the code was associated with the Wall-Adapting Local Eddy Viscosity (WALE) model, while encouraging results were achieved for turbulent flame plume structure and the near-wall boundary field predictions in medium-scale compartment fire scenarios [25]. The objectives of this study are as follows:

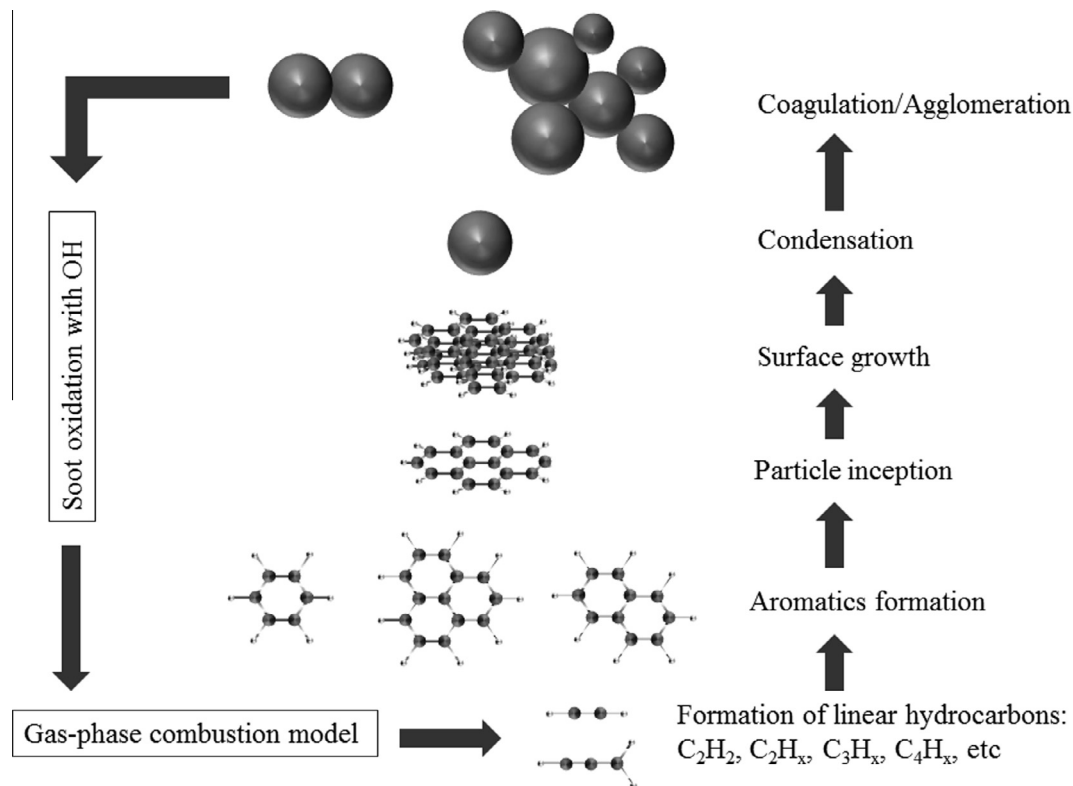


Fig. 1. Illustration of the soot particle generation and reduction processes.

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