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Extension of the turbulent flame speed closure model to ignition in multiphase flows

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ABSTRACT

An extension of the turbulent flame speed closure model rendering the model applicable to multiphase flow and ignition is presented. As formerly no coupling between reaction progress variable and enthalpy was existent, except through the temperature dependency of the laminar flame speed, an adaptation is proposed which offers an interface to initiate the combustion process. The modification to incorporate multiphase conditions is achieved by substituting the mixture fraction variable as representation of the composition in the original implementation of the turbulent flame speed closure model with independent species. Source terms to correlate the species progress to the reaction progress variable are derived in this work. The additional transport equations serve a higher generality of the model and enable the proper treatment of vaporizing fuel droplets. It is demonstrated that limitations which arise in the standard formulation of the model, stemming from differences in the transport equation for the reaction progress variable and the mixture fraction, are addressed and resolved by the new approach. Regarding the initiation of the flame, an additional source term for the reaction progress variable is introduced, which relates the reaction progress to the auto-ignition time. This allows the development of the flame without imposing artificial boundary conditions. The correct model behavior is established by means of a series of widely used test cases. The results of these simulations show that the model's potential to predict flame growth and more generally the flame evolution as a function of time and space is preserved. At the same time more sophisticated test case boundary conditions involving multiphase conditions and variable inflows in terms of composition can be incorporated. As a thorough assessment of the extended model capabilities, a multiphase lab scale set-up, which provides a comprehensive data set, is presented. The good agreement of the obtained results underline the range of applicability of the extended model and its accuracy, albeit its simplicity, for multiphase conditions.

1. Introduction

Low-order methods for the treatment of combustion processes in numerical simulations have a long history. With low-order we refer to combustion models in contrast to those using a detailed description of the gas phase chemistry, e.g. Di Domenico et al. [1], which considers complex kinetic schemes and requires the transport of a multitude of species. Indeed, since the development of global reaction schemes, e.g. Westbrook and Dryer [2], the use of such models is widely acknowledged. Concurrently, the demand of numerical work for investigating problems involving complex fluid dynamics has increased. Due to the improvement made in LES modeling [3,4] a large part of modeling strategies focuses on implementing a multiphase combustion model within a LES context to simulate full scale gas turbine combustion chambers [5–7]. However, as this essentially proves very costly in terms of computation time, a large number of calculations on supercomputers is usually out of scope. Specifically, studies involving parameter variations are predestined for a fast and efficient computation for which simplified turbulence modeling (e.g. URANS) and simplified combustion models such as the eddy dissipation concept [8] or the flamelet model [9] can be utilized. However, there are certain aspects of combustor development, also demanding a large number of simulations, as for instance the optimum position of an igniter or more generally, estimating lean blow out [10], which pose special requirements on the combustion modeling capabilities. For resolving ignition processes, an accurate description of the flame propagation is necessary, see e.g. Levebvre [11] whereas the simulation of lean blow out requires a precise prediction of the flame quenching phenomenon [12]. Thus, there is still a great need for low-order combustion models to be able to deal with the modern challenges of aero-engine design.

Within the context of igniter location, a significant number of experimental investigations which focus on determining the

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ignition probability within simplified geometries have been recently published [13–17]. The starting point in such series of experiments is marked with the analysis of the basic gaseous jet-flame configuration [15] for the development of numerical tools. Then, technically relevant applications such as a swirl-stabilized spray flame [17] are investigated. The interest of aircraft's engine original equipment manufacturers (OEMs) regarding this topic is demonstrated through studies published by Stow et al. [18], Mosbach et al. [19] and Fyffe et al. [10]. With the combustion systems' concept changing from rich toward lean primary zone combustion in order to address policy measures regarding pollutant emissions reduction, in particular nitrogen oxides (NO_x), the issue of ignitability of the engine is more pronounced. Actually, lean-burn low NO_x combustors have an operating envelope closer to the stability limits with respect to rich-burn systems. Specifically, high-altitude relight and cold start where adverse conditions prevail are thoroughly investigated experimentally in dedicated facilities during OEMs lean combustion system research programs [10]. Thus, there is a growing interest in dealing with this matter at an early stage of the combustor design cycle entraining a demand for numerical tools to support the development and allow a multitude of simultaneous computations. In this context, ad hoc ignition models as proposed by Neophytou et al. [20] and Weckering et al. [21] were recently developed.

The numerical work which has been done with more complex models concerning the ignition probability of some of the test cases [13–17] has shown that a good agreement for distinct points can be achieved in terms of the ignition probability of that specific location and the subsequent flame behavior, see e.g. [22]. However, in summary, most of the numerical studies involved a LES-based approach and were thus limited to a very small number of calculations. As a consequence, the results only comprised a confined set of locations at which the ignitability could be elucidated and can therefore, at the current state of still restricted computational power, not be employed to yield a complete spatial map of the ignitability of a combustor. On the other hand, by means of URANS simulations based on the extended TFC model presented here, a reasonable reproduction of the ignition map of the jet flame test case studied by Ahmed et al. [16] has been achieved, see Boyde et al. [23].

Hence, in order to bridge the gap until the computational power becomes available to allow LES computations for numerous stoichiometric and air flow conditions at the igniter positions, we present a reacting multiphase flow combustion model which is applicable to a standard RANS/URANS environment. Our approach is based on the turbulent flame speed closure model, hereafter termed TFC model, which was first proposed by Zimont [24] and offers the advantage that it is of a very reasonable accuracy and robustness for premixed flames. This was successfully demonstrated by the work of Zimont et al. [25]. Its extension to non-premixed conditions was realized by Polifke et al. [26], Flohr and Pitsch [27] and Knudsen and Pitsch [28] among others. Usually, the aforementioned low-order models are optimized for a single characteristic of the combustion process; for instance certain species concentrations and pollutant emissions or ignition delay times or soot prediction. In this work, the TFC model offers the essential advantage that it captures the flame propagation speed. Precisely, the source term in the reaction progress variable transport equation is closed using a velocity scale dependent upon the physical–chemical properties of the local mixture. With the inclusion of the laminar flame speed as an intrinsic chemical property and the local turbulence quantities, a correlation is derived which approximates the propagation behavior of the flame also in laminar and turbulent regimes. Through the dependence on the laminar flame speed, detailed chemistry effects are taken into account yet retaining the simplicity of the model. The second detailed chemistry effect accounted for in our model for the reaction progress variable source term is the ignition delay time. It has been identified by Lefebvre [11] that three phases determine the success of the gas turbine light-off. Phase 1, which represents the deposition of energy to achieve a sufficiently large initial flame kernel is addressed in our ignition model extension. Phase 2, corresponding to the propagation and growth of the flame kernel into the primary zone and, Phase 3 the "light around" where flame kernels from an ignited fuel injector propagate circumferentially around the annular combustor both directly depend on the flame speed. Thus, with our focus on relight or light-off modeling, the TFC model represents a very adequate choice among the low-order combustion models.

The TFC model itself has undergone a series of enhancements since its formulation by Zimont [24]. One of the improvements made by Zimont and Lipatnikov [29] limits the turbulent flame speed needed for the source term in the presence of high turbulence. Formerly, the increase of turbulence fluctuations would also cause a rise in the absolute value of the turbulent flame speed, which is only valid for Karlovitz numbers less than one. Up to this condition, the small eddies of the size of the Kolmogorov length scale are larger than the inherent reaction zone of the flame front. Beyond that point, for Karlovitz numbers greater than one in case of stronger turbulence, the chemical reactions are affected by the small scale turbulence, which reduces and ultimately quenches the flame. A further contribution to the flexibility of the model was accomplished by Polifke et al. [26] and also Cokljat et al. [30] who proposed the transport of the mixture fraction and the sensible enthalpy in order to adapt the model to non-premixed environments and to incorporate non-adiabatic effects. The model can also be used in the context of LES simulations, as demonstrated by Knudsen and Pitsch [28].

To the best of the authors knowledge, simulations involving the TFC model for multiphase flows are not present in the literature, nor the common model implementation apt to incorporate multiphase reactants phenomena. Thus, our contribution is the extension of the model formulation to allow the treatment of multiphase reactants in turbulent flows.

Furthermore, there are some shortfalls associated with the standard model implementation. A numerical study performed by Wood and Moss [31] revealed that problems arise for example in situations where a fully burnt lean mixture connects with pure air. Pure air is difficult to describe with a reaction progress variable. In the original model, c corresponds to the normalized ratio of the current local product mass fraction to the value of the maximum attainable local product mass fraction: $c = Y_p/Y_{p,b}$. Hence, under premixed conditions c is unity within the flame and zero outside the flame. The situation becomes more complex in a non-premixed scenario. Without the presence of fuel, pure air cannot react and the reaction progress variable is undefined. Thus, capturing the dilution of products from lean combustion with air constitutes a challenge. This process should not alter the reaction progress variable considering that a further chemical reaction cannot occur since only fuel is scarce. In the original model, the reaction progress variable is nevertheless reduced due to the mixing of air with a flame progress variable value of zero and combustion products with a flame progress variable value of unity. We will demonstrate that this dilemma is solved by applying the extended model formulation presented in this paper. The approach we propose, demands the transport of selected species which enables the determination of the physical reaction progress and avoids an erroneous influence of mixing effects. The improvement of a low order model by adding a second non-normalized flame progress variable (which can be derived from the transported species in our case) to the already existing normalized one, has been successfully applied to other models previously, see e.g. Colin and Benkenida [32],