DEVELOPMENT OF THE STREAM RECOGNITION MODEL OF TRANSPORTED PROBABILITIES FOR TURBULENT FLAMES

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Preface. The objective of reported development was to work out a model leading to a relatively simple engineering method to calculate estimates for probabilistic properties of turbulent combustion. The road taken is based on the features of Multi-Fluid Model of turbulent mixing put forward by D.B. Spalding [1], which are close to Multi-Environment Method invented by D.O. Fox [2]. The latter was applied by B.H. Hjertager et al. [3] to turbulent mixing under the title of Multi-Spike Model. The central idea of all three above is basically the same. It is that of discretization of composition space into a finite (typically large) number of separate sub-spaces, called environments in MEM or fluid population introduced in MFM, linked with each other by the chain of interchanging probability fluxes. The Stream Recognition Model developed by present author focuses on prediction of probabilities of just three major streams which initiate and maintain the combustion, namely, fuel, oxidant and product. By doing its predictions SRM has managed to combine MEM and MFM in such a way that the use is made of advantages of latter two without so much inheritance of their drawbacks. SRM constitutes a transported probability approach to combustion which requires a coarser discretization of variable space compared to MFM, and involves more accurate treatment of probability fluxes than in both MEM and MFM. The main advantage of SRM is that it can preserve efficiency and accuracy of fluctuating property calculations within reasonable computer-time demand. It has been demonstrated that using SRM it is possible to calculate fluctuating mixing properties, as well as probabilistic turbulence-chemistry interactions, and assess details of thermal and polluting performance of a combustion units - all simultaneously with relative easy. The text below, after some introductory remarks, presents an overview of the physical concept, theory and methodology of the SRM technique, and provides a brief discussion of significance of currently available results of its testing, validation and applications relevant to simulation of turbulent combustion. The detailed technical description of the SRM and its applications is now publicly available elsewhere [4, 5].

Introduction. Over past three decades the industry standard practice is to use the commercial general-purpose CFD codes such as, PHOENICS (http://www.cham.co.uk), FLUENT or CFX (http://www.ansys.com), and others for providing solutions of engineering design problems of industrial combustion.

It is well known that the turbulent mixing of fuel and air to form industrial flames is dominated by turbulence-chemistry interactions. Existing demand of higher reliability and accuracy of computations, and also concern with the sensitivity of important reaction kinetics to the fluctuating nature of temperature and composition distributions has laid special emphasis on the need for an evaluation of this behavior of turbulent flames. However, in engineering practice of combustion analysis the modeling of fluctuating characteristics is often avoided, mainly because (i) it involves complex mathematics needing an appropriate training ; (ii) it usually requires the computer power exceeding what is normally available for project engineers; (iii) it uses, in majority of cases, prohibitively high computational time, and (iv) it possesses a significant uncertainty concerning guidance to the right values of often numerous modeling constants and functions. The most popular engineering model of turbulent combustion remains to date an Eddy Dissipation Method or EDM of direct calculation of flow average reaction rates through physically-controlled mixing mechanisms. It completely ignores any modeling of fluctuating characteristics.

The inability of engineering computational models, such as EDM, of gaseous combustion to calculate the fluctuating heat and mass flow properties has been one of their main disadvantages with respect to more complex methods using, mostly presumed, PDF, i.e. Probability Density Functions. The superiority of employing more sophisticated full methods of transported PDF lies in the fact that unlike presumed PDF methods, full PDFs do not require *a priori* knowledge of neither the shape of the composition PDF nor the distribution of mixture fraction fluctuations, but they are much more computer-time hungry.

The present development provides combustion engineers with a reasonably simple and computationally economical yet realistic and comprehensive way of predicting the fluctuating structure of industrial flames as well as their mean field distributions of mixture composition. To this end it has introduced a SRM, the Stream Recognition Method. SRM combines the multi-environment, MEM, approach proposed by Rodney Fox [1] and the multi-fluid, MFM, model adapted and adopted by Brian Spalding [2].

SRM constitutes a transported probability technique of combustion simulation with accurate treatment of probability fluxes. SRM has an advantage over widely used EDM-type calculations of being capable of calculating, uncomplicatedly, the fluctuating flow properties. The main strength of SRM is that it can preserve efficiency and accuracy of numerical calculations of fluctuating properties within reasonable computer-time demand.

Model concept. The central idea behind SRM is simple. It is that a combusting flow is assumed to comprise homogeneous blend of three streams sharing the same set of flow velocities, as well as mixture density and specific heat, namely, that of the fuel gas, referred below as 1, of oxidant, 2, and of producer stream, denoted as 3. The first two streams usually act as donors providing the third, in probabilistic manner, with reactants to produce combustion products by thermo-chemical transformations. The latter are assumed to take place mainly within producer, acceptor stream.

Conservation equations. Mathematically, SRM is based on the set of Eulerian conservation and transport equations to provide probabilistic tracking of three streams. The local probabilities of each *i*-stream, p_i, are obtained from the special sort of transport equations:

$$\frac{\partial}{\partial t}\left(\rho p_i\right)+ div\left(\rho\vec{U}p_i\right)- div\left(\Gamma_p\ grad\ p_i\right)= R_{p,i} \qquad (1)$$

The latter are of standard format of general conservations, but with sources terms, $R_{p,i}$, formed by probability fluxes transferred from reactant streams into a producer one. The conditions of p_3 at the fuel gas and oxidant inlets are zero. The conditions of p_1 and p_2 are unity at respective stream inlets, and are zero at the others.

The sources created by probability fluxes comprise inter-stream turbulence-probability interactions. Two kinds of such interaction are considered, as illustrated on picture at Fig.1c, a direct mass transfer from streams 1 and 2 to stream 3, and also mass transfer to stream 3 resulted from the collision of two other streams. Such a representation provides the truly indiscriminate interactions between streams, in contrast with MEM direct mechanism only shown in Fig.1a, and solely collision-driven MFM's [10] *modus operandi* , illustrated by Fig.1b, of two predecessors of the current model. The stream probabilities are further related to each other through the summation-to-unity rule.

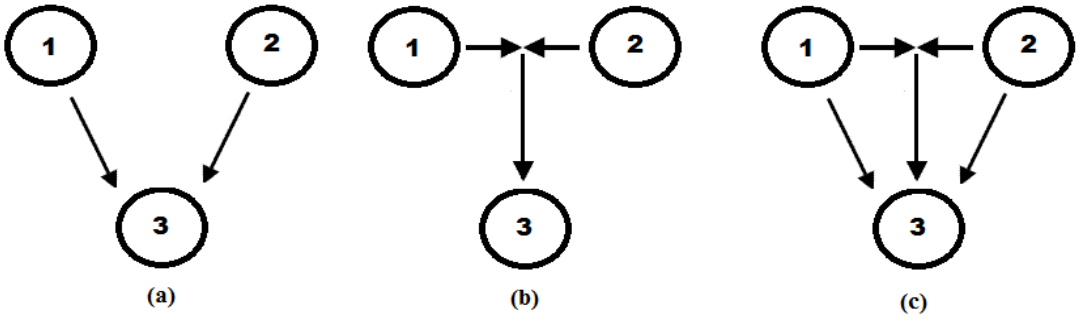

Figure 1. Probability fluxes for three-stream system: (a) - Multi-Environment Mechanism; (b) - Multi-Fluid Mechanism; (c) - Stream Recognition Method.

The additional conservation equations are used to calculate in- stream attributes, such as enthalpy, temperature, element and species mass fractions etc., collectively known as ϕ_i:

$$\frac{\partial}{\partial t}\left(\rho\, p_i\phi_i\right)+ div\left(\rho\vec{U}p_i\phi_i\right)- div\left(\Gamma_\phi\, grad\ p_i\phi_i\right)= R_{\phi_i}+S_{\phi_i} \qquad (2)$$

where S_{ϕ_i} represents other (non-inter-stream) sources.

The stream-weighted, mean and fluctuating characteristics are then readily computed. The details of complete set of transport equations as well as auxiliary and additional calculations can be found elsewhere [4,5].

Presentation of results. The just referenced papers detail the computational algorithm used to compute the transported stream probabilities, flow field, and stream-attribute results. The results of some currently available testing, validation and application cases are also shown in there in terms of

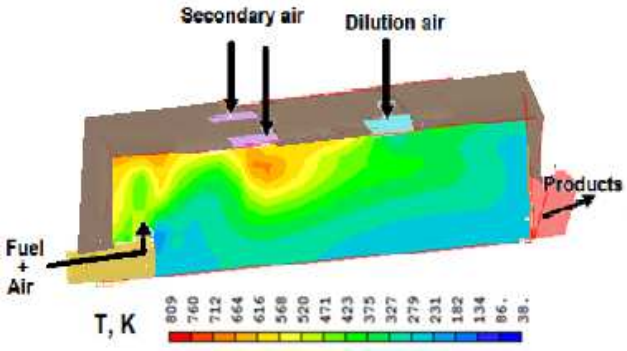

Figure 2. Distribution of RMS of temperature fluctuations in a gas turbine model combustor : taken from [5] .

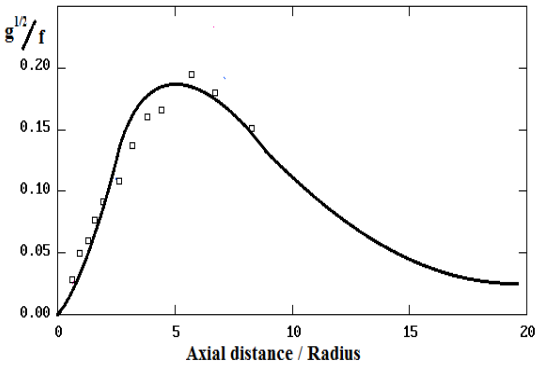

Figure 3. Time mean value of concentration fluctuations in coaxial jets [4]: line - predictions; points-experiment.

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plots for stream probability distribution, temperature , mass fraction contours such as shown on Fig. 2, and distributions of their fluctuations and related correlations, fuel and air utilisation, pollution indices, and also flow field velocity vectors. The SRM-based method is validated against experimental data as seen in Fig.3, the comparisons have been made with EDM and MFM-based numerical calculations. The details can be found in [4] and [5]. The significance of these results is discussed below with further steps required to extend the current methodology.

Discussion of results. The existing, earlier models of transported probabilities have been combined, and seemingly widely applicable computational procedure has been developed for predictions of fluctuating properties of mixing and chemical transformation in turbulent reacting flows. It is, perhaps, the simplest kind of a model that permits predictions of both magnitudes and probabilities of fluctuating properties; it successfully accounts for most practically important fundamental features of turbulence-chemistry interactions; and its use has led to satisfactory predictions of mixing in inert turbulent flows as well as those of reacting kind. The capability of the present uncomplicated set of equations to predict complex changes in the magnitude of fluctuating properties as well as their probabilities in real-life industrial equipment is very encouraging. The SRM analysis generate meaningful results for all the spectrum of case studies and practical applications considered so far. The approach developed permits the quantitative calculation of slow pollutant-forming reactions, simultaneously with finite rate and relatively fast combustion reactions.

Convergence was achieved, by and large, unproblematically for all case studies considered. Some oscillations were observed in the residual plots, though these did converge without difficulty, when reasonable relaxation was used. This is , undoubtedly, mainly due to the fact that the sum-to-zero rule is strictly applied to the related sources in all conservations governed by or involving probability transports.

The conservation equations (1) and (2) for stream probabilities and related attributes are easy to use and interpret because all of them are of familiar type. The terms of equations employ formulations of probability fluxes with little or no calibration constants (elsewhere present author has successfully connected the main empirical constant of SRM with value of unity).

The field distributions of stream probabilities generated by SRM provide valuable insight into the fluctuating nature of combusting flow. So, it is well known that turbulent combustion processes are characterized by intermittency which is ignored in most of the industry-standard models of

turbulent-chemistry interactions. Computations of fluctuating properties and their correlations which are inexpensively derived from present approach allow the intermittency factors to be calculated through the probabilities of different streams present in a flow system.

A theoretical model developed is based on conservation equations of conventional format, and, therefore, is easy to implement in computational loops of available finite-volume CFD solvers. Moreover, the predictions are performed much more economically than with any calculation procedure of similar kind known to the present author. And yet the computations provide detailed information of each stream recognized to be present in the flow system, regarding three-dimensional fields of their presence probabilities, of stream temperatures, of stream compositions, and their fluctuations.

Concluding remarks. The current development has demonstrated the capabilities of a novel approach to modeling of turbulent combustion processes. A combustion solver of PHOENICS equipped with SRM, the probabilistic flow–chemistry module, is used in this study, and calculation procedure has been built around it for the combusting flow involving fast, finite and low reaction rates. The main advantage of the SRM is that it allows reliable calculations of transported probabilities and resulting fluctuated fields to be obtained at a fraction of the computational cost needed to perform calculations using existing methods of similar descriptiveness.

The developed procedure is broad in its capabilities, and is, in particular, readily applicable to both premixed and diffusion flame computations. The procedure has been successfully applied to a number of laboratory case studies and those of realistic three-dimensional geometry and operating conditions. It has been demonstrated that it is possible to calculate fluctuating *in-stream, stream-weighted* and *mean* flow properties, as well as probabilistic turbulence-chemistry interactions, and assess details of thermal and polluting performance of combustion units - all simultaneously with relative easy.

A further systematic validation of the model with reference to experimental quantitative observations of laboratory and industrial equipment performance seems to be very desirable. Successful practical validation will allow this approach to be used with confidence in determining detailed temperature and composition of combustion-product patterns in real-life industrial equipment. In any case, the investigation of the SRM is still in progress; and its new approach needs to be combined with an appropriate model of thermal radiation, and the latter will have to be taught to interact probabilistically with turbulent chemistry before it can be said that the main acceptability

tests of the model have been successfully passed.Yet it is maintained that the achieved level of agreement between predictions and measurements is satisfactory, and the model is already sufficiently detailed to justify the use of present methodology for many engineering purposes.

However, there is substantial scope for further model development and improvement: larger number of participating streams can be accounted for, using more general stream interaction mechanisms; the boundary heating effects (at the internal and external walls) need to be represented as a separate additions to the stream enthalpies; again the inclusion of radiation model to handle turbulence-radiation interaction should perhaps be given a preferential consideration. If it is worth taking into consideration, finer discretization of producer stream could also be thought over, perhaps, to improve the accuracy of temperature calculations and related computations of fluctuating thermo-physical flow properties, as well as those of finite-rate chemistry effects of multi-step reactions. The assumption of homogeneous nature of stream mixture can also be relaxed by allowing different streams or groups of them to move with their own velocities. All of these developments would be a natural extensions to the work described in this article, and it is not very hard, although not entirely effortless either, to extent the present theory in those directions.

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