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# A parametric turbulence closure for simple gas phase chemistry in an extended Eddy Break-Up combustion model

Peter P. Breithaupt

This thesis deals with mathematical modelling of gaseous turbulent diffusion flames by means of computational fluid dynamics (CFD). Emphasis is laid on fuel efficiency measures, because improvements in process efficiency often provide the benefits of pollutant reduction as well. However, only few companies can accept the cost and risk of undertaking cutting-edge technological developments and testing in full scale facilities. The industry-wide need to develop or to retrofit new gas-fired combustion equipment into either novel, or existing production facilities gives rise to the need to predict with reasonable accuracy the effect of both combustion equipment modification and process operation upon general combustion performance. As time-to-market cycles become even more shorter, engineering practice demands solutions either over “lunch-time” or over “night”. At present, industrial combustion analysis is only obtainable through the application of Reynolds-averaged Navier-Stokes (RaNS) equation together with single- or reduced multi-step reaction mechanisms. Although Eddy Break-Up (EBU) combustion models are known for their reasonable performance in predicting strongly stabilized industrial flames, model improvements are required when strong turbulent combustion flow fields in flames are chemistry-stabilised as is the case in modern gas-fired combustion systems.

A general method to tackle this kind of prediction is to apply the combination of the EBU model with global Arrhenius multi-step reaction mechanisms to account for slow reaction kinetics. However, as it is shown in this thesis, the simple application of published global Arrhenius formulations for methane combustion fail to predict values of turbulent in-flame reaction rates by order of magnitudes.

The major objective of this thesis is to show, theoretically, that a solution to this problem could be derived from an earlier attempt by Borghi: the moment closure-method, when incorporating turbulent effects in Arrhenius equations. A factor is derived which approximates the closure of all higher-order correlations with regard to turbulent effects. However, this factor has no analytic solution and the form of the function and its parameters have to be derived from computational data. This closure function is called here a “*parametric turbulence closure*”.

Consequently, the next objective is to obtain a sufficient number of turbulent reaction rate data which allow for a detailed statistical analysis to deduce a model for the parametric turbulence closure. These data are generated from validated CFD predictions of a swirl-stabilized 2 MW, natural gas flame by means of the Eddy Break-Up combustion model only. Since the computations are performed using a global 2-step reaction mechanism for the combustion of gaseous hydrocarbon, it may be called a “*simple gas phase chemistry*”.

The analysis of computed reaction rates versus various flow field quantities leads to the proposal of a model for the parametric turbulence closure. Multiple linear regression is applied to probe the model's ability to predict the results of the original data. The model replaces the standard Arrhenius formulation “*in an extended form of the EBU combustion model*”.

Finally, the last objective of this thesis is fulfilled, namely, to test the “novel” combustion model against an independent sample space. The agreement between predictions and measurements is found to be superior over comparable models. Most remarkable is that, although statistically derived from a type-2 swirl-stabilised natural gas flame, the “novel” combustion model is also able to predict lifted turbulent jet flames with accuracies needed to support engineering decisions. Further application of this “novel” combustion model to predict various turbulent flame structures is needed to gain more confidence in its performance.