Curve matching: a generalized framework for combustion model validation.

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The increasingly higher size of combustion kinetic mechanisms, in terms of the number of involved species and reactions, makes any critical analysis of the provided output a difficult task. Moreover the validation of these models over a wide range of operating conditions with the available experimental data, is often the most time consuming part of models development. In fact a critical analysis of the obtained results is not always compatible with an iterative process of variables refinement.

Therefore, the reduction of the time required for a continuous human guided validation through an automatized process, would significantly speed up the whole model development. This would improve the overall performances, thus allowing to focus on more fundamental aspects of chemical kinetics.

The state of the art automatic approaches for assessing the quality of a model are usually based on Sum of Squares Methods (SSM). Nevertheless in several cases this method may provide misleading feedbacks, preventing a direct generalization in the extensive validation of a mechanism.

Moving from these issues, in this work, a new framework for model comparison is presented, in the attempt to overcome the limitations of the current approaches. This method is focused on the computation of four distances between the experimental points and each model. Every distance provides different information about the adherence of the model curve to the data, thus allowing a precise analysis of its characteristics. Eventually, the quantitative evaluation of the aforementioned distances allows to create a proper ranking.

Moreover, when a database of models describing the same experiment is available, the method can detect the outliers: for example, in a variable refinement process, it is possible to detect those steps which are significantly improving or worsening their performances.

The benefits of such a generalized approach are wide. Beyond the most direct applications discussed above, it can provide a significant breakthrough in several related fields: an immediate use for reduced mechanism development and validation has been identified, as well as ranking models of different nature aimed at reproducing the same set of experimental data and phenomena.