Validation of Detailed Chemical Kinetic Models

H. J. Curran

National University of Ireland, Galway, Ireland

Abstract

Stricter emissions legislation combined with the need to reduce greenhouse gas emissions in order to militate against climate change drives fundamental research to produce cleaner more efficient systems. Chemical kinetic mechanisms are used by relevant industries to predict and optimize the operating behaviour of experimental facilities such as internal combustion engines, gas turbines and other combustion devices. More practically, detailed chemical mechanisms are reduced so that they reproduce the relevant target be it ignition delay time, flame speed, etc., and then combined with computational fluid dynamics simulations in order to accurately represent the whole combustion environment.

However, in order to validate and produce accurate detailed chemical kinetic mechanisms in the first instance, a wide range of data is needed, and which is normally generated under well-controlled physical conditions of temperature, pressure, fuel/air ratio and dilution. These data include (i) ignition delay times recorded in shock tubes and in rapid compression machines, (ii) speciation data from flow reactors, jet-stirred reactors and flame experiments and (iii) flame measurements of laminar burning velocity. Typically, these mechanisms for hydrocarbon and oxygenated hydrocarbon systems are generated in a hierarchical way, starting first with the hydrogen/oxygen system, thereafter adding a carbon monoxide/carbon dioxide subset, followed by formaldehyde, methane and other larger C_1-C_n species.

This work will discuss the development of detailed chemical kinetic mechanisms in the context of hierarchy and range of validation. Some typical problems associated with these mechanisms will be discussed and some ideas on how they may be addressed will be explored. Moreover, the application of detailed kinetic mechanisms to fuel flexibility in gas turbines will be explored in some more detail.