2013 AAAS (American Association for the Advancement of Science) Annual Meeting

Chemical Models for Combustion: Abstract

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The requirement to reduce greenhouse gas emissions is a necessary driver for the development of many new technologies and increasing passenger demands within the transport sector make it a priority area. In a rapidly developing world where the number of vehicle miles travelled is constantly increasing, there will be a reliance on technical solutions to lower engine emissions of both greenhouse gas, and pollutants of relevance to human health such as nitrogen oxides and soot. Within the internal combustion engine, the use of alternative fuels such as biofuels and Fischer Tropsch derived fuels has the potential to lower overall emissions. However, such fuels must be used efficiently and cleanly requiring the development of new engine technologies such as homogeneous compression charged ignition (HCCI) or direct injection systems. The HCCI engine combines the advantages of spark ignition engines with those of compression ignition ones (used in Diesel engines). The homogenous fuel/air mixtures leads to low particulate emissions whereas high dilution leads to low NOx production, while still maintaining high efficiencies. The successful design and operation of such engines depends on controlling the timing of the auto-ignition process which is known to be governed by complex chemical processes. It is important therefore that engine models used in design are able to incorporate chemical processes at sufficient levels of detail and for a wide variety of possible future fuels. The presentation will address the types of chemical models that can be used within the engine design process for current and future fuels. A particular focus will be the confidence with which we can use such complex models which contain many detailed reaction steps each requiring a quantification of reaction rates over the range of temperature and pressure conditions experienced within engines. Methods for identifying the sources of uncertainty in predicting ignition characteristics will be addressed. New methodologies based on the optimisation of reaction mechanisms which aim to reduce such uncertainties will be introduced.