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Chemistry Aspects of Alternative Energy Carriers Utilization

par

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The increasing scarcity of conventional fossil energy carriers, increasing energy needs and the need to mitigate environmental concerns are major societal challenges of the first half of the 21st century. The substitution of conventional fossil fuels requires diversification of energy carrier sources and increase of conversion efficiency. These needs call for new chemical energy carriers, extending toward molecules from alternative sources, and advanced combustion technologies that are fuel flexible and efficient under conditions (low/high temperatures, extreme lean/rich/diluted mixtures, high pressures) significantly different than those of conventional combustion modes and where chemical knowledge/models is limited/unknown even for conventional fuels.

The present work presents an overview of chemical aspects of alternative energy carriers utilization. The starting point is the chemistry of small C_1-C_2 hydrocarbons, some of which, such as methanol, ethanol and DME, are also potential alternative transportation fuels. Further development and application of a comprehensive detailed kinetic mechanism for the combustion of small hydrocarbons and oxygenated species in flames is presented and discussed. The mechanism is further utilized in order to explore synergies in the combustion of e.g. methane-hydrogen and methane-higher hydrocarbon mixtures which are pivotal when considering dual-fuel engine combustion with EGR. The reforming potential and efficiency of natural gas is also considered in detail and the study supports design guidelines aiming towards identification of optimum operating conditions, for particular fuels.

The introduction of novel fuels with not well known behaviour, also imposes the need for development of appropriate experimental and numerical combustion metrics. A review of heat release metrics is presented. The detailed kinetic mechanism is used to assess correlations between heat release rate and appropriate chemical markers (e.g. species mole fraction and/or elementary reaction rates) in laminar premixed flames. Detailed kinetic computations are interrogated through suitable analysis tools (such as rate-of-production and sensitivity analyses) to assess the validity and generality of proposed correlations.

The final part of the paper deals with issues related to catalysis and after-treatment. There are also specific challenges faced by the exhaust gas after-treatment systems of natural gas engines. The major concerns are the low exhaust temperatures and the unreactive methane in the exhaust stream (methane slip). Catalysts and systems that can be used to address the above challenges are discussed. Soot formation is less of a problem in natural gas engine. However it can still be formed during on-board reforming and little is yet known about its properties. The paper presents data on morphology and chemical characterization of soot formed from natural gas mixtures. Results from preliminary work on fuel effects on soot are presented. Finally, a brief review of studies related to the health impacts of exhaust emissions of engines operated with conventional and alternative fuels is presented.

Prochain séminaire prévu 17/04/2014, 11h
Modelling & numerical simulation of low Nox pulverized coal burners, par Erinç KAPUSUZ, doctorant co-tut. ICARE/Marmara U.

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