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Alternative fuels: challenges and opportunities of combustion research

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With more than 85% of the current world energy being converted by combustion, the use of alternative fuels with increased energy efficiency is among the most important solutions for energy sustainability and has posted a grand challenge in combustion research to develop robust and predictive tools for innovative engine design. The lecture will discuss several technical challenges and opportunities in combustion research arising from the use of alternative fuels and their complex chemical kinetics, modeling, diagnostics, and ignition control at extreme conditions.

The first challenge of a drop-in alternative fuel is how it will impact engine performance and emissions. As the future engines are designed for higher pressure, lower temperature, and dual and multiple fuels, how do we control and predict the ignition and heat release rate to achieve better efficiency and lower emissions? In this lecture we will present a generic surrogate fuel modeling approach and concepts of radical index and transport weighted enthalpy to rank the fuel reactivity and model real fuel combustion with a few component fuel mixtures.

The second challenge is that combustion of a realistic alternative fuel and its blends often involves thousands of species and ten thousands of reactions. Many of the combustion properties and elementary reactions are strongly pressure dependent. How do we develop a kinetic model to be applicable to practical engine conditions? How do combustion diagnostics and ab initio quantum chemical computation play a role in kinetic model development? The lecture will use hydrogen, dimethyl ether, and biodiesel as a few examples of the gap of knowledge in high pressure combustion and introduce the opportunities of new combustion diagnostics such as the mid-infrared Faraday rotational spectroscopy and ab initio quantum chemical computation.

The third challenge is how to understand turbulence-chemistry interaction at low temperature and how to model turbulent combustion with hundreds and thousands of species. The lecture will discuss a new turbulent diagram and experimental method to address high pressure and low temperature turbulent combustion, and present a multi-time scale method (MTS) with a correlated-dynamic adaptive chemistry (CO-DAC) approach to improve drastically the computation efficiency of combustion with large kinetic mechanisms. Finally, opportunities using plasma assisted combustion to activate low temperature chemistry and enable ultra lean combustion will be presented.

Keywords: alternative fuels; combustion research; challenges and opportunities

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替代燃料：燃烧研究的挑战和机遇

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当前世界能源的 85％以上是通过燃烧转化。使用具有高能源效率的替代燃料，是能源可持续性的首选解决方案之一。它将在燃烧研究上引起大挑战，即为新发动机设计发展强健的预测工具。本次讲座将讨论使用替代燃料进行燃烧研究中遇到的几个技术挑战和机遇，以及替代燃料中复杂的化学反应动力学，建模，诊断，及极端条件下的点火控制。

第一个挑战是关于直接替代燃料如何影响发动机的性能和排放。未来发动机为高压、低温、双重和多重燃料所设计，那么我们将怎么控制和预测点火和热释放速率，以实现高效率和低排放？本次讲座中我们将提出一个通用的替代燃料的建模方法，和使用激进指数和运输加权焓来排名燃料反应的概念，并且模拟真实的有若干组成部分的混合物燃料的燃烧。

第二个挑战是因为真实替代燃料及其混合物的燃烧往往涉及几千种上万次的反应。许多燃烧性能和基本反应都有强压力依赖性。我们应如何建立适用于发动机实际条件的动力学模型？燃烧诊断和量子化学从头计算在动力学模型发展中如何发挥作用？本次讲座将使用氢气，二甲醚，生物柴油作为几个例子来看高压燃烧的不同，并引进新的燃烧诊断方法，如通过中红外法拉第旋转光谱和量子化学从头计算。

第三个挑战是如何理解低温下湍流与化学反应之间的相互作用，以及如何模拟具有数百千种类的湍流燃烧。讲座将讨论新的湍流图和实验方法来解决高压低温下的湍流燃烧，并提出多时间尺度方法（MTS）与相关动态自适应化学（CO-DAC）的方法，大大提高对含有大型动力学机制燃烧的计算效率。最后，提出使用等离子体辅助燃烧来启动低温化学和启用超稀薄燃烧的可能性。

关键词：替代燃料；燃烧研究；挑战和机遇