Droplets autoignition simulations of ethanol mixtures with a reduced kinetic mechanism

A. Millán-Merino a,*, E. Fernández-Tarrazo a, M. Sánchez-Sanz a, F.A. Williams b

Droplet ignition and combustion is a very relevant problem in combustion applications. Many studies have been conducted in the past, both theoretical [1, 2] and experimental [3, 4]. In view of the increasing use of biofuels, either as pure fuels or mixed with hydrocarbons, accurate modelling of vaporization and chemistry of such fuels is needed in order to optimize the systems to be used with biofuels and thus, facilitate their introduction. Ethanol is, by large, the most used biofuel, because it is easy to produce and because it is adequate to be used with present-day systems, considering both engine technology and fuel storage aspects.

In typical combustion applications involving liquid fuels, the fuel is injected, in the form of a spray, in the combustion chamber, where the prevailing conditions include recirculated exhaust gases at high temperatures. In these conditions, heat transfer from the produces fuel vaporization and a fuel mixture evolves in the gas phase until either ignition is forced or autoignition is achieved.

In this work we will focus on the vaporization and autoignition of a single multi-component droplet in realistic high temperature ambient conditions, in the absence of microgravity. With the aim of obtaining realistic autoignition times, accurate submodels for the different inter-coupled physical phenomena are required. Especial attention is given to the chemistry, where a multipurpose 14-steps chemical model, previously developed [5] is used, while adequate models are used for molecular transport, thermodynamics and phase change.

Numerical results are obtained using an unsteady finite volume discretization. Effects of droplet size, ambient temperature and humidity content -both in the ambient and in the liquid fuel- on autoignition times are analyzed.

- [1] A. Kazakov, J. Conley, F. L. Dryer, Detailed modeling of an isolated, ethanol droplet combustion under microgravity conditions, Combust. Flame 134 (2003) 301-314.
- [2] V. Nayagam, D. L. Dietrich, F. A. Williams, Unsteady droplet combustion with fuel thermal expansion. Combust. Flame 195 (2018) 216-219.
- [3] A. Lee, C. K. Law, An experimental investigation on the Vaporization and Combustion of Methanol and Ethanol Droplets, Combust. Sci. Tech. 86 (1992) 253-265.
- [4] C. L. Vang, B. D. Shaw, ISS Experiments on Combustion of Heptane/Hexadecane Droplets. AIAA J. (2018) 1-12.
- [5] A. Millan-Merino, E. Fernandez-Tarrazo, M. Sanchez-Sanz, F.A. Williams, A Multipurpose Reduced Mechanism for Ethanol Combustion, Combust. Flame, 193 (2018) 112-122.

^a Departamento Ingeniería Térmica y de Fluidos, Universidad Carlos III de Madrid, Madrid, Leganés 28911, Spain

^b Department of Mechanical and Aerospace Engineering, University of California San Diego, La Jolla, USA