A Preliminary Assessment of Alternative Fuels for Marine Engines using Combustion Chemistry Tools

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Introduction

The de-carbonization of the shipping industry is critical in the context of low-carbon economy and the mitigation of the adverse effects of GHG emissions. The shipping industry is under increasing pressure to act upon the Paris Agreement and reduce greenhouse gas (GHG) emissions and other emitted hazardous pollutants at local level, such as NOx, SOx and particulate matter.

Conventional oil-based fuels will remain the main fuel option for most vessels in the near future: in a 10-15 year perspective HFO, LSHFO and MGO will still be the most used fuels for ships due to their cost effectiveness.

Reducing emissions from shipping is a challenging task that requires the use of energy efficiency measures, the increased penetration of alternative renewable fuels as well as the deployment of advanced aftertreatment technologies [e.g. 1, 2].

The introduction of alternative fuels will also have a positive effect on local air quality in ports, harbours and coastal areas as it will lead to significant reductions in sulphur emissions. However, the effect of fuel substitution on pollutants, including nitrogen oxides and unburned hydrocarbons, cannot be readily quantified and dependent not only on fuel/fuel mixture properties but also on engine operating conditions.

LNG will be a suitable fuel for new built ships in certain areas were logistics are well developed. A large number of LNG fuelled ships and LNG tankers sailing the oceans today have been certified and classed by the international verification bodies. LNG offers huge advantages, especially in the light of ever-tightening emission regulations, as it can provide a smart way to meet existing and upcoming requirements for the main types of emissions (SOx, NOx, PM, CO2). Moreover, LNG can be competitive pricewise with distillate fuels and, in many cases does not require the installation of additional process technology.

On the other hand, there is a number of projects implemented by international maritime companies that demonstrate the growing interest and potential of methanol as a marine fuel. As an example, the Stena Germanica passenger ferry is mentioned, which runs on methanol [3].

Methanol features Hydrogen to Carbon (H/C) ratio of 4/1 (similar to the H/C ratio of LNG), which allows classifying it as a low carbon content fuel. Accounting on molar mass and lower heating value, this results in around 20% less CO2 emitted while combusting methanol, compared to diesel with similar efficiencies. This result is similar to LNG (for LNG, methane slip creates additional GHG

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issue) and along with sustainable production potential (from captured CO2 and electricity) predefine methanol as one of short-term transition fuels for transport [4].

While there are no projects directly focusing on the use of ethanol, or other oxygenated fuels such as DME, on ships, the long interest on the use of these fuels in diesel engines in road transport for many years, makes them candidates for maritime applications as well [1].

The objective of the present work is to provide a decision support methodology for the assessment of potential alternative fuels for the shipping industry in terms of combustion efficiency and pollutant formation using a kinetic approach.

This involves assembly and validation of both in-house [5] and literature [6, 7] combustion chemistry models of various complexity for small hydrocarbon species also incorporating a comprehensive nitrogen chemistry sub-mechanism and appropriate sub-models for PAH and soot formation. The assessment will be based on kinetic computations in fundamental reactors mirroring marine engine operation both in terms of key operating parameters (pressure, temperature, mixture composition) and residence time distribution. The effects of Exhaust Gas Recirculation on the mixture and exhaust gas compositions will be also considered in detail.

Computations are performed for a wide range of gaseous fuels including natural gas (also LNG), LPG, biogas (CO_2-CH_4 mixtures) and methanol. Results obtained in the form of global performance indicators (such as burning velocities and ignition delay times) and exhaust speciation data (including the potent CH_4 and N_2O GHG). Chemical aspects of the fuel conversion processes are investigated through rate-of-production path and sensitivity analyses.

The work concludes with the definition of appropriate metrics for the quantification of the effects of fuel substitution on combustion performance and emissions under typical marine engine operating conditions.

Methodology and approach

In a previous study an optimized skeletal chemical kinetic mechanism for methane combustion, for conditions relevant to dual-fuel marine engines was developed. The mechanism was developed on the basis of a systematic approach that considered (a) the assessment of available mechanisms, (b) their analysis through reaction path and sensitivity analyses, (c) production of a skeletal mechanism by means of the simulation error minimization connectivity method, (d) uncertainty analysis of the rate constants of important reactions, and (e) optimization of the skeletal mechanism for the rate constant parameters of the important reactions. The model has been validated against (i) laminar flame speeds, (ii) ignition delay times, and (iii) speciation data from JSRs for methane combustion, in a wide range of conditions, relevant to dual-fuel marine engine operation in the gas mode. Figure 1 presents indicative results from [8].

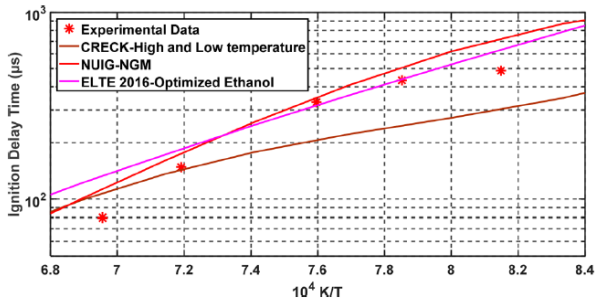

Figure 1 (a): Ignition delay time profiles versus initial temperature for P = 85 atm and φ = 3.0, with mixture composition per volume of 20.0% CH4, 13.3% O2, and 66.7% Ar (see [8] for details).

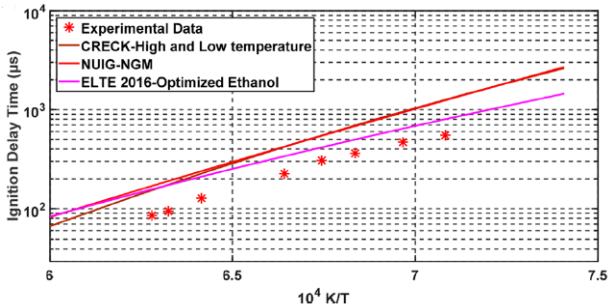

Figure 1 (b): Ignition delay time profiles versus initial temperature for φ = 0.5 and P = 39.5 atm, with mixture composition per volume of 1.0% CH4, 4.0% O2, and 95.0% Ar (see [8] for details).

In the frame of this work, the mechanism is further developed on the basis of the oxygenated chemistry part of the model in [5] and is further validated against experimental data from methanol combustion in fundamental configurations. The model also includes a Poly Aromatic Hydrocarbon (PAH) sub-mechanism taking into account the combustion of naphthalene and toluene selected in the present work as solvent representative species. Indicative validation campaigns are presented for: (a) stoichiometric premixed C_1-C_2 oxygenated flames of formaldehyde, methanol, acetaldehyde and ethanol (Figure 2).

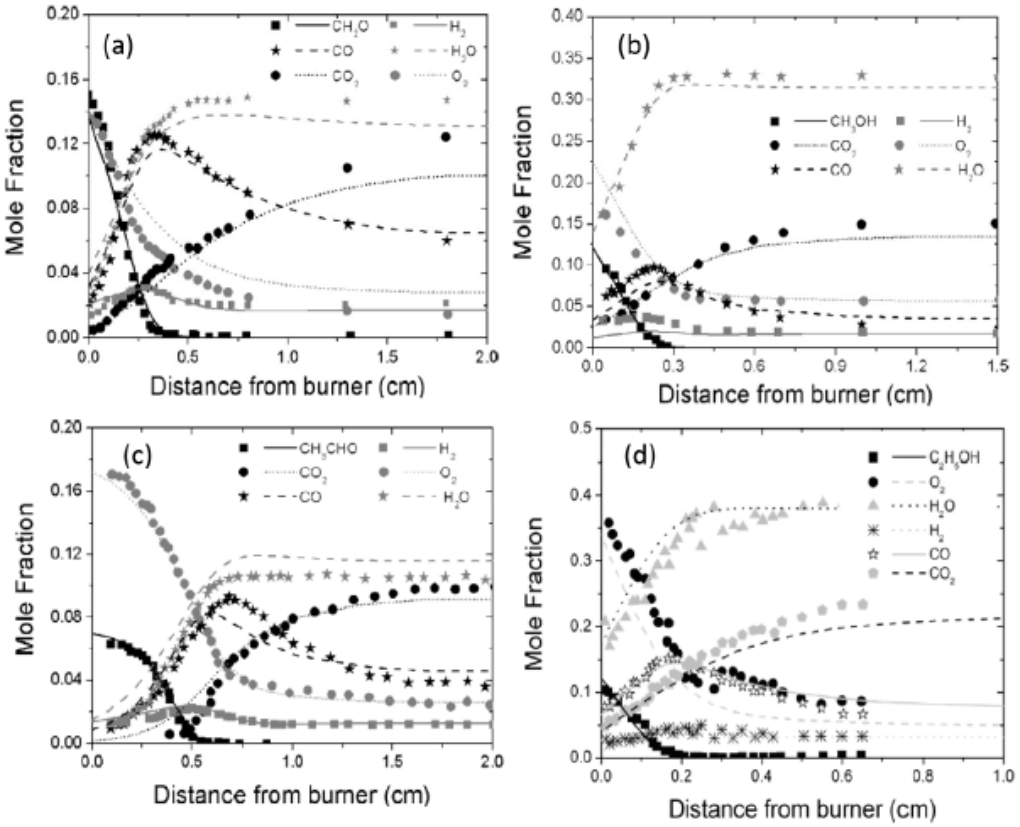

Figure 2: Computed (lines) and experimental (symbols) of major species profiles in: (a) formaldehyde flames, (b) methanol flames, (c) acetaldehyde flames, (d) ethanol flames (see [5] for details).

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