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Modelling of temporal and spatial evolution of sulphur oxides and sulphuric acid under large, two-stroke marine engine-like conditions using integrated CFD-chemical kinetics

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HIGHLIGHTS

- A reduced sulphur mechanism, consisting of 4 species and 5 reactions is developed.
- SO_2 to SO_3 conversion and sulphuric acid formation in a marine engine are simulated.
- The conversion at varying fuel sulphur contents and engine conditions is predicted.
- The absolute values of simulated and measured SO_2 to SO_3 conversion levels are close.
- Sulphur acid condensation may begin early at the top part of the cylinder liner.

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ABSTRACT

In this work, three-dimensional computational fluid dynamics (CFD) studies of sulphur oxides (SO_x) and sulphuric acid (H_2SO_4) formation processes in a large, low speed two-stroke marine diesel engine are carried out. The current numerical study aims to investigate the conversion of sulphuric dioxide (SO_2) to sulphuric trioxide (SO_3) and the possibility of H_2SO_4 condensation which are the prerequisites to better understand the corrosion-induced wear phenomenon. This is achieved with the aid of the implementation of a multicomponent surrogate model, which comprises a skeletal *n*-heptane mechanism and a reduced sulphur subset mechanism. In the present work, performance of the coupled CFD-chemical kinetic model is evaluated using both qualitative and quantitative methods. The modelling results show that the temporal and spatial evolutions of SO_x predicted by the skeletal model are similar to those by the base mechanism. Predictions of the variations of SO_x and the associated SO_2 to SO_3 conversion in response to the change of fuel sulphur content, swirl velocity, start of injection, scavenge pressure and humidity qualitatively agree with numerical and experimental results from the literature. The model is further evaluated using the measured SO_2 to SO_3 conversion levels in a low load, low scavenge pressure case and a low load, high scavenge pressure case. The absolute values of simulated and measured conversion levels are close, although the former appear to be higher. The current results show that the flame impinges at the cylinder liner near top dead centre. The gas is cooled rapidly by the wall temperature and H_2SO_4 is produced in the region where the local temperature is less than 600 K. Based on the flue gas correlation, the acid dew point temperature is higher than the wall temperature, suggesting that acid condensation may begin early at the top part of the cylinder liner. The predicted distribution corresponds well with the distribution of corroded parts observed in service engines. The model is expected to serve as an important tool to simulate the rates of SO_2 absorption into lubricating oil film and H_2SO_4 condensation in this combustion system.

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1. Introduction

The majority of the world trade is carried out by the international shipping industry. The de-facto standard propulsion technology for large commercial vessels, for instance container ships, bulk carriers and tankers, is the large, low speed two-stroke marine diesel engine. The two-stroke concept offers a thermal efficiency of above 50% despite the fact that the commonly used fuel, heavy fuel oil (HFO), is of low quality. Sulphur is generally present as an impurity in HFO. During the in-cylinder combustion process where air is in excess, most of the sulphur is oxidised to sulphuric dioxide (SO_2). The absorption of SO_2 into the engine lubricating oil film may play a role in cylinder wear [1]. Meanwhile, a fraction of SO_2 is subsequently oxidised to sulphuric trioxide (SO_3) [2] and SO_3 reacts with water vapour (H_2O) to form sulphuric acid vapour (H_2SO_4). The latter condenses as aqueous sulphuric acid on engine cylinder liners where the local temperature is low. This promotes corrosive wear on the cylinder liner. The present solution is to apply lube oil which contains limestone additives to neutralise the acid and hence to impede corrosion on liner surfaces. This however increases the operational costs. Also, the rate of acid condensation is dependent on engine operating conditions and fuel sulphur content. Practical evaluations of acid reaction on cylinder liners are therefore not straightforward and optimising the lube oil treatment becomes complicated. In order to prolong the engine lifespan with minimal expenses on lubrication, an improved understanding of the formation of sulphur oxides (SO_x) in HFO combustion as well as the subsequent H_2SO_4 formation, condensation, and corrosion processes is essential.

While the influences of H_2SO_4 on the physical and chemical behaviour of marine diesel engine lube oils and piston ring were investigated [3,4], engine-out measurements of SO_x from large, low speed two-stroke marine engines, to date, remain rare [5]. The experimental investigations of emissions have been focusing on nitrogen oxides (NO_x) and/or particulate matter [6–9]. Even though Tsukamoto et al. [9] measured the conversion rate of sulphur in fuel to sulfate in particulate matter in their two-stroke marine diesel engine experiment, their study concentrated more on the effects of sulphur on particulate formation but not explicitly the formation of SO_x [9]. The most relevant experimental work was carried out by Cordtz et al. [10] who investigated the tailpipe SO_3 formation of HFO in a medium speed four-stroke test engine. A series of SO_3 measurements were carried out in the exhaust gas produced by a single-cylinder test engine with a rated speed of 1500 revolution per min (rev/min). The measurements covered a range of operating conditions from low to full load under steady-state conditions, wherein start of injection (SOI) timing, engine speed and air-fuel ratio were varied to alter the combustion history. In another study, Engel et al. [11] investigated exhaust gas compositions sampled from five large diesel engines over a range of engine operating conditions using fuels with 0.05–0.8% sulphur. The influences of fuel sulphur contents and engine operating conditions on SO_3 formation were studied. In both studies, variation of the SO_3 production with respect to the change of operating condition and fuel sulphur content was indicated by the conversion of SO_2 to SO_3 (ε), calculated using Eq. (1),

$$\varepsilon = \frac{[SO_3]}{[SO_2] + [SO_3]} \quad (1)$$

This expression assumes the H_2SO_4 concentration is lumped with the SO_3 concentration. Both studies suggested that the conversion levels varied within the range of 1.0–8.0%.

Other investigations on the SO_x formation in marine diesel engines rely mostly on theoretical models [5,12]. For these numerical studies, the fuel oxidation model is different from the typical pure hydrocarbon oxidation model used in gasoline or diesel engine simulations. Instead, accurate high temperature sulphur chemistry is required to be coupled with the fuel oxidation model. Previous research on sulphur kinetics in flames has provided an overall understanding of the general aspects of the associated high temperature chemistry [13–17]. However, early models suffered from a lack of accurate thermodynamics and kinetic data. Glarborg and co-workers [2,16,17] proposed a detailed hydrogen/sulphur/oxygen (H/S/O) reaction mechanism, using laboratory reactor experiments and theoretical predictions to support the model formulation. Although the validation of the H/S/O mechanism was carried out under atmospheric pressure, it would be expected to extrapolate well to higher pressure levels. Cordtz et al. [5] as well as Andreasen and Mayer [12] combined the mechanism with a multi-zone model for the investigation of SO_x formation under large, two-stroke marine diesel engine conditions. In their work, the mechanism did not account for the decomposition or oxidation of hydrocarbons. Solely the post flame phenomena were simulated and chemical reactions were initiated by equilibrating the species at stoichiometric conditions. One of the main limitations of these studies [5,12] or in general multi-zone models [18] was the absence of detailed information of the temperature and combustion product distributions. In addition to this, a mixing constant had to be calibrated for different engine speeds [5].

Alternatively, three dimensional (3-D) computational fluid dynamics (CFD) modelling of marine engines is a promising tool to provide a more comprehensive insight into in-cylinder events [19,20]. Nonetheless, several issues have to be addressed beforehand. First of all, the simulation has to initiate from fuel injection, followed by fuel evaporation, ignition and combustion. An accurate yet compact surrogate model which describes both hydrocarbon and sulphur oxidation has to be constructed. It is noteworthy that, although different reduced mechanisms for sulphur oxidation have been proposed [5,21], they are not coupled with hydrocarbon subsets or validated under engine-like conditions. Another challenge is to simulate the thermal boundary layers on the cylinder wall liner during the high temperature flame jet impingement where the temperature gradient is usually steep [22,23]. The peak temperature in the flame jet can reach above 2700 K while the cylinder liner wall temperature is much lower at approximately 400 K [19]. Based on the steady-state Reynolds-averaged Navier–Stokes (RANS) simulation on heat transfer from combustion gaseous to the piston surface in a large marine engine performed by Jensen and Walther [24], it was found that both the magnitude and the distribution of the predicted wall heat transfer varied significantly when different wall models were applied. This indicates that such calculation was strongly dependent on the empirical models. The local temperature near the cold wall is however crucial for the computation of H_2SO_4 formation rates and has to be properly simulated.

Set against these backgrounds, the objective of this work is to develop numerical models for the investigation of SO_x and H_2SO_4 formation in a large, low-speed two-stroke marine engine. As aforementioned, a compact multicomponent surrogate model that accounts for SO_x formation is not available from the literature. A reduced sulphur subset mechanism is first developed in the current work and is incorporated with the skeletal *n*-heptane model which was previously built [19]. Apart from this, the near wall spatial resolution is also carefully examined to ensure that the thermal boundary layers along the cylinder liner are properly resolved. The coupled CFD-chemical kinetic model is then evaluated using both qualitative and quantitative methods. Finally, temporal and spatial distributions of SO_2 and H_2SO_4 on the cylinder liner are investigated using the model.

The remainder of the paper is structured such that the formulation of the skeletal chemical mechanism and CFD models are next

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