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Numerical simulation of condensation of sulfuric acid and water in a large two-stroke marine diesel engine

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HIGHLIGHTS

- The film condensation affects the total mass of acid vapor.
- The scavenging air humidity has a strong influence on the condensation of water.
- The total condensed sulfuric acid scales linearly with the fuel sulfur content.
- The present CFD model allows spatial analysis of the condensation.

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ABSTRACT

In the present study, three-dimensional (3D) computational fluid dynamics simulations are performed to examine the process of sulfuric acid (H_2SO_4) and water (H_2O) condensation in a large two-stroke marine diesel engine. A skeletal n-heptane chemical mechanism is coupled with a sulfur (S) subset to simulate the combustion process as well as the formation of sulfuric oxides (SO_x) and H_2SO_4. The condensation process is simulated using a fluid film model which is coupled with the in-cylinder gas phase. Prior to the engine simulations, the fluid film condensation model is validated using the experimental data of sulfuric acid condensation rate in a laminar pipe flow. Next, the engine model is validated against the experimental sulfur dioxide (SO_2) to sulfur trioxide (SO_3) conversion obtained from the corresponding test engine. Both of the validation studies show a good agreement with the experimental data. The engine model is then utilized to simulate condensation for different operating conditions. The engine simulation results reveal that the fluid film has a significant effect on the total mass of sulfuric acid vapor and a marginal effect on the total mass of water vapor. A close to linear correlation is found between the fuel sulfur content and the total condensed mass of sulfuric acid. The level of humidity of the scavenging air does not affect the condensation of sulfuric acid considerably, relative to the humidity increase, but it has a high impact on water condensation. The study of the scavenging pressure level reveals a counter intuitive behavior where the condensation rates decrease with higher scavenging pressures due to the flow regime and flame size. Next, increasing the cylinder liner temperature decreases significantly the water condensation contrary to the sulfuric acid condensation which is marginally affected. The increase in lubricant film thickness results in a decrease for both the sulfuric acid and water condensation with a more pronounced reduction for water. Finally, a comparison between the high and low load operating conditions reveals a small drop in the total condensed mass of sulfuric acid and water for the low load conditions.

1. Introduction

The shipping industry is responsible for the majority of the world trade transportation. The main source of propulsion is two-stroke diesel engines due to their high efficiency and reliability. The present configuration of these marine diesel engines utilizes low cost heavy fuel oil (HFO). However, HFO contains a certain level of sulfur (S). In the Diesel process, the fuel sulfur oxidizes to large amounts of sulfur dioxide (SO_2)

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and a small portion of SO_2 subsequently oxidizes to sulfur trioxide (SO_3). The latter reacts with water (H_2O) and produces sulfuric acid (H_2SO_4) in the gas phase. As the piston moves towards the bottom dead center (BDC) the bulk gas pressure decreases, due to the volume expansion, lowering the dew point temperature of sulfuric acid and water. When the cylinder liner temperature is lower than the aforementioned dew point temperature condensation of sulfuric acid and water on the cylinder liner ensues forming an aqueous solution. This can result in cold corrosion which may be the leading wear mechanism under these conditions [1,2]. Cold corrosion degrades the engine efficiency and consumption, see Yahagi [2]. Moreover, it can significantly shorten the life span of vital engine components thus increasing downtime for maintenance and operational costs. As a counter measure, the lubricants are enriched with an alkaline reserve of surfactants and limestone in order to neutralize the sulfuric acid, see Sautermeister and Priest [3]. The lubricant feed rate is also an important parameter against cold corrosion. An optimum feed rate can maximize the refreshing of the lubricant and thus guarantee an adequate alkaline reserve for the sulfuric acid neutralization. Over-lubrication can lead to high lubricant consumption (i.e. high operational costs and emissions) and excessive calcium deposits on the piston and piston rings (i.e. high wear and low engine component life) while under-lubrication can lead to mechanical wear and cold corrosion, see Chew and McGeary [4]. The challenges of calculating an appropriate feed rate are also analyzed by García et al. [5].

Due to the aforementioned reasons, sulfuric acid condensation and cold corrosion for HFO fueled marine engines is an active ongoing research field [6–10]. Nevertheless, there is no open literature to date for engine sulfuric acid condensation simulations using three-dimensional (3D) computational fluid dynamics (CFD) modeling. The previous studies [6–8] are limited to simplified phenomenological models related to the present work and only two CFD simulation studies [11–13] on unrelated applications. A diesel engine zero-dimensional (0D) model of corrosive wear due to sulfuric acid was developed by van Helden et al. [6] without considering the condensation of sulfuric acid. Next, McKinley [7] studied sulfuric acid and water condensation in diesel engine exhaust gas recirculation (EGR) coolers using a 0D model with a simple one reaction chemistry model. The first numerical study concerning the present analyzed problem was carried out by Cordtz et al. [8] who applied a 0D multizone model for a large two-stroke marine diesel engine. The chemical model includes a single hydrocarbon decomposition reaction, a detailed sulfur mechanism and a single reaction for H_2SO_4 formation. The condensation of H_2SO_4 and H_2O is simulated with a two-phase vapor liquid equilibrium (VLE) model using activity coefficients derived from the nonrandom two-liquid (NRTL) equation by Renon and Prausnitz [14]. However, this approach neglects the flow field inside the engine and consequently its mixing effects. For this reason the model compensates by the introduction of a mixing factor thus reducing the robustness of the model. Moreover, the model only provides a quantitative outlook on the condensation of sulfuric acid and water but not the spatial distribution of the condensation rate on the cylinder liner.

One of the early attempts to model condensation of sulfuric acid with CFD was performed by Perujo [11], who coupled a commercial CFD solver (ANSYS FLUENT) with a simple VLE condensation model, in order to simulate the condensation of sulfuric/nitric acid and water in boilers. The dew points of the species were calculated in a preprocessing step for specific conditions and used as constants thus decreasing the fidelity of the results. Next, Han et al. [12] introduced a VLE condensation solver using the model of Gmitro and Vermeulen [15] coupled with ANSYS FLUENT through user defined functions. The purpose of that study was to simulate the condensation of sulfuric acid and water on heat exchanger surfaces. The model was first validated using the experimental measurements of a test case of sulfuric acid condensation in a laminar pipe flow performed by Wilson [16] and reasonably accurate results were obtained. Following validation, the model was applied to study condensation on heat exchangers. The exact same method (from Han et al. [12]) was used by Wang and Tang [13] for a different heat exchanger geometry.

In the present work, numerical experiments are conducted by modeling the combustion and condensation processes using 3D CFD models. The main goal is to identify the critical parameters which affect sulfuric acid and water condensation on the cylinder liner. This can provide insight into the design parameters that can be taken into account to achieve large two-stroke diesel engines with low levels of cold corrosion and optimal lubricant feed rate. The importance of the engine design parameters, operating conditions and their connection to the lubricant feed rate is highlighted by [4,5,17]. Additionally, the present study aims to explore the capabilities of the 3D CFD models with respect to condensation coupled with engine combustion simulations which is a topic so far unexplored (to the knowledge of the authors). In the forthcoming sections a description of the main numerical models is presented. A validation study of the fluid film model is then conducted using the experimental measurements of a test case of sulfuric acid condensation in a laminar pipe flow performed by Wilson [16] and the numerical results of Han et al. [12]. Upon validation of the fluid film model, the marine diesel engine model is validated against the experimental SO_2 to SO_3 conversion obtained from the corresponding test engine. Next, a parametric study is performed for different engine operating conditions, which includes the influence of the lubricant film, fuel sulfur content, scavenging air humidity, scavenging pressure, cylinder liner temperature, lubricant film thickness and engine load. Finally, concluding remarks are provided.

2. Numerical model

Condensation is simulated with a fluid film model coupled with a condensation model both of which are provided by STAR-CCM+ version 10 [18]. The fluid film model comprises of conservation equations of the mass (Eq. (1)), momentum (Eq. (2)) and energy (Eq. (3)) which are derived with respect to the fluid film thickness h_f assuming a parabolic velocity profile across the film [18]

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho_f \mathrm{d}V + \int_A \rho_f(\mathbf{u}_f-\mathbf{u}_{gr})\cdot\mathrm{d}\mathbf{a} = \int_V \frac{\dot{m}_v}{h_f}\mathrm{d}V \tag{1}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho_f \mathbf{u}_f \mathrm{d}V + \int_A \rho_f \mathbf{u}_f(\mathbf{u}_f-\mathbf{u}_{gr})\cdot\mathrm{d}\mathbf{a} = \int_A \mathbf{T}_f\cdot\mathrm{d}\mathbf{a} - \int_A \rho_f \mathrm{d}\mathbf{a} + \int_V \rho_f \mathbf{g}\mathrm{d}V \tag{2}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho_f E_f \mathrm{d}V + \int_A [\rho_f H_f(\mathbf{u}_f-\mathbf{u}_{gr}) + \mathbf{u}_{gr}p_f]\cdot\mathrm{d}\mathbf{a} = \int_A \dot{Q}_v\cdot\mathrm{d}\mathbf{a} + \int_A \mathbf{T}_f\cdot\mathbf{u}_f\mathrm{d}\mathbf{a} + \int_V \rho_f \mathbf{g}\cdot\mathbf{u}_f\mathrm{d}V \tag{3}$$

Here, ρ_f denotes the film density while $\mathbf{u}_f$ and $\mathbf{u}_{gr}$ are the film and grid velocity, respectively. For the engine model, the grid velocity represents the cylinder volume expansion which involves deformation of the computational grid. The integrals are with respect to the fluid film volume V and surface area A, where $\mathbf{a} = \mathbf{n}A$ is the vector surface area and $\mathbf{n}$ is the unit vector normal to this surface. The fluid film stress tensor is represented by $\mathbf{T}_f$ while $\mathbf{g}$ denotes acceleration due to gravity. Moreover, $\dot{Q}_v$ represents the heat flux at the interface between the fluid film and the gas phase. Also, p_f denotes the pressure in the film. Finally, E_f is the total energy and H_f is the total enthalpy of the fluid film [18] described by

$$E_f = H_f - \frac{p_f}{\rho_f} \tag{4}$$

$$H_f = h_f - \frac{|\mathbf{u}_f|^2}{2} \tag{5}$$

$$h_f = \sum_i h_{f,i} Y_{f,i} \tag{6}$$