

# MODELING OF CONDENSATION OF SULFURIC ACID AND WATER IN A LARGE TWO-STROKE MARINE DIESEL ENGINE

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**Summary.** In the present work, three-dimensional computational fluid dynamics simulations are performed to examine the process of sulfuric acid and water condensation in a large two-stroke marine diesel engine.

## 1 INTRODUCTION

The majority of the world freight transportation is carried out by ships, using mainly two-stroke diesel engines. These engines operate with heavy fuel oil (HFO) due to its low cost. Nevertheless, the HFO contains sulfur (S) which during combustion oxidizes and forms sulfur oxides ( $\text{SO}_x$ ). One of the sulfur oxides ( $\text{SO}_3$ ) reacts with water ( $\text{H}_2\text{O}$ ) and forms sulfuric acid ( $\text{H}_2\text{SO}_4$ ). During the combustion cycle sulfuric acid and water may condense on the cylinder liner. As a consequence, cold corrosion ensues which is the main wear mechanism under these conditions<sup>1,2</sup> and thus decreases the life expectancy of critical engine parts (e.g. cylinder liner). The present study aims to provide some insight into the critical parameters that affect the condensation of sulfuric acid and water as well as assist the design of cold corrosion resistant engines.

## 2 NUMERICAL MODELS

The process of condensation is described by the fluid film model coupled with the condensation model provided by STAR-CCM+<sup>3</sup>. The condensation model solves the conservation equations governing mass and energy at the film interface, in order to calculate the condensation rates of the condensable species. The model relates the gas phase

to the film phase using Raoult's equation

$$X_{gas,i} = \gamma_i X_{film,i} p_{sat}(T) \quad (1)$$

where  $X_{gas,i}$  and  $X_{film,i}$  are the mole fractions of  $i$ -th condensable species in the gas and film phase, respectively. The activity coefficient is represented by  $\gamma_i$  and the saturation pressure of the pure liquid species by  $p_{sat,i}$ . The main assumption of the built-in condensation model is that  $\gamma_i \approx 1$ , thus the liquid film solution is assumed to be ideal. However, this does not hold true for this case, thus the model of Gmitro & Vermeulen<sup>4</sup> is used to account for the non ideal behavior of the aqueous sulfuric acid solution.

### 3 VALIDATION

A simple test case of sulfuric acid and water condensation in a laminar pipe flow is used to validate the fluid film condensation model against the experiments performed by Wilson<sup>5</sup> and the numerical model of Han et al.<sup>6</sup>. The results show a good agreement with both the result of Wilson<sup>5</sup> and Han et al.<sup>6</sup>, as illustrated in Fig. 1.

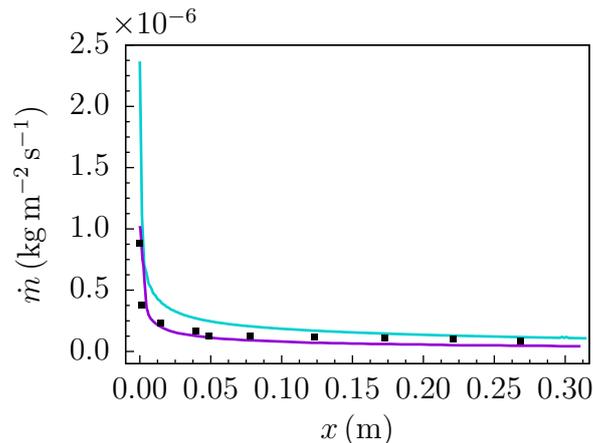


Figure 1: Condensation rate ( $\dot{m}$ ) of sulfuric acid with respect to the pipe axial position ( $x$ ) using the current condensation model (—) compared with the numerical model of Han et al.<sup>6</sup> (—) and the experimental results of Wilson<sup>5</sup> (■).

### 4 ENGINE MODEL

The model uses a reduced n-heptane skeletal chemical mechanism coupled with a sulfur subset to simulate the combustion process and the formation of  $\text{SO}_x$  and  $\text{H}_2\text{SO}_4$ . Upon validation of the models, the engine simulations are set up accordingly. Next, a parametric study is performed to examine the influence of the fluid film, the fuel sulfur content, the scavenging air humidity, the scavenging pressure and the cylinder liner temperature. The fluid film influence is examined by performing an engine simulation with and without the fluid film model. The tests reveal that the fluid film has a significant effect on the total

mass of sulfuric acid vapor and a minimal effect on the total mass of water vapor. This shows the importance of condensation for the overall prediction of reacting condensable species. Next, the effects of sulfur content in the fuel are examined by varying its mass fraction. The results exhibit a linear correlation between the fuel sulfur content and the total condensed mass of sulfuric acid. Furthermore, a study on the effects of level of the scavenging air humidity is conducted by altering the water vapor concentration at the top dead center (TDC), where the engine simulations start. The study shows that the level of the scavenging air humidity is not greatly affecting the condensation of sulfuric acid, but it has a high impact on the condensation of water. The effect of the scavenging pressure is investigated by varying the cylinder pressure at TDC. The tests reveal a counter intuitive trend, which is the inverse correlation between the scavenging pressure and the resulting condensation rates. This is due to the nature of the flow and more specifically the flame propagation speed, cf. Gol'denberg & Pelevin<sup>7</sup>. Fig. 2 illustrates the contour of the condensation rate of sulfuric acid on the film along with the isolines of temperature in the gas phase and represents a prime example of the interaction between the gas phase and the film. It can be seen that the areas where the flame impinges the cylinder liner have zero condensation rate. Finally, increasing the cylinder liner temperature decreases significantly water condensation, contrary to sulfuric acid condensation which is unaffected.

## 5 CONCLUSIONS

The present study identifies the critical design parameters for engines with low levels of cold corrosion. Moreover, it demonstrates the potential of 3D CFD models to capture trends that phenomenological models fail to do, like in the case of the scavenging pressure findings, providing a better insight.

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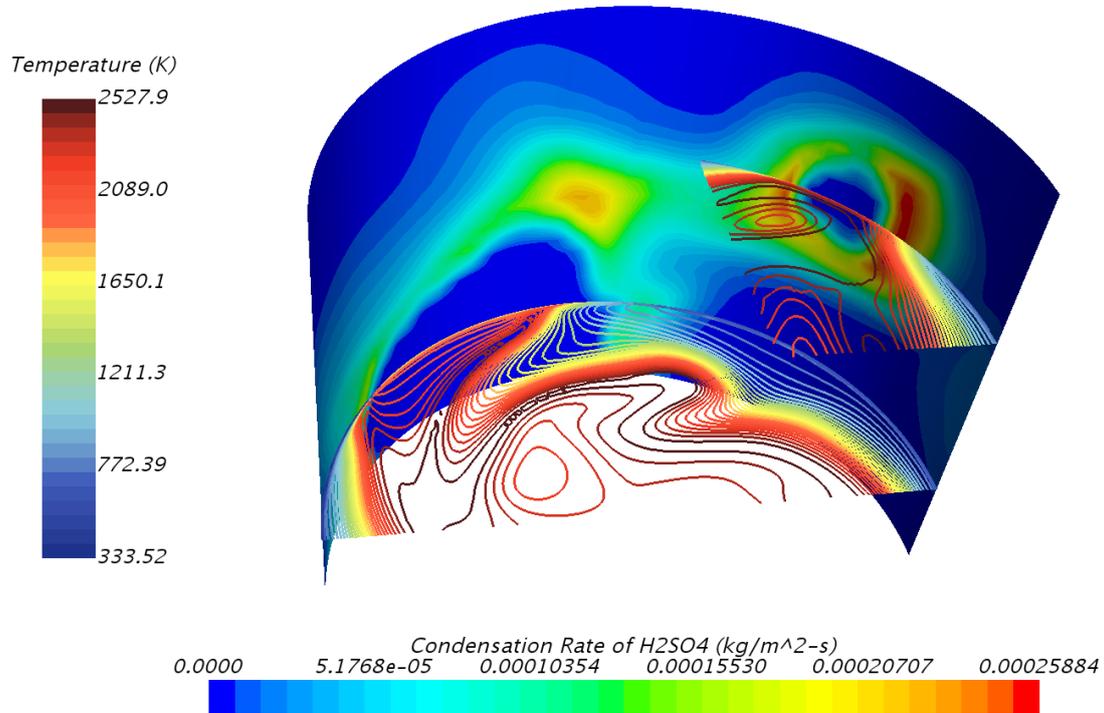


Figure 2: Contour of the condensation rate of sulfuric acid ( $H_2SO_4$ ) on the film and isolines of temperature in the gas phase at 35 crank angle degrees after TDC.