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Numerical and experimental investigation of evaporation and mixture uniformity of urea–water solution in selective catalytic reduction system

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ABSTRACT

Selective catalytic reduction (SCR) technology for the control of NOx emissions has become an attractive option for marine diesel engine applications because of the International Maritime Organization (IMO) Tier III regulation. SCR systems are effective over a wide temperature range in reducing NOx emissions during rich and lean operations. This study investigated the evaporation and thermal decomposition processes of urea–water solution (UWS) in an SCR system both experimentally and via simulation. It was found that a wall film forms at the inlet and outlet of the mixer in the mixing pipe as a result of deposition or splashing after impingement of urea droplets. A model of the evaporation and thermal decomposition of UWS to form the wall film developed in this study and utilized in simulations. Although the conversion rate of NOx reduction presented in the simulation case was slightly higher than that obtained experimentally, the simulation results were in good agreement with the experimental results. The results prove that it is possible to effectively predict the actual NOx reduction rate of an SCR system via simulations.

1. Introduction

To meet the stringent future emission regulations from the Environmental Protection Agency (EPA) (Kota et al., 2014; Skalska et al., 2010), especially with respect to reducing nitrogen oxides, various technologies such as basic internal engine modifications (Lee and Lee, 2007a, 2006, 2007b), fuel switching (Winnes and Fridell, 2009), water emulsions (Ithnin et al., 2014), exhaust gas recirculation (Verschaeren et al., 2014; Bhaskar et al., 2014; Jafarmadar, 2014), and selective catalytic reduction (SCR) (Guo et al., 2015; Cimino et al., 2015) have been recommended for marine diesel engines. The several internal modifications to reduce NOx (nitrogen oxides) and other pollution was employed to simulate the operation cycle and characterized the exhaust gas composition. After a preliminary validation process was carried out using experimental data from a four-stroke, medium-speed marine engine, the numerical model was employed to study the influence of several internal modifications, such as water addition from 0 to 100% water to fuel ratio (Ithnin et al., 2014), exhaust gas recirculation of 0–100% EGR rate (Verschaeren et al., 2014; Jafarmadar, 2014), modification of the overlap timing from 60 to 120 CA

Abbreviations: ASOI, after starting of injection; CFD, computational fluid dynamics; EGR, exhaust gas recirculation; IMO, International Maritime Organization; NOx, nitrogen oxides; SCR, selective catalytic reduction; UWS, urea-water solution; UI, uniformity index.

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(Lee and Lee, 2007a), modification of the intake valve closing from 510 to 570 CA (Lee and Lee, 2006), and modification of the cooling water temperature from 70 °C (Lee and Lee, 2007b). NOx was reduced by nearly 100%. The International Maritime Organization (IMO) regulates NOx emissions from marine vessels. The IMO's Tier III emission standard (Herdzik, 2011; MARPOL Convention 73/78) requires that marine vessels must reduce NOx emissions by 80% between 2010 and 2016. SCR is one of the most promising technologies for accomplishing this aggressive regulation. As a reducing agent, urea is preferred in marine SCR applications because of its safety and low toxicity.

In SCR technology based on urea–water solution (UWS, containing 40 wt% urea), the solution is injected into the hot exhaust gas and subsequently the reducing agent (ammonia, NH_3) is generated by evaporation of water, thermolysis reaction of urea, and hydrolysis reaction of isocyanic acid (HNCO) Koebel et al., 1996. Homogeneous distribution of the reducing agent upstream of the catalyst is an important factor for the conversion of NOx. This study (Lee, 2016) presented a steady kinetic model of urea-SCR with vanadium-based catalyst. The simulation results with modeling urea-selective catalyst reduction based on NH_3 temperature programming desorption experiment using a commercial 1D-aftertreatment code coupled with an optimizer produced generally good agreement with experiment measurement of NH_3 and NOx reactions under different temperatures, NO/NO_2 ratios, space velocities and NH_3/NOx ratios.

The used spray/wall interaction model of Kuhnke (2004a) accounts for dry and wet as well as for cold and hot walls by using dimensionless numbers that are influenced by the thermo-physical properties of the droplets. Because of the complexity involved in modeling the interaction between an impinging spray and a wetted wall, empirical and phenomenological models are best used for the simulation of impingement. Heat transfer between spray and wall is described according to Wruck (1998). The film on the wall is modeled as a two-component fluid of urea and water coupled by momentum, species, and energy balance to the gas phase and the walls. Koebel et al. (2000), Birkhold et al. (2006) discussed spatial enthalpy variations due to evaporation, thermolysis, and hydrolysis of UWS, and derived a model to determine various SCR system configurations for conversion and local distribution of the reducing agent. The application of numerical modeling in the area of environmentally friendly technology mobile SCR was incorporated into the wall film module of the commercial computational fluid dynamics code FIRE for description of urea-water-solution injection into hot exhaust gases of diesel engine and compared experimental data. Results of the conducted numerical study support the feasibility of commercial application (Baleta et al., 2015).

A model of the evaporation and thermal decomposition of UWS to form a wall film is developed in this study. The model accounts for all relevant processes from the injection point to the entrance of the SCR catalyst:

- Momentum interaction between gas phase and droplets.
- Evaporation and thermolysis of droplets.
- Hydrolysis of HNCO in gas phase.
- Heat transfer between wall and droplets and spray/wall interaction.
- Two-component wall film formation including interaction with gas phase and exhaust pipe.

Computational fluid dynamics (CFD) simulations of an SCR system conducted and compared with experimental data to determine the uniformity of NH_3 concentration, wall film interaction, and trajectory of droplets in the mixing pipe. Finally, uniformity index of temperature at the outlet of catalyst measured and compared with simulation results at the same location.

2. Numerical and experimental methods and conditions

2.1. Numerical methods

The flow of a viscous heat conducting fluid is governed by momentum equations, also called Navier-Stokes equations, supplemented by continuity and energy equations. The term Navier-Stokes equations is applied for the entire set of governing equations, i.e., momentum, continuity, and energy. Eqs. (1) and (2) comprise the set of governing equations, with continuity governed by Eq. (1), and momentum by Eq. (2):

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0 \tag{1}$$

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = -\frac{\partial p \delta_{ij}}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} \tag{2}$$

The viscous stress is given by Eq. (3):

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{1}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij} \tag{3}$$

The model used in this study is a nonlinear eddy viscosity model, κ-ζ-f, and is based on the set of equations given below. The turbulent viscosity is given by Eq. (4) and the transport equation for ξ is given by Eq. (7).