Autoignition And NOx Generation on Burning of Diesel Oil

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1. INTRODUCTION

Nitrogen Oxides (NO_x) are among the major pollutants causing smog, acid rains and damaging the ozone layer. Most of the NO_x is produced by combustion systems (automobile and stationary sources).

2. MATHEMATICAL MODEL

2.1 Dimensional Equations Governing the Heat and Mass Transfer

Since attention is focused on the axisymmetric case, the dimensional energy balance equation for the particle and gas-phase can be written in one-dimensional form

$$\frac{\partial(\rho_d c_d T_d)}{\partial t} = r^{-2}\frac{\partial}{\partial r}\left(r^2\frac{\partial(k_d T_d)}{\partial r}\right) + \frac{3\alpha_{abs,(\lambda)}}{4\pi r_d^3}\frac{\partial E}{\partial t} \tag{1}$$

and

$$\frac{\partial(\rho_g c_g T_g)}{\partial t} = r^{-2}\frac{\partial}{\partial r}\left(r^2\frac{\partial(k_g T_g)}{\partial r}\right) \tag{2}$$

where c_d ($J\ kg^{-1}\ K^{-1}$), k_d ($W\ m^{-1}\ K^{-1}$), $\square\square_d$ ($kg\ m^{-3}$) and T_d (K) are the specific heat capacity, thermal conductivity, density and temperature of the droplet. c_g, k_g, T_g and $\square\square_g$ are the specific heat capacity, conductivity, temperature and density of the gas-phase. E (J) is the radiative energy of the external source and t (s) is time.

Equations (1) and (2) are coupled through the following initial and boundary conditions

$$\kappa T_d = T_g = T_a \quad \text{at } t = 0$$

$$\frac{\partial T_d}{\partial r} = 0 \quad \text{on } r = 0$$

$$T_g = T_d \quad \text{on } r = r_d$$

$$\alpha_{ads,(\lambda)}q = k_d \frac{\partial T_d}{\partial r} + h(T_d - T_a) + \frac{LD(C_e - C_\infty)}{r_d} \quad \text{on} \quad r = r_d \quad (\text{here } q = \partial E / 4\pi r_d^2 \partial t)$$

$$\frac{\partial T_g}{\partial r} = 0 \quad \text{as} \quad r \to \infty$$

Here $a_{ads,(l)}$ is a non-dimensional adsorptivity coefficient of the droplet with respect to wavelength l, , T_a is the initial gas-phase temperature, r_d (m) is the radius of the droplet, L $(J\ kg^{-1})$ is the latent heat of vaporisation, D $(m^2\ s^{-1})$ is the binary diffusion coefficient, C_e $(kg\ m^{-3})$ is the concentration of vapour in equilibrium with the droplet and C_∞ $(kg\ m^{-3})$ is the concentration of vapour at infinite distance from the droplet. k is the ratio between droplet and gas-phase initial temperatures.

The effect of droplet vaporisation was taken into account, while the effect of droplet/gas-phase radiative energy exchange was neglected. Note that a detailed consideration of $a_{abs,(l)}$ and $a_{ads,(l)}$ dependence on media properties, radiation wavelength and temperature was beyond the interests of the current work.

The binary diffusion coefficient that controls the fuel-vapour/air mixing is proportional to $T_g^{3/2}$ and inversely proportional to the pressure, see Incroperra *et al.* (1996). Hence

$$D = \frac{D_0 p_{atm}}{T_a^{3/2}} \frac{T_g^{3/2}}{p} \tag{3}$$

where p (Pa) is gas-phase pressure and p_{atm} is the atmospheric pressure.

Strictly speaking the evaporation of a droplet cannot be a stationary process since the radius and hence the rate of evaporation is decreasing. However, as shown in Chapman *et al.* (1939), when $C_e \ll \rho_d$ the evaporation can be regarded as quasi-stationary, i.e. it can be assumed that the energy balance on the droplet surface at a given moment is independent of time. Assuming C_e is independent of temperature in the temperature region of interest, $C_\infty = 0$, $T_g = T_d$ on $r = r_d$, and considering an isobaric process, the energy balance on droplet surface becomes

$$\alpha_{ads,(\lambda)}q = k_d \frac{\partial T_d}{\partial r} + h(T_d - T_a) + \frac{LC_e}{r_{d,0}} \frac{D_0 T_d^{3/2}}{T_a^{3/2}}$$

where $r_{d,0}$ (m) is the initial radius of the droplet.

Material properties of the gas-phase were taken to be functions of the temperature

$$k_g = k_{g,a}\tilde{k} \tag{4}$$

$$\rho_g = \rho_{g,a}\tilde{\rho} \tag{5}$$

$$c_g = c_{g,a}\tilde{c} \tag{6}$$

where $k_{g,a}$, $r_{g,a}$ and $c_{g,a}$ are the thermal conductivity, density and heat capacity of the gas-phase at the ambient temperature, T_a. The non-dimensional parameters $\tilde{k}$, $\tilde{\rho}$ and $\tilde{c}$ are written in a polynomial form that fits the thermophysical data provided by Perry (1997) for air. The data is validated for the temperature range 300-1000 K and a constant pressure of 0.1 MPa. Normally the volume fraction of fuel in vaporised stoichiometric mixture does not exceeds 2%, Diesel Fuel Oils (1987), therefore it can be assumed that the polynomial coefficients change little with the changes in fuel/air composition.

2.2 The Dimensionless Form of the Governing Equations

In order to place the system of dimensional equations (1) and (2) into non-dimensional form, which is suitable for computational purposes, new independent variables and constants were defined:

$$T_1 = \frac{T_d}{T_a} \qquad T_2 = \frac{T_g}{T_a} \qquad \tau = t\frac{k_g}{\rho_g c_g r_{d,0}^2}$$

$$J = \frac{k_{g,a}}{k_d}\frac{\rho_d c_d}{\rho_{g,a}c_{g,a}}$$

$$x = \frac{r}{r_{d,0}}, \text{ where } \quad x = \begin{cases} \left(\dfrac{r}{r_{d,0}}\right) : 0 \le \left(\dfrac{r}{r_{d,0}}\right) \le 1 \\ \left(\dfrac{r}{r_{d,0}}\right)^{-1} : \left(\dfrac{r}{r_{d,0}}\right) \ge 1 \end{cases}$$

$$\frac{\partial J_1}{\partial \tau} = \frac{3\alpha_{abs,(\lambda)}}{4\pi r_{d,0}^3 \rho_d c_d T_a}\frac{\partial E}{\partial \tau} \qquad J_2 = \frac{\alpha_{ads,(\lambda)}q r_{d,0}}{k_d T_a}$$

$$J_3 = \frac{LC_e D_0}{k_d T_a}, \text{ and the Nusselt number } \quad Nu = \frac{h r_{d,0}}{k_d}$$

Here $\rho_g c_g r_{d,0}^2/k_g$ is the natural "diffusion" time-scale for the droplet.

The dimensionless equation governing the temperature within the droplet then becomes

$$\frac{\partial T_1}{\partial \tau} = J^{-1}x^{-2}\frac{\partial}{\partial x}\left(x^2\frac{\partial T_1}{\partial x}\right) + \frac{\partial J_1}{\partial \tau} \tag{7}$$

The gas-phase energy balance equation is expressed as

$$\frac{\partial(\tilde{\rho}\tilde{c}T_2)}{\partial \tau} = x^{-2}\frac{\partial}{\partial x}\left(x^6\frac{\partial(\tilde{k}T_2)}{\partial x}\right) - 6x^3\frac{\partial(\tilde{k}T_2)}{\partial x} \tag{8}$$

Equations (7) is coupled with equation (8) in the following initial and boundary conditions

$$\kappa T_1 = T_2 = 1 \text{ at } \tau = 0$$

$$\frac{\partial T_1}{\partial x} = 0 \text{ on } x = 0$$

$$T_2 = T_1 \text{ on } x = 1$$

$$J_2 = \frac{\partial T_1}{\partial x} + Nu(T_1 - 1) + J_3 T_1^{3/2} \text{ on } x = 1$$

$$\frac{\partial T_2}{\partial x} = 0 \text{ as } x \to \infty$$

2.3 Examination of power flux requirements

Let consider the case, in which the droplet and the surrounding gas-phase have the same initial temperature ($\kappa = 1$). In this case the increase of the temperature of the droplet will be a result of the external radiative heating only. The internal energy of the gas-phase that surrounds the droplet will increase until the autoignition temperature, T_{ign} of the combustible mixture is reached.

The power flux requirement for a droplet to reach T_{ign} was calculated for the steady state case in which the differential equation (7) is automatically satisfied, as there is no flux boundary condition at $x = 0$ and $T_1(x,\tilde{t}) \to \tilde{T}_e$ as $\tilde{t} \to \infty$. Here $\tilde{T}_e = T_e/T_a$ is the normalised equilibrium temperature and T_e is a constant to be determined. Setting $T_1 = \tilde{T}_e$, the boundary condition on $x = 1$ becomes

$$J_2 = Nu(\tilde{T}_e - 1) + J_3\tilde{T}_e^{3/2}$$

it can be found that $T_e \geq T_{ign}$ at q = 24.7 $kW\ m^{-2}$ (Figure 1). A substantial increase of the radiative heat flux of ~75 $kW\ m^{-2}$ is required to double the binary diffusivity of the fuel-vapour/air mixture, and therefore, to decrease heterogeneity of the system in a measurable scale.

In addition, $a_{abs,(l)}$ and $a_{ads,(l)}$ depend on radiation wavelength. Data about diesel

fuel spectral properties (Dombrovsky *et. al*, 2003) is used to calculate the power flux requirements to increase the temperature of a droplet ($r_{d,0}$ = 25 mm) from 300 to 590 K (the autoignition temperature) and to double the binary diffusivity of the fuel-vapour/air mixture. Results are plotted in Figure 2. The power flux of a 10 W laser with a diameter of the cross-section of the beam of 10 mm is also shown for comparison. Substantial external radiative power flux must be applied in order to increase the binary diffusivity of fuel-vapour/air mixture in a measurable scale. Except for the wavelength of ~3.4 mm, the power flux requirements cannot be satisfied in laboratory conditions.
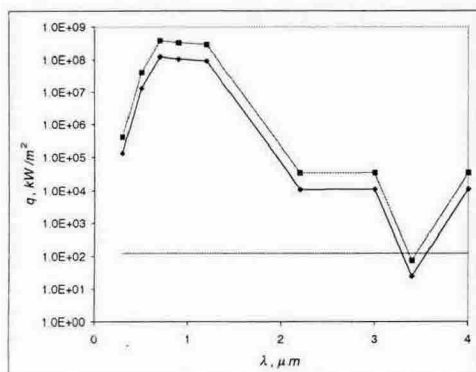
Figure 2. Power flux versus radiation wavelength.
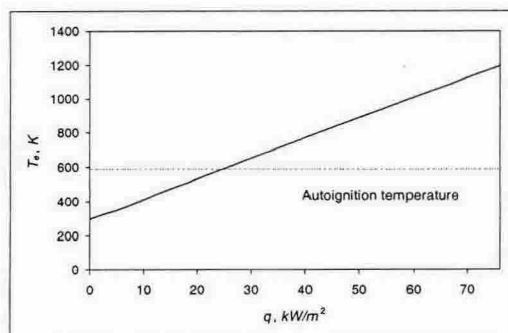
Figure 1. Equilibrium temperature of a diesel fuel droplet ($r_{d,0}$ = 25 mm) versus radiative heat flux.

3. PRELIMINARY EXPERIMENTS

A set of preliminary experiments using a simple experimental set up was done in order to determine whether a laser radiation of limited power (0.97 W) could have any measurable effect on gas emissions from a diffusion flame.

Two identical, spherical, cellulose (cotton) balls were soaked in fuel (~0.1 ml). The diameter of the balls was ~ 2 mm. Functions of the balls were to contain the fuel, to accumulate the heat energy and to increase the optical thickness of the fuel. Two cases were examined. In the first case the fuel ball was burned with no external radiative power applied. In the second case the fuel ball was burned in the presence of external laser radiation. A frequency doubled, single cavity, Nd:YAG laser, pulsed at a repetition rate of 10 Hz, was used to produce a cylindrical beam to irradiate the ball. Only one side of the ball was irradiated. The laser was operating at 532 nm wavelength. It was found that the fuel ball is non-transparent to this wavelength of the laser. The laser was capable of

producing a maximum energy per pulse of 200 mJ with a pulse width of approximately 6 ns. It was normally operated at 75% of its maximal power. A system of lenses was used to collimate the beam and to keep the diameter of the beam equal to the initial diameter of the ball.

In both cases the fuel balls were burned at atmospheric pressure in a combustion chamber with dimensions of $0.1 \times 0.1 \times 0.2$ m. The hood of the chamber was connected through a filter, to a gas-analyser. The function of the filter was to collect the soot particulates, preventing the gas-analyser from damaging. The flow rate of the sampled gases to the gas-analysed was 1.510^{-5} m^3/s. Concentrations of O_2 and CO_2 in the exhaust gases were measured every second in order to provide data about the burning rate of the flame. NO_x emissions were also measured in order to provide indirect data about fuel/air mixing rate. Note that the energy provided by the laser was sufficient to evaporate the outer layers of the fuel. Therefore, the external radiation, added to the thermal radiation from the flame was able to increase the evaporation rate of the fuel and to intensify fuel/air mixing. This, in turns, could lead to a reduction of the flame temperature and consequently, to a reduction of NO_x emission.

4. CONCLUSIONS

Results from mathematical simulation show that at otherwise identical conditions, the external radiative heating of a semi-transparent fuel droplet surrounded by quiescent gas-phase causes a faster increase of surface temperature of the droplet and an increase of the mass transfer between the droplet and the surrounding gas-phase.

Substantial external radiative power flux must be applied in order to increase the binary diffusivity of fuel-vapour/air mixture in a measurable scale. The power flux requirement can be minimised if the external radiative source irradiate the droplet with a wavelength of approximately 3.4 mm.

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