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Mathematical Modeling of the Effect of External Radiative Heating on Heat and Mass Transfer Between A Semi-transparent Diesel Fuel Droplet and Quiescent Air

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Abstract : The system considered in this model consists of a single,semi- transparent, diesel fuel droplet, which is immobile in the heating area and surrounded by a quiescent air. A uniform external radiation field surrounds the droplet. Results from mathematical simulation suggest that because of the higher surface temperature, the external radiative heating of the droplet can promote an earlier ignition of the fuel vapour/air mixture. The radiative heating of the droplet increases the mass transfer from the droplet to the surrounding gas-phase, thus, decreasing the heterogeneity of the fuel droplet/air system.

Key words: Combustion, Ignition, DeNOx, Mathematical model

1. Introduction

The contribution of thermal radiation that results from combustion processes to the heat transfer processes in Diesel engines has received a great deal of attention. The works of Lage *et al.* (1993), Chang *et al.* (1995), Dombrovsky (1996), Marchese *et al.* (1997) and Sazhin, *et al.* (2000) show that the effect of heating of droplets by thermal radiation can contribute significantly to the process of droplet evaporation. Recently, Dombrovskya *et al.*(2001) applied approximated absorption and scattering spectral efficiency factors for spherical semi-transparent fuel droplets to the modelling of thermal radiation transfer in Diesel engines. The average absorption coefficient of droplets is shown to be proportional to the droplet radii and gas temperature. The effect of thermal radiation on heating and evaporation of semi-transparent diesel fuel droplets is shown to be considerably smaller when compared with the case of black opaque droplets.

While the effect of heating of droplets by thermal radiation that results from combustion processes in Diesel engines is widely discussed in the literature, currently there are no investigation of the effects of droplets external radiative heating (i.e. laser heating) on latest stages of diesel fuel atomisation and ignition.

The system considered in this model consists of a single, semi-transparent, radiation-heated droplet immobile in the heating area. The droplet is surrounded by a quiescent gas-phase. The heat and mass-tranfer processes, which take place in the system, obey Fourier's law of heat conduction, newton's law of cooling and Fick's law of diffusion. A spherical co-ordinate system is adopted. The effect of external radiative heating on droplet surface temperature, droplet radius change and fuel-vapour/air diffusivity is modelled.

2. Mathematical Model

2.1 General Model Assumptions

The following assumptions concerning the properties of the droplet in the temperature range of interest (300-1000 *K*) are adopted within the mathematical model:

1. The droplet is spherical.

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2. The droplet is situated in the centre of a spherical radiative field and its surface is uniformly heated.
3. The droplet is immobile in the heating area.
4. The droplet is homogeneous and isotropic. There is a single liquid phase without inclusion of gaseous matter. Furthermore, no mass transfer processes occur within the droplet volume.
5. There is no chemical transformations of the droplet in the temperature range of interest.
6. The thermal linear expansion of the droplet is ignored and the values of the heat capacity, thermal conductivity, density, spectral absorptivity, emissivity and other physical properties of the droplet are taken to be independent of the temperature.
7. The droplet surface does not absorb the gas-phase.
8. The droplet is semi-transparent to the wavelength of the radiative heating source.

The assumptions that are adopted within the mathematical model for the properties of the gas-phase are:

1. The gas-phase is isotropic and follows the ideal gas law.
2. The gas-phase has a volume infinitively larger than the volume of the droplet.
3. The gas-phase is not forced to flow.
4. Initially the gas-phase is homogeneous, i.e. the components of the gas composition are uniformly mixed.
5. The thermodynamic property change of mixing is negligible.
6. There is no heat impact by the chemical reactions during the pre-heating of the droplet, prior tothe ignition, since the concentration of the fuel in the oxidiser is below the flammability limits of the fuel/oxidiser system, and temperature of the fuel/oxidiser mixture is too low to initiate fuel oxidation.
7. The gas-phase is fully transparent to the wavelength of the radiative heating source.
8. The gas-phase transparency remains constant during the heating.

2.2 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 $c_d(J\ kg\text{-}1\ K\text{-}1)$, $k_d(W\ m\text{-}1\ K\text{-}1)$, $\rho_d(kg\ m\text{-}3)$ and $T_d(K)$ are the specific heat capacity, thermal conductivity, density and temperature of the droplet. $\alpha_{abs,(\lambda)}$ is the absorptivity ratio of the droplet with respect to wavelength λ of the external radiative source. c_g, k_g, T_g and ρ_g are the specific heat capacity, conductivity, temperature and density of the gas-phase. $E(J)$ is the radiative energy of the external source, $t(s)$ is time and $r(m)$ is the radial distance.

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

$$\kappa T_d = T_g = T_a \quad t = 0$$

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

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

$$\alpha_{ads,(\lambda)q} = k_d\frac{\partial T_d}{\partial r} + h\left(\frac{T_d}{\kappa} - T_a\right) = \frac{LD(C_e - C_\infty)}{r_d} \quad \text{on } r = r_d$$

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

Here $\alpha_{ads,(\lambda)}$ is the adsorptivity ratio of the droplet with respect to wavelength λ, q $(W\ m\text{-}2)$ is the radiative heat flux, T_a is the initial gas-phase temperature, $r_d(m)$ is the radius of the droplet, $L(J\ kg\text{-}1)$ is the heat of evaporation, $D(m2\ s\text{-}1)$ is the binary diffusion coefficient, $C_e(kg\ m\text{-}3)$ is the concentration of vapour in equilibrium with the droplet and $C_\infty(kg\ m\text{-}3)$ is the concentration of vapour at infinite distance from the droplet. κ is the ratio between droplet and gas-phase initial temperatures.

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

The binary diffusion coefficient that controls the fuel-vapour/air mixing, D $(m2\ s\text{-}1)$ is proportional to $T_g^{3/2}$ and inversely proportional to the pressure, see Incropera *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 can not 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

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

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

Material properties of the gas-phase are taken to be functions of the temperature. The expression for the thermal conductivity, density and heat capacity, k_g, ρ_g and c_g are given by

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

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

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

where $k_{g,a}$, $\rho_{g,a}$ and 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 polynomial form

$$\tilde{k} = 1 + B_{i,k}(T_2 - 1) + B_{2,k}(T_2 - 1)^2 + B_{3,k}(T_2 - 1)^3 \tag{7}$$

$$\tilde{\rho} = 1 + B_{i,\rho}(T_2 - 1) + B_{2,\rho}(T_2 - 1)^2 + B_{3,\rho}(T_2 - 1)^3 \tag{8}$$

$$\tilde{c} = 1 + B_{i,c}(T_2 - 1) + B_{2,c}(T_2 - 1)^2 + B_{3,c}(T_2 - 1)^3 \tag{9}$$

where $T_2 = T_g/T_a$ and

$B_{i,k} = 3.1210^{-03}$ $B_{2,k} = -9.9910^{-07}$ $B_{3,k} = 5.1510^{-10}$;

$B_{1,ro} = -2.7710^{-03}$ $B_{2,ro} = 4.4410^{-06}$ $B_{3,ro} = -2.7210^{-09}$;

$B_{1,c} = 2.7910^{-04}$ $B_{2,c} = 5.91\ \ 10^{-07}$ $B_{3,c} = -5.4210^{-10}$.

The polynomials (7), (8) and (9) fit the thermophysical data that is 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). It is assumed that the polynomial coefficients, $B_{i,k}$, $B_{i,\rho}$ and $B_{i,c}$ change little with the changes in fuel/air composition.

2.3 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 are defined:

$$T_1 = \frac{T_d}{T_a} \quad \tilde{t} = t\frac{k_g}{\rho_g c_g r_{d,0}^2} \quad J = \frac{k_{g,a}}{k_d}\frac{\rho_d c_d}{\rho_{c,a} c_{g,a}}$$

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

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

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

The dimensionless equation governing the temperature within the droplet then becomes

$$\frac{\partial T_1}{\partial \tilde{t}} = J^{-1} x^{-2} \frac{\partial}{\partial x}\left(x^2 \frac{\partial T_1}{\partial x}\right) + \frac{\partial J_1}{\partial \tilde{t}} \tag{10}$$

The gas-phase energy balance equation is expressed as

$$\frac{\partial(\tilde{\rho}\tilde{c}T_2)}{\partial \tilde{t}} = x^{-2}\frac{\partial}{\partial x}\left(x^6 \frac{(\tilde{k}T_2)}{\partial x}\right) - 6x^3 \frac{\partial(\tilde{k}T_2)}{\partial x} \tag{11}$$

Equations (10) is coupled with equation (11) in the following initial and boundary conditions

$\kappa T_1 = T_2 = 1$ at $\tilde{t} = 0$

$\dfrac{\partial T_1}{\partial \tilde{t}} = 0$ on $x = 0$

$T_2 = T_2$ on $x = 1$

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

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

3. Results from Numercal Simmulation

3.1 Effect of Radiative Heating on Droplet Surface Temperature

The system of partial differential equations (10) and (11) is solved for two test cases. In the first test case no radiative heating of the droplet is considered (J_1=J_2 =0), while in the second case the values of J_1 and J_2 are changed to 1, taking into account the radiative heating of the droplet. The Nusselt number has the value for pure convection through an infinite stagnant fluid surrounding the sphere, $Nu = 2$, $J_3 = 1$, and $\kappa = 3$ are kept constant.

The solution is obtained using the routine D03PCF from the NAG suite of subroutines. This routine employs a finite difference discretisation in the spatial direction and the method of lines is used to reduce the partial differential equations to a system of ordinary differential equations. The resulting system of time dependent ordinary differential equations is solved using a backward differentiation formula method. Full details of this method can be found in Berzins *et al.* (1989) and the NAG suite of subroutines.

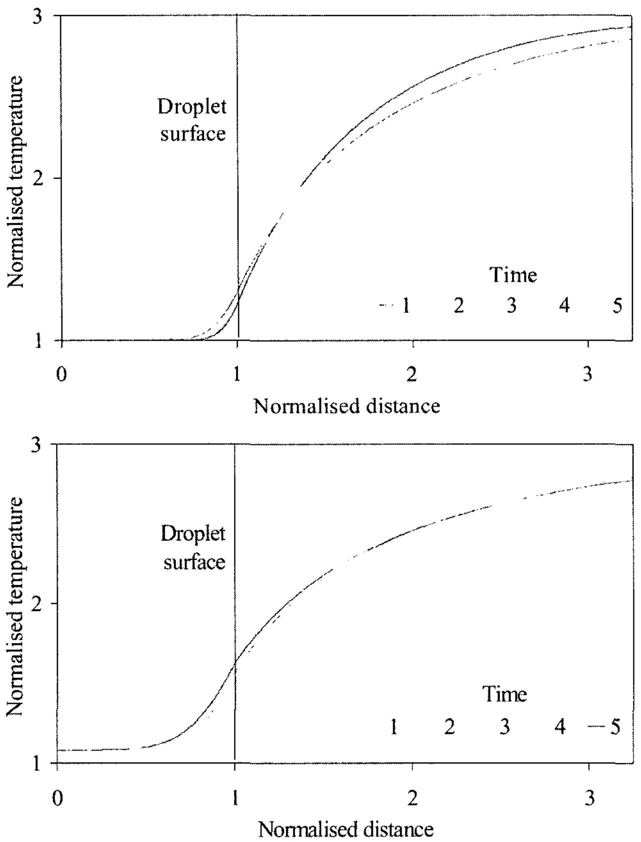

Fig. 1. Temperature distribution in droplet and gas-phase. in the case of a) $J_1 = J_2 = 0$, b) $J_1 = J_2 = 1$.

The system is solved on a staggered grid chosen to ensure good resolution in the vicinity of the droplet surface. It was found that a thousand grid pointsin the range of integration more than adequately resolved the structure with both the droplet and the gas phase. After some experimentation the following distribution of grid points was chosen

$$x = \sin\left(\frac{\pi(n-1)}{2(N-1)}\right), \text{ where } n = 1, \ldots N$$

The result of the numerical simulation is shown in Figure 1a,b. It gives the temperature distribution in droplet and gas-phase. The surface temperature increase is plotted in Figure 2. The result indicates that, at otherwise identical conditions, the droplet surface temperature increases faster in the case of external radiative heating.

3.3 Effect of Radiative Heating on Fuel-Vapour/Air Diffusivity

The solution of the system of partial differential equations (10) and (11) is used to examine the influence that the radiative heating could have on fuel-vapour/air mass transfer.

The binary diffusion coefficient, D is proportional to $T_g^{3/2}$ and inversely proportional to the pressure, see equation (3). Hence the ratio between the diffusion coefficients in a case of radiative heating, D_{irr} anda case of no radiative heating $D_{n\text{-}irr}$, become

$$\phi = \frac{D_{irr}}{D_{n-irr}} = \sqrt{\frac{T_{g,irr}}{T_{g,n-irr}}} \qquad (12)$$

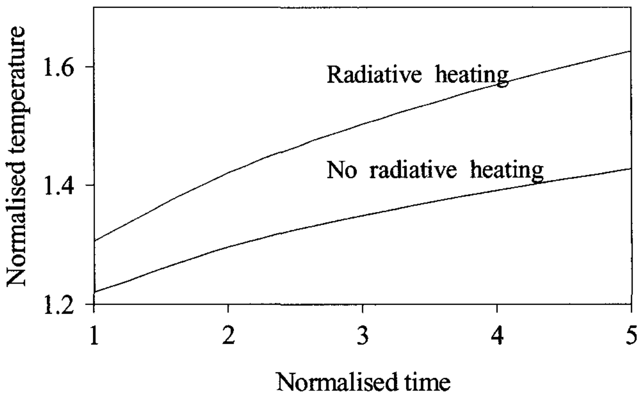

Fig. 2. Normalised surface temperature of the droplet versus normalised time in the case of $J_1 = J_2 = 0$ (no radiative heating) and $J_1 = J_2 = 1$ (radiative heating).

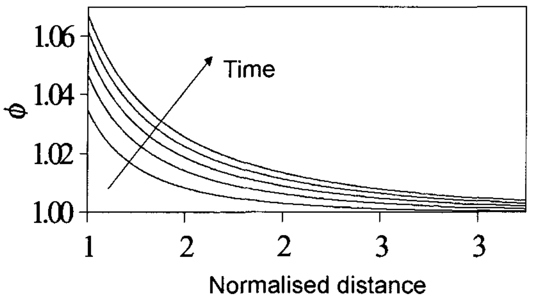

Fig. 3. Dependence of ratio ϕ on normalised distance and time.

The dependence of ratio ϕ on normalised distance and time is plotted in Figure 3. From this figure is clear that the radiative heating of the droplet increase the mass transfer from the droplet to the surrounding gas-phase, thus decreasing the heterogeneity of the system.

3.4 Effect of Radiative Heating on Droplet Radius Change

Fuchs (1959) gives the following equation for the radius change of a spherical droplet during its stationary evaporation

$$r_{d,0}^2 - r_d^2 = \frac{2D}{\rho_d}(C_e - C_\infty)t \tag{13}$$

This equation is based on the Maxwell equation for the rate of stationary evaporation, assuming that $C_e \ll \rho_d$.

The ratio, $\gamma = r_{d,irr}/r_{d,n-irr}$ where $r_{d,irr}$ and $r_{d,n-irr}$ are the radius of the droplet in the case of radiative heating, and in the case of absence of such a heating, is

$$\gamma = \sqrt{r_{d,0}^2 - \frac{(C_{e,irr} - C_\infty)}{(C_{e,n-irr} - C_\infty)}\frac{D_{irr}}{D_{n-irr}}} \tag{14}$$

Since $D_{irr}/D_{n-irr} = \sqrt{T_{g,irr}/T_{g,n-irr}}$ (see equation 12), assuming that vapour obeys the ideal gas law and $C_\infty = 0$ equation (14) becomes

$$\gamma = \sqrt{r_{d,0}^2 - \sqrt{\frac{T_{g,n-irr}|_{x=1}}{T_{g,irr}|_{x=1}}}} \tag{15}$$

The effect of radiative heating on the ratio γ is shown in Figure 4.

From Figure 4 is evident that at otherwise identical conditions, the external radiative heating promotes significantly higher evaporation rate of the droplet. This result is consistent with the observations from previous researches (Dombrovskya *et al.* (2001)).

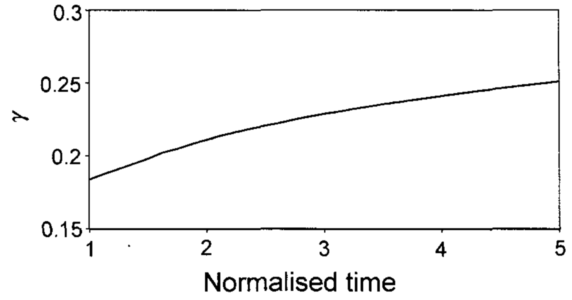

Fig. 4. Dependence of ratio γ on normalised time.

4. Experiments

Fuel was burned at atmospheric pressure in the presence of external laser radiation and without it. The concentrations of O2, CO2 and NOx were measured using gas-analyser. Concentrations of O2 and CO2 were measured in order to obtain data about the flame burning rate. Higher concentration of CO2 and lower concentration of O2 mean higher burning rate and visa versa. Time was normalised against the duration of the flame post-ignition period. The concentration of the species is normalised against the maximal concentration of the given specie for the period of time of interest.

The experimental set up is shown in Figure 5. A small cellulose (cotton) ball is soaked in fuel (~0.1 *ml*). Functions of the ball are to contain the fuel, to accumulatethe heat energy and to increase the optical thickness. The ball is placed on a thin metal hook under a metal funnel, which is connected through a filter to the gas-analyser. The ball is ignited using a gas torch. After ignition, the exhaust gases samples are collected. Experiments are then repeated while a laser beam irradiates the ball.

Figure 6 shows the normalised concentrations of O2, CO2 and NOx as a function of the normalised time.

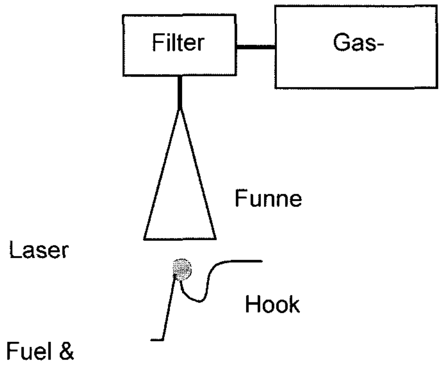

Fig. 5. A schematic diagram of the experimental set up.

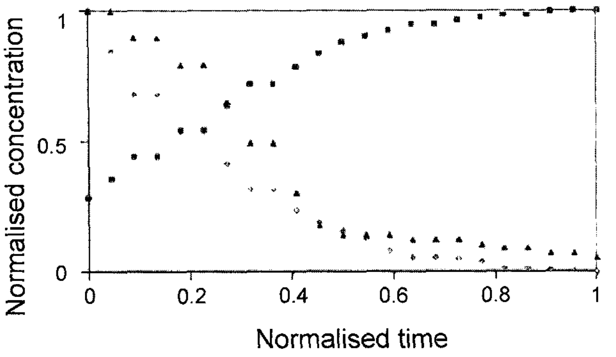

Fig. 6. Normalised concentration of CO2 (◇), O2. (●) and NOx (△) versus time with no external radiation applied.

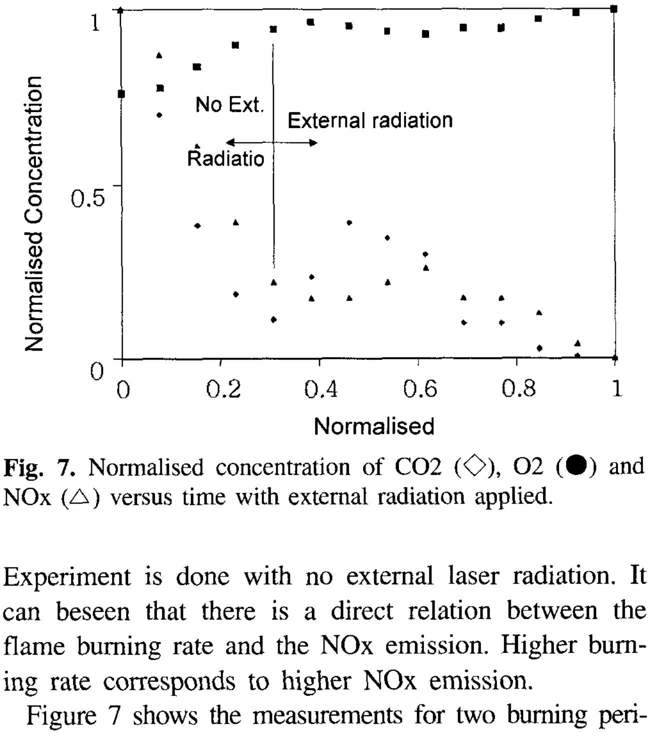

Fig. 7. Normalised concentration of CO2 (◇), O2 (●) and NOx (△) versus time with external radiation applied.

Experiment is done with no external laser radiation. It can beseen that there is a direct relation between the flame burning rate and the NOx emission. Higher burning rate corresponds to higher NOx emission.

Figure 7 shows the measurements for two burning periods of a droplet. During first 1/3 of the time the laser beam did not irradiate the droplet. Then, for the rest of the time, a collimated, 532 *nm*, 0.97 *W*, laser beam was directed towards the droplet. It can be seenthat during the period of non-irradiation (first 1/3), the burning rate of the flame and the NOx emission strictly follow the normal burning behaviour, similar to that shown in Figure 1. The system behaviour changes significantly when the irradiation commence. The external irradiation causes an increase of the burning rate, see the increase of CO2 concentration and the decreased concentration of O2 immediately after the irradiation commence. However, the increased burning rate in this case does not leadto an immediate increase in the NOx concentration. There is a slight increase of NOx during the latest stages of flame extinction, which is not related with the flame burning rate, and which might results from a local thermal fluctuation.

5. CONCLUSIONS

The results from mathematical simulation show that at otherwise identical conditions, the external radiative heating of a semi-transparent fuel droplet surrounded by a quiescent gas-phase cause a faster increase of surface temperature of the droplet, consequently increasing the mass transfer between the droplet and the surrounding gas-phase and decreasing the heterogeneity of the system.

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