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Control of Soot Emission from Diesel Engines

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Abstract

Soot emission is a problem in major cities in the world. The number of diesel cars raised a lot in last years in Palestine, were 57,3% of the new cars in 2010 were equipped with diesel engines. This evolution was motivated by diesel engine excellent fuel economy and durability. This paper discusses soot combustion fundamental processes in term of the in-cylinder combustion and emission. The new research requested both simulation and experimental researches to study fundamental process involved in diesel engines in order to decrease the soot emissions of diesel engines and to contribute to the global emission reduction.
This project of soot modeling is developed to integrate to the conception cycle the ability of predicting the soot particle concentration from combustion in diesel engines. The goal is to develop a model that can be applied during the concept phase of the engines; this model has for vocation to predict the soot concentration during the combustion cycle.

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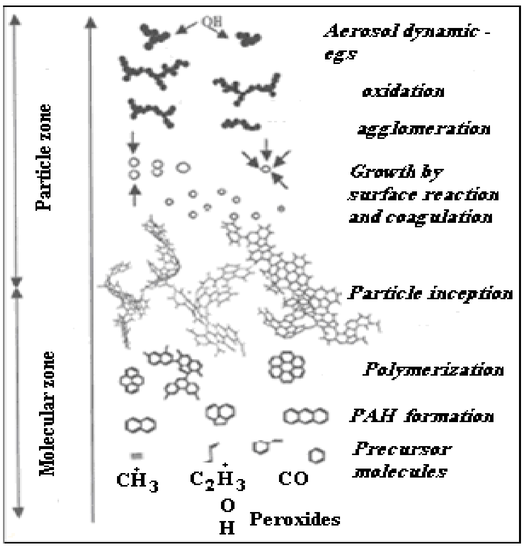
Keywords**:** harm emission reduction, soot combustion proces, diesel engines.

1. Introduction

Diesel is also responsible of emission, in particulate diesel particulate matter which includes soot particulates. These very fine particulates are considered as responsible for damaging health effects as cardiac, pulmonary and cancer effects. The effect of the particulates was also underlined; soot warms arctic in two primary ways.' When it is in the atmosphere, soot absorbs incoming solar radiation and warms the atmosphere while possibly decreasing cloudiness. On the ground, it blackens snow and ice, making it less reflective so that absorbs more warning radiation'[2]. In order to regulate the soot emissions different norms were created including soot, the Euro norms shown in table (1).
Soot particles are commonly believed to be formed by coagulation of PAH species, the resulting small particles essentially grow by heterogeneous surface reactions with acetylene being the most important growth species. These reactions are commonly modeled by the reaction mechanism. The combustion of soot particles occurs mainly by heterogeneous reactions with OH radicals and molecular oxygen [3-5].
In the present study numerical simulation of soot particles formation in diesel cylinder are presented, the kinetic model used to describe physical chemistry interactions, the formation and combustion of soot particles is described by detailed kinetically based soot model, In order to develop this model, all the formation and oxidation steps shown in fig(1) have to be described in the model from the gas phase to the solid interactions:
-The gas phase
-The formation of the first particles from the gas phase by collision of two pyrenes (molecules with four aromatic rings), this step is called nucleation or inception
-The condensation of the PAHs on the surface of the first particles
-The coagulation which accounts for the collisions of the particles between them to form bigger ones
-The surface growth and oxidation based on the Hydrogen Abstraction Carbon Addition mechanism [1,7].



Fig(1) soot formation steps

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Norms	Years	Exhaust emission standard, g/kW.h			
		NO_X	Smoke	Solid particles	CO
EURO-3	2000	5,0	0,8	0,100	2,1
EURO-4	2005	3,5	0,5	0,02	1,5
EURO-5	2008	2,0	0,5	0,02	1,5
EURO-6	2013	0,13	-	0,01	1,5

Table(1) exhaust emission norms for diesel heavy-duty, automobiles and buses

In the present study of soot particles formation in diesel cylinder are presented the chemical kinetics used to describe physical chemistry interactions, the formation and combustion of soot particles described kinetically, different assumptions for soot particles concentration are applied and the results are discussed in a comparison with experimental data provided.

2-Mathimatical Model Of Soot Formation

A predictive model of soot formation in flames is being developed by using elementary reaction to describe the basic flame chemistry, soot particles growth and combustion in the case of application fuel additives. Sectional equations for soot formation, growth and oxidation are expressed in a form suitable for concurrent soot modeling [4,7].
By using additives, which contain Ba, K, Ca and other metals, and by conserved general model construction, provided only summary about metal's character. The primary carbonyl fraction with appearance particular soot Ċ, growing and burning their surface, considered in the following form:

$C_XH_Y \rightarrow C_3H_6+C_2H_6+C_2H_4+CH_4+H_2$ (1)

$C_3H_6 \rightarrow C_2H_4+CH_4+H_2$ (2)

$C_2H_6 \rightarrow C_2H_4+H_2$ (3)

$CH_4 \rightarrow C_2H_4+H_2$ (4)

$C_2H_4 \rightarrow C_2H_2+H_2$ (5)

$C_5H_5Me(CO)_3+C_5H_5 \rightarrow (C_5H_5)_2Me+CO_3$ (5a)

$(C_5H_5)_2Me+C \rightarrow Me+C_5H_5$ (5b)

$C_2H_2 \rightarrow C_2\dot{H}+\dot{H}$ (6)

$C_2+C_2H_2 \rightarrow C_{m+2} \rightarrow (nC)_{sur.}+H_2$ (7)

$(nC)_{sur.}+C_4H_2 \rightarrow (C_{n+4})_{sur.}+H_2$ (8)

$(nC)_{sur.}+C_2H_2 \rightarrow (C_{n+2})_{sur.}+H_2$ (9)

$C+O_2 \xrightarrow{\underline{Me}} CO_2$ (10)

$C+O_2 \xrightarrow{\underline{Me}} CO$ (11)

$C+CO_2 \xrightarrow{\underline{Me}} CO$ (12)

$C+H_2O \xrightarrow{\underline{Me}} CO+H_2$ (13)

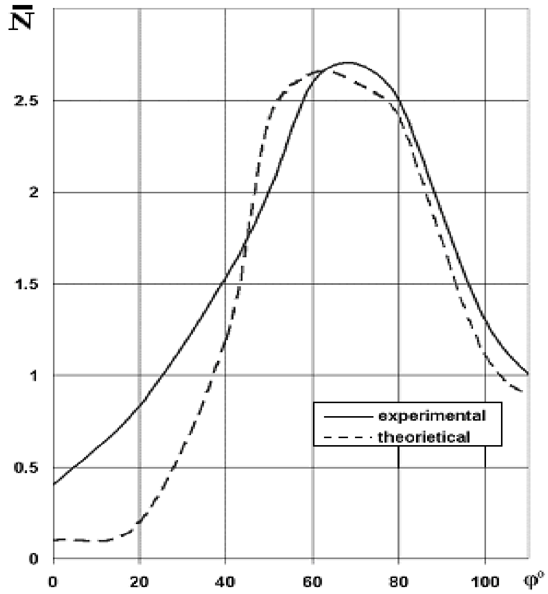
$H_2+O_2 \rightarrow H_2O$ (14)

$Me+CO \rightarrow MeO+C$ (14a)

In presented system, equation(1) describes the primary fraction of fuel to individual hydrocarbons, equations(2-5) describe high-temperature of fraction individual hydrocarbons to acetylene C_2H_2, equation(5a) illustrates isolate carbonyl groups then joining radicals, equation (5b)shows isolation metal by carbon, equation(6) describes the decomposition of acetylene with generation embryonic charged soot particles, equation(7) process carbonation and appearance physical embryonic acetylene, equations(8-9) self-accelerated growth the surface of soot particles, equation (10-14)show burning of soot particles, equation(14a) restores metal oxide by oxides of carbon[3,6,7].
Provided system kinetic equations in the form of differential equations to describe in-cylinder processes, Computer simulation gives possibility to solve the equations with high accuracy to define the instantaneous rational amount of soot $\bar{N}$ relative to crank angle position (φ^o), presented simulation describes in-cylinder processes soot generation and the combustion in diesel engine.
A part study described by the model was performed for C_2H_2-soot which correctly predicted experimental soot mass concentration, the study included cases in which only C_2H_2 added to the soot.
Mathematical model (Index 2) considers the change of soot particles concentration with crank angle position in degrees (φ^o) and so when exhaust valve opens estimated the quantity of soot particles with exhaust gases[3,7].

3. Results

The high-quality of computing results indicated in comparison with experimental data. In fig(3) presented experimental and computing rational amount of soot formation in diesel cylinder as a function of crank angle position in degrees (φ^o). Graphics show good agreement for soot particles concentration in diesel cylinder, so it confirm our assumption of chemical kinetics[3,6].



Fig(3) Soot emission with exhaust gases (rational amount of soot). Pe=3bar

In fig (2) presented experimental results of soot concentration (rational amount of soot) in diesel cylinder as a function of φ^o. An 8-cylinder diesel engine study of water-in-diesel emulsion was conducted to investigate the effect of water emulsification on soot emission with exhaust gases. Emulsified diesel fuel 17% water/diesel ratio by volume, were used direct injection diesel engine, operating at 1700 rpm and molti-loads (Pe=1,21…4,85). Graphics indicate that the addition of water in the form of emulsion decreases soot emission with exhaust gases to 20% [7,8,10].

In the result of dripping emulsified fuel increases mixture quality. Decreasing temperature on account of water Dissociation and sharply decelerate chemical reactions of soot formation. The system saturates with hydrogen's radicals which assist to suppress formation of chains at the stage of sootier radical formation so the burning speed of soot particles increases on account of increasing of carbon gasification[8,10].

Fig(2) the effect of water emulsification on soot emission with exhaust gases(rational amount of soot). 1-Pe=1,21bar 2-Pe=2,42 bar 3-Pe=3,64 bar 4-Pe=4,85 bar, ___diesel fuel, ---- Emulsified diesel fuel, 1700rpm

The results of numerical simulation show soot particles concentration (rational amount of soot) in diesel cylinder as a function of crank angle positioning in degrees (φ^o). In fig(4) presented computing results of soot formation in diesel cylinder. A single cylinder diesel engine study of metallo-organic compound fuel additives for diesel was conducted to investigate the effect of antismoking additives on soot emission with exhaust gases. Modified diesel fuel 0,5% additive/diesel ratio by mass, were used direct injection diesel engine, operating at multi-loads (Pe=2bar, Pe=5bar, and Pe=7bar) and 1300 rpm Graphics indicate that the addition of antismoking additives (SLD) decreases soot emission with exhaust gases to 40% [7].

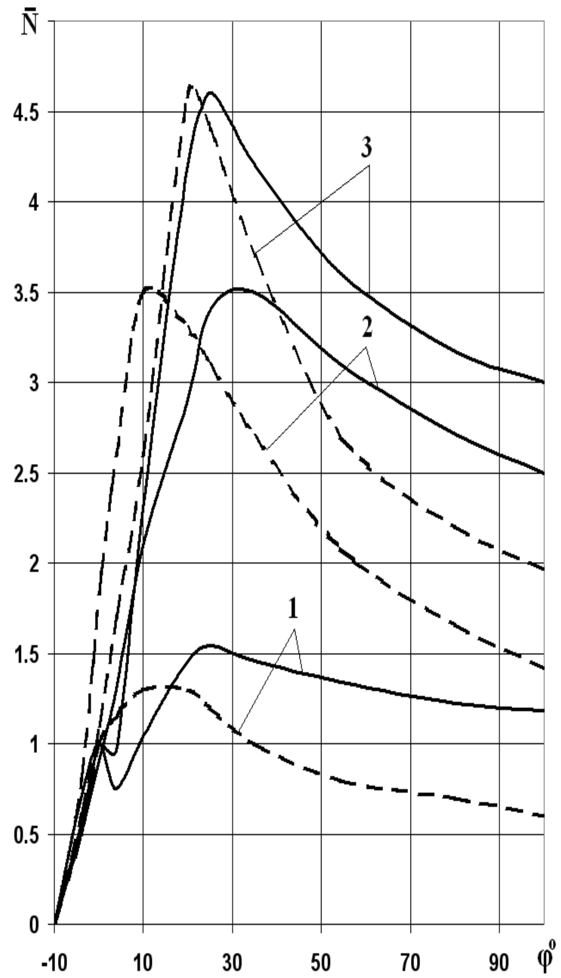


Fig (4) the effect of antismoking additives on soot emission with exhaust gases(rational amount of soot). 1-Pe=2bar 2-Pe=5 bar 3-Pe=7 bar, ____diesel fuel, ---- modified diesel fuel, 1300rpm

The soot particles reducing effects of many additives are well-known, but little is understood about the details of soot particles suppression mechanism, a laminar diffusion flame burning was seeded with a metallo-organic additive, by evaporating the additive from a crucible placed in the heated fuel gas flow, found that additives suppress the formation of PAH and accelerate the burning process[7,8,10].

4. Conclusions

The test for computer matrix simulations was developed, and parametric test results were obtained by using standard fuel and fuel with metallo-organic compound fuel additives. Simulation results indicate the following:

- Antismoking additives is effective in reducing soot.
- In period of time, metallo-organic compound fuel additives suppress the formation of PAH, but in period diffusion flame accelerate burning process, this reduce PM in exhaust gases at least 40%.
- Achieved a fundamental understanding of the formation and description in diesel particulate matters.

The presented work confirmed effective of modifications on processes of soot formation in diesel cylinder, and permit to make conclusion about mechanism their effect on the actual processes of soot formation in diesel engine, and by using dripping emulsified fuel, decreased harm emission with exhaust gases in atmosphere. A mechanism for the catalysis is proposed. We hope that this paper stimulates interest in pursuing further solutions of environmental problems.

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Index (1): List of Symbols:

Sur.	surface
F	Specific surface of soot particles, M^2/kg
n	Engine angular speed, min^{-1}
$N_{comb.}$	Soot particles combustion
$N_{form.}$	Soot particles formation
φ^o	Crank angle position
α	Theoretical air fuel ratio
α_{comb}	Actual air fuel ratio
σ	Equivalence ratio
X	Specific heat generation (Combustion efficiency)
N_n	Initial value of soot particles concentration in diesel cylinder at firing instant
R_5	Reaction speed of soot particles growth
P	Pressure of gases in diesel cylinder
r_5	Acetylene volumetric concentration
G_{air}	Cyclic entered air for 1kg fuel, m^3
G_D	Soot particles concentration with exhaust gases kg/m^3
Me	Metal
M	Metal molecule
PM	Particulate Matter
$\dot{C}$	Particular Soot
$\bar{N}$	Rational amount of soot particles
1H13/14	One Cylinder KAMAZ Engine, Cylinder Diameter 13cm, Length of Stroke 14 cm.
SLD	Antismoking Additive, which contains Barium.
rpm	Revolution per minute
Pe	Effective Pressure
TDC	Top Dead Center

Index (2): mathematical model of soot formation

1- $$\frac{d\Gamma}{d\varphi}C_{14}H_{30} = \left(-K_{+1}\Gamma_{C_{14}H_{30}} + K_{-1}C_{\Sigma}^{5,5}\cdot\Gamma_{C_3H_6}^{2}\cdot\Gamma_{CH_4}\cdot\Gamma_{C_2H_4}^{3,5}\right)/6n,$$

2- $$\frac{d\Gamma}{d\varphi}C_3H_6 = \left(\left(-K_{+2}\Gamma_{C_3H_6} + K_{-2}C_{\Sigma}\cdot\Gamma_{C_2H_4}\cdot\Gamma^{0,5}{}_{C_2H_2}\cdot\Gamma^{0,5}_{H_2}\right) - 2\frac{d\Gamma}{d\varphi}C_{14}H_{30}\right)\Big/6n,$$

3- $$\frac{d\Gamma}{d\varphi}CH_4 = \left(\left(-K_{+3}\Gamma_{CH_4} + K_{-3}C_{\Sigma}^{0,5}\cdot\Gamma_{C_2H_4}\cdot\Gamma_{H_2}\right) - \frac{d\Gamma}{d\varphi}C_{14}H_{30}\right)\Big/6n,$$

4- $$\frac{d\Gamma}{d\varphi}C_2H_4 = \left(\left(-K_{+4}\Gamma_{C_2H_4} + K_{-4}C_{\Sigma}\cdot\Gamma_{C_2H_2}\cdot\Gamma_{H_2}\right) - 6\frac{d\Gamma}{d\varphi}C_{14}H_{30} - \frac{d\Gamma}{d\varphi}C_3H_6 - 0,5\frac{d\Gamma}{d\varphi}CH_4\right)\Big/6n,$$

5- $$\frac{d\Gamma}{d\varphi}H = \left(\begin{array}{l}\left(K_{+5}C_{\Sigma}\Gamma_{H_2}\Gamma_M - K_{-5}C_{\Sigma}^2\Gamma_H^2\Gamma_M^2\right) + 7\frac{d\Gamma}{d\varphi}C_{14}H_{30} + \\ +1,5\frac{d\Gamma}{d\varphi}C_3H_6 + 0,5\frac{d\Gamma}{d\varphi}CH_4 + \frac{d\Gamma}{d\varphi}C_2H_4 + \frac{o\Gamma}{d\varphi}C_2H_2\end{array}\right)\Big/6n,$$

6- $$\frac{d\Gamma}{d\varphi}C_2H_2 = \left(\begin{array}{l}\left(-K_{+6}C_{\Sigma}\Gamma_{H_2}\Gamma_{C_2H_2} + K_{-6}C_{\Sigma}\Gamma_{H_2}\Gamma_{\dot{C}_2H}\right) - 7\frac{d\Gamma}{d\varphi}C_{14}H_{30} - \\ -1,5\frac{d\Gamma}{d\varphi}C_3H_6 + 0,5\frac{d\Gamma}{d\varphi}CH_4 + \frac{d\Gamma}{d\varphi}C_2H_4\end{array}\right)\Big/6n,$$

7- $$\frac{d\Gamma}{d\varphi}H_2 = D'\left(K_{+7}\Gamma_{C_2H_2} + 0,5K_{+8}\Gamma_{\dot{C}_2H}\right)/6n,$$

8- $$D' = \frac{\left(10^{-3}P_{\Sigma}\Sigma_{\mu_i}\Gamma_i\cdot N\cdot \mathrm{F}\cdot 10^4\right)}{\left(12\cdot 1,003\cdot G\cdot(\sigma - x)(\alpha_{\mathrm{com.}} + 1)\right)},$$

$$\Gamma_{\dot{C}_2H} = \left(1 - \sum_{i=1}^{8}\Gamma_i\right),$$

9- $$\frac{dN}{d\varphi} = \frac{10^4 P_{\Sigma}\cdot N''\cdot \mathrm{F}}{1,033\cdot 6n}\cdot\left(K_{+7}\Gamma_{C_2H_2} + 0,5K_{+8}\Gamma_{\dot{C}_2H}\right),$$

10- $$\frac{dN}{d\varphi} = \frac{10^4 P_{\Sigma}\alpha_{Д}\cdot N''\cdot S_{уд.}}{6nRT(1+N_3)(1+N_1+N_2)}\left(\begin{array}{l}\Gamma_{O_2}\left(N_1''(1+2N_3)+2N_2(1+N_3)\right)+ \\ +\Gamma_{CO_2}N_3(1+N''+N_2)+\Gamma_{H_2O}N_4\cdot \\ \cdot(1+0,5N_1+N_3)\end{array}\right),$$

11- $$\frac{dN}{d\varphi} = \frac{d\Gamma_i}{d\varphi}\cdot\Big|_{x}^{i} + \Gamma_i\frac{1}{\sigma + x}\cdot\frac{d\sigma}{d\varphi} - \Gamma_i\frac{1}{\sigma - x}\cdot\frac{dx}{d\varphi},$$