Modeling, Simulation and Experimental Study of Soot Combustion Process

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Our investigations can be divided into groups, which are however closely linked with each other:
1. The application of chemical kinetics to problems relating to the theory of combustion and explosion processes.
2. Mathematical formulation of the concentration of reactants.
3. Experimental and simulation results of soot in-cylinder concentration.
4. The influence of antismoking additives on thermal and combustion efficiencies.

This paper presents data from tests conducted by internal combustion diesel engines, a testing laboratory and results of numerical simulation. The results of calculation are compared to experimental data showing good agreement for soot particles concentration in diesel cylinder.

Keywords: harmful emission reduction and soot combustion process.

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Modeling, Simulation and Experimental Study of Soot Combustion Process

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Abstract: The formation of soot particles is one of the most complex problems in combustion science, still by for not well understood. However, intense experimental and theoretical researches within the last two decades improved the fundamental understanding and led to detailed picture of the soot particles formation process. 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 define possible strategic scenario toward zero emission level.

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I. Introduction

The heterogeneous air-fuel mixture and heterogeneous diffusion of flame stream in diesel cylinder always be accompanied with appearance of solid carbon in the form of soot particles, which estimate smog with diesel exhaust gases, the importance of studying soot particles formation not only in decreasing harm emission with exhaust gases but in increasing engine efficiency too.

Researchers on diesel particulate matters (PM) has probed and provided unprecedented details about the atomic microstructure of (PM), researchers used scattering spectroscopy with a highly sensitive optical analysis technique that can study atomic microstructures in carbonaceous material (fig.1), they have thus far concluded that higher combustion temperatures and pressure conditions within the engine are the factors contributing most to the production of diesel exhaust emission with (PM) characterized by small, agglomerated, oxidized/graphitic (sootier) particles. [U.S. Department of Energy- Drexel University-August 26, 2004]

Figure 1: The transmission electron microscope can reveal the presence of graphitic structures in PM sampled under high engine loads.

Soot particles are commonly believed to be formed by coagulation of polycyclic aromatic hydrocarbons PAH species, the resulting small particles essentially grow by heterogeneous surface reactions with acetylene being the most important growth species. The combustion of soot particles occurs mainly by heterogeneous reactions with OH radicals and molecular oxygen, the formation and oxidation steps have to be described in fig(2).

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In diesel engines, soot particles formation occurs essentially under complex heterogeneous conditions, predictions of soot particles in numerical simulations become even more difficult because of unresolved question in the treatment of physical chemistry interactions, even though some progress has been made recently, applying for reaction rate and physical state in a chemical reaction.

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.

II. SOOT PARTICLES FORMATION

Chemical kinetics take a part in process of flame stream diffusion in diesel cylinder, when reactants (mixture) are in different phases, one is liquid and the other is gas, contact can only occurs at the interface, in other words at the surface of the liquid, so this means that the more final divided a solid or liquid particles, the formation of soot particles is growing with growing particles (carbon radicals) surface.

Radicals are atomic or molecular species unpaired electrons, these unpaired electrons are usually highly reactive, so radicals are likely to take part in chemical reactions, and a radical plays an important role in combustion. The formation of radicals requires covalent bonds to be broken homiletically, a process requires by thermal cracking where complex carbonyl group (fuel) converted simpler molecules (acetylene) as shown in following reactions shown in equations (1-5).

\[
\begin{align*}
C_2H_6 & \rightarrow V_{11}C_3H_6 + V_{12}C_2H_6 + V_{13}C_2H_4 + V_{14}CH_4 + V_{15}H_2 \\
C_2H_4 & \rightarrow V_{21}C_2H_4 + V_{22}CH_4 + V_{23}H_2 \\
C_2H_6 & \rightarrow V_{31}CH_4 + V_{32}H_2
\end{align*}
\] (1-3)

CH\textsubscript{4} \rightarrow V_{41}C_2H_4 + V_{42}H_2 \quad (4) \\
C_2H_4 \rightarrow V_{51}C_2H_2 + V_{52}H_2 \quad (5)

In this type of processes, the corresponding reactive intermediates (radicals, ions) are permanently regenerated, and thus they proceed by a self-propagation chain mechanism, the chain of reactions is eventually terminated by radicals or ions recombination, the main reactions that take place include:

**Initiation** reactions are those which result in a net increase in the number of free radicals, the formation occurs at low-temperature mechanism, with appearance carbon radical C\textsubscript{6}H\textsubscript{5}-phenyl, therefore, from acetylene formed the following reactions shown in equations (6-9):

\[
\begin{align*}
C_2H_2 & \rightarrow \hat{C}_2H_5 + \hat{H} \\
C_2H_2 & \rightarrow \hat{C}_2H_2 + H \\
C_2H_2 & \rightarrow \hat{C}_2H_3 \\
C_2H_2 & \rightarrow \hat{C}_2H_3 + \hat{C}_2H_3
\end{align*}
\] (6-9)

**Isolation Metal** in the case of application metallo-organic compound antismoking fuel additives, where carbon radical removes the metal from cyclopentane compound, turning the second molecule into a free radical as shown in equation (10).

\[
(C_6H_5)Me + \hat{C} \rightarrow Me + \hat{C}_6H_5
\] (10)

**Hydrogen decomposition**, where a free radical breaks a part into two molecules, one is cyclopentane the other is a free radical as shown in equation (11).

\[
\hat{C}_6H_5 \rightarrow C_5H_5 + \hat{H}
\] (11)

**Radical addition**, the reverse of radical decomposition at T<700°C in which a radical reacts with a phenyl radical \(\hat{C}_6H_5\) to form a single or larger free radicals, these processes are involved in forming the polycyclic aromatic hydrocarbons (PAH) and other products, which a result of low-temperature processes at temperature below 1500K, as shown in the following reaction considered by equation (12):

\[
\hat{C} + \hat{C} \rightarrow \hat{C}_6H_5
\] (12)

**Termination reactions**, which happen when two free radicals react with each other to produce products that are not free radicals, high-temperature (T>1500°K) process growth aromatic hydrocarbons structure with the formation of soot particles. General scheme for reaction mechanism of soot particles formation shown in fig.(3).

Analyzing the influence of different reaction conditions gives information about the chain reaction and the transition state of matters in a chemical
reaction. Thus, expressed reaction equation (13) for carbon's concentration rate.

\[ i = \frac{12P}{8.514} \left[ (1 + 2 + 11) + 12K_{12} + 12K_{13} \right] \]  

Where: \( r_{O_2}, r_{CO_2}, r_{H_2O} \) - volumetric concentration of \( O_2, \ CO_2, \) and \( H_2O \)

Kinetic deals with experimental determination of reaction rates from which constants are derived for soot particles combustion as shown in equation (14):

\[ K_i = K \exp \left[ \frac{F_i}{E_i T_m} (1 - T_m) \right], \text{ n/s} \]  

Products of chemical reactions considered by reaction rate, the rate equations are differential equations named mathematical model, and it can be integrated in order to obtain the in-cylinder concentration of soot particles. The main differential equation describes the change of soot particles concentration in diesel cylinder as shown in equation (15):

\[ \frac{dN}{dt} = \left( \frac{dN}{dt} \right)_t + \left( \frac{dN}{dt} \right)_{k} - \left( \frac{dN}{dt} \right)_{x} \]  

Where:

\( \left( \frac{dN}{dt} \right)_t, \ \left( \frac{dN}{dt} \right)_{k}, \ \left( \frac{dN}{dt} \right)_{x} \): The change in soot particles concentration by instantaneous evaporation of the mixture, by transition state of the mixture, and based on combustion.

The rates of soot particles concentration in diesel cylinder calculated as the sum of two components are characterized soot particles formation and soot particles combustion shown in equation (16):

\[ \left( \frac{dN}{dt} \right)_{\text{form}} - \left( \frac{dN}{dt} \right)_{\text{comb}}. \]  

Mathematical model (Index 1) considers the change of soot particles concentration with crank angle position in degrees (\( \phi^o \)) and so when exhaust valve opens estimated the quantity of soot particles with exhaust gases.

III. Results

In fig (4) presented experimental results of soot concentration (rational amount of soot) in diesel cylinder as a function of \( \phi^o \). 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 r.p.m. and multi-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%.

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.

The high-quality of computing results indicated in comparison with experimental data. In fig.(5) presented experimental and computing rational amount of soot formation in diesel cylinder as a function of crank angle position in degrees (\( \phi^o \)). Graphics show good agreement for soot particles concentration in diesel cylinder, so it confirm our assumption of chemical kinetics.
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). In fig (6) 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 r.p.m. Graphics indicate that the addition of antismoking additives (SLD) decreases soot emission with exhaust gases to 40%.

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.

The results indicate that antismoking additives improve combustion efficiency (X) and brake thermal efficiency (ηth.) as shown in fig.(7). The average increase in the brake thermal efficiency is approximately 4% over the use of diesel for the engine range studied. The proper brake specific fuel consumption and gases exhaust temperature decreased.
IV. Conclusion

The results presented in this paper are those that have been carried out by sources from Altai State Technical University. The new detailed kinetic model of soot particles formation in the diesel cylinder and aromatic hydrocarbons is proposed, the model based on comprehensive of PAH formation and growth.

The new pathways were introduced into the kinetic mechanism of the soot particles formation and the new concepts of soot particles nucleation and soot particles surface growth implemented in the new model made it possible to improve considerably the agreement between the results of calculations and experimental measurements. A mechanism for the catalysis is proposed. We hope that this paper stimulates interest in pursuing further solutions of environmental problems.

V. Acknowledgement

During the planning and preparation of this, the authors had advice and assistance of many people researchers, educators, and specialists. The authors offer their sincere thanks. Special thanks are owed to the following organizations for information: Ministry of Education and Higher Education, and Palestinian Polytechnic University.

REFERENCES Références Referencias

**Index 1: List of Symbols**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi_0$</td>
<td>Crank angle position</td>
</tr>
<tr>
<td>$N$</td>
<td>Rational amount of soot particles</td>
</tr>
<tr>
<td>$\text{1H13/14}$</td>
<td>One Cylinder KAMAZ Engine, Cylinder Diameter 13cm, Length of Stroke 14 cm.</td>
</tr>
<tr>
<td>$F$</td>
<td>Specific surface of soot particles, $\text{m}^2/\text{kg}$</td>
</tr>
<tr>
<td>$G_{\text{act}}$</td>
<td>Cyclic entered air for 1kg fuel, $\text{m}^3$</td>
</tr>
<tr>
<td>$G_P$</td>
<td>Soot particles concentration with exhaust gases $\text{kg}/\text{m}^3$</td>
</tr>
<tr>
<td>$K^*$</td>
<td>8m/sec</td>
</tr>
<tr>
<td>$n$</td>
<td>Engine angular speed, min$^{-1}$</td>
</tr>
<tr>
<td>$N_{\text{comb}}$</td>
<td>Soot particles combustion</td>
</tr>
<tr>
<td>$N_{\text{comb}}$</td>
<td>Soot particles formation</td>
</tr>
<tr>
<td>$N_{\text{ini}}$</td>
<td>Initial value of soot particles concentration in diesel cylinder at firing instant</td>
</tr>
<tr>
<td>$P$</td>
<td>Pressure of gases in diesel cylinder</td>
</tr>
<tr>
<td>$M_e$</td>
<td>metal</td>
</tr>
<tr>
<td>r.p.m.</td>
<td>Revolution per minute</td>
</tr>
<tr>
<td>$R_e$</td>
<td>Reaction speed of soot particles growth</td>
</tr>
<tr>
<td>$L_0$</td>
<td>Acetylene volumetric concentration</td>
</tr>
<tr>
<td>SLD</td>
<td>Antismoking additive, which contains Barium.</td>
</tr>
<tr>
<td>$T^*$</td>
<td>$2500 \text{ K}$</td>
</tr>
<tr>
<td>TDC</td>
<td>Top Dead Center</td>
</tr>
<tr>
<td>$T_m$</td>
<td>Average temperature in the center of flame.</td>
</tr>
<tr>
<td>$\chi$</td>
<td>Specific heat generation (Combustion efficiency)</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Theoretical air fuel ratio</td>
</tr>
<tr>
<td>$\alpha_{\text{comb}}$</td>
<td>Actual air fuel ratio</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Equivalence ratio</td>
</tr>
</tbody>
</table>

**Index 2: Mathematical model of soot formation**

1. $\frac{d\Gamma}{d\phi} C_{i1H_{30}} = \left( -K_i \Gamma C_{i1H_{30}} + K_i C_i ^{55} \cdot \Gamma_i C_{iH_i} \cdot \Gamma_i C_{H_i} \right) \frac{1}{6n},$

2. $\frac{d\Gamma}{d\phi} C_{i2H_i} = \left( C_{i2H_i} ^{55} \cdot \Gamma_i C_{iH_i} \cdot \Gamma_i C_{H_i} - \frac{1}{2} \frac{d\Gamma}{d\phi} C_{i1H_{30}} \right) \frac{1}{6n},$

3. $\frac{d\Gamma}{d\phi} C_{iH_i} = \left( -K_i \Gamma C_{iH_i} + K_i C_i ^{55} \cdot \Gamma_i C_{iH_i} \cdot \Gamma_i C_{H_i} \right) \frac{d\Gamma}{d\phi} C_{i1H_{30}} \frac{1}{6n},$

4. $\frac{d\Gamma}{d\phi} C_{iH_i} = \left( C_{iH_i} ^{55} \cdot \Gamma_i C_{iH_i} \cdot \Gamma_i C_{H_i} + \frac{1}{2} \frac{d\Gamma}{d\phi} C_{i1H_{30}} \right) \frac{1}{6n},$

5. $\frac{d\Gamma}{d\phi} H_2 = \frac{1}{6n} \left( -K_{iH_2} \Gamma C_{iH_2} + K_{iH_2} C_i ^{55} \cdot \Gamma_i C_{iH_i} \cdot \Gamma_i C_{H_i} \right) / 6n,$

6. $\frac{d\Gamma}{d\phi} H_i = \frac{1}{6n} \left( -K_{iH_i} \Gamma C_{iH_i} + K_{iH_i} C_i ^{55} \cdot \Gamma_i C_{iH_i} \cdot \Gamma_i C_{H_i} \right) / 6n,

7. $\frac{d\Gamma}{d\phi} H_2 = \frac{1}{6n} \left( -K_{iH_2} \Gamma C_{iH_2} + K_{iH_2} C_i ^{55} \cdot \Gamma_i C_{iH_i} \cdot \Gamma_i C_{H_i} \right) / 6n,$

8. $D^* = \frac{10^{-3} P \sum \Gamma_i \cdot N - F \cdot 10^4}{12 \cdot 1003 \cdot \chi \cdot (\alpha_{\text{comb}} + 1)},$

9. $\frac{\partial N}{\partial x} = \frac{10^4 P_e \cdot N^* F}{1003 \cdot 6n} \left( K_{iH_2} C_{iH_2} + 0.5 K_{iH_i} C_{iH_i} \right),$

10. $\frac{\partial N}{\partial x} = \frac{10^4 P_e \cdot N^* F}{6n} \left( \frac{\partial \Gamma_i \cdot \partial N}{\partial x} \right),$

11. $\frac{d\Gamma}{d\phi} \cdot \frac{1}{x} + \frac{1}{x} \cdot \frac{d\Gamma}{d\phi} / \frac{1}{x} = \frac{d\Gamma}{d\phi} / \frac{1}{x} \cdot \frac{d\Gamma}{d\phi} / \frac{d\phi}{d\phi}$