

## **MATHEMATICAL MODELLING OF FUEL COMBUSTION IN DIESEL ENGINES. II. INFLUENCE OF OPERATION PARAMETERS ON THE EMISSIONS OF EXHAUST GASES**

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**Abstract.** By using the statistical method for analysis, equations were worked out describing the dependence of exhaust gases on the amount of the air introduced in the combustion chamber. Experimental data for diesel fuels containing Ca, Ba or Mg salt of a nitrated fraction were used in this study. The results obtained make it possible to model diesel fuel combustion more accurately.

**Keywords:** diesel engines, operation parameters, diesel fuel, smoke gases.

### **AIMS AND BACKGROUND**

Internal combustion diesel engines are the main source of air pollution. The problem of decreasing the harmful components in exhaust gases from diesel engines can be solved in two ways: by optimising the construction of diesel engines and improving the quality of fuels and oils<sup>1</sup>.

The characteristics of modern diesel fuels can be improved by better production technologies and also by using various additives<sup>2</sup>. The main types of additives, used to improve the operation characteristics of diesel fuels, are compounds able to facilitate fuel combustion and to decrease smoke, carbon deposit, sediment formation in the combustion system of the engine, the cold filter plugging point and the pour point<sup>3</sup>.

With regard to this, the aim of the present study is to model the combustion process in a diesel engine by using additives synthesised from oil fractions treated with nitric acid<sup>4</sup>.

“Statistica” program is used to process the experimental data obtained in order to work out mathematical models for calculating some of the parameters of the fuels.

### **RESULTS AND DISCUSSION**

The experimental results for the combustion of the exhaust gases from the engine show a decrease in the amount of the products of the incomplete combustion:

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\* For correspondence.

Table 1. Mathematical models describing the dependence of exhaust gases on the air-excess coefficient

Pure DF	Parameters			DF+0.5% nitr. fraction	Parameters		
	correl. coeff.	mean abs.err.	mean relat.err. (%)		correl. coeff.	mean abs.err.	mean relat.err. (%)
1	2	3	4	5	6	7	8
$HC\% = 0.109 - 0.022\alpha - 0.36\alpha^2 + 0.447\alpha^3 - 0.191\alpha^4 + 0.027\alpha^5$	0.997	0.00046	2.78	$HC\% = 0.499 - 0.059\alpha - 1.53\alpha^{-1} + 2.379\alpha^2 - 1.950\alpha^3 + 0.808\alpha^4 - 0.132\alpha^5$	0.999	0.00012	1.88
$CO\% = -0.049 + 0.012\alpha + 0.642\alpha^2 - 1.157\alpha^3 + 0.79\alpha^4 - 0.174\alpha^5$	0.999	0.0022	2.74	$CO\% = 0.07 - 0.012\alpha + 0.037\alpha^2 - 0.029\alpha^3 + 0.081\alpha^4 - 0.024\alpha^5$	0.999	0.00098	1.03
$D = -660.655 + 101.527\alpha + 1860.082\alpha^1 - 2518.28\alpha^2 + 1805.238\alpha^3 - 647.541\alpha^4 + 91.688\alpha^5$	0.999	0.0007	0.002	$D = -212.919 + 35.139\alpha + 565.377\alpha^1 - 739.414\alpha^2 + 525.791\alpha^3 - 190.238\alpha^4 + 27.492\alpha^5$	0.999	0.001	0.007
$CO_2\% = -100.571 + 17.241\alpha + 269.066\alpha^1 - 346.145\alpha^2 + 240.465\alpha^3 - 85.761\alpha^4 + 12.236\alpha^5$	0.999	0.0003	0.005	$CO_2\% = 30.882 - 3.125\alpha - 70.252\alpha^1 + 102.879\alpha^2 - 76.712\alpha^3 + 27.968\alpha^4 - 4.025\alpha^5$	0.999	0.00008	0.0012
$HC\% = 0.109 - 0.022\alpha - 0.36\alpha^2 + 0.447\alpha^3 - 0.191\alpha^4 + 0.027\alpha^5$	0.997	0.00046	2.78	$HC\% = -0.661 + 0.1\alpha + 1.798\alpha^{-1} - 2.451\alpha^2 + 1.749\alpha^3 - 0.611\alpha^4 + 0.082\alpha^5$	0.999	0.0002	2.42

to be continued

Continuation of Table 1

1	2	3	4	5	6	7	8
$CO\% = -0.049 + 0.012\alpha + 0.642\alpha^2 - 1.157\alpha^3 + 0.79\alpha^4 - 0.174\alpha^5$	0.999	0.0022	2.74	$CO\% = -4.147 + 0.599\alpha + 11.478\alpha^1 - 15.642\alpha^2 + 11.27\alpha^3 - 4.01\alpha^4 + 0.562\alpha^5$	0.999	0.0018	1.58
$D = -660.655 + 101.527\alpha + 1860.082\alpha^1 - 2518.28\alpha^2 + 1805.238\alpha^3 - 647.541\alpha^4 + 91.688\alpha^5$	0.999	0.0007	0.002	$D = 104.959 - 9.056\alpha - 329.969\alpha^1 + 551.396\alpha^2 - 465.081\alpha^3 + 192.919\alpha^4 + 30.873\alpha^5$	0.999	0.00044	0.0023
$CO_2\% = -100.571 + 17.241\alpha + 269.066\alpha^1 - 346.145\alpha^2 + 240.465\alpha^3 - 85.761\alpha^4 + 12.236\alpha^5$	0.999	0.0003	0.005	$CO_2\% = 14.986 - 0.812\alpha - 26.966\alpha^1 + 43.353\alpha^2 - 33.709\alpha^3 + 12.443\alpha^4 - 1.839\alpha^5$	0.999	0.000031	0.00053
$HC\% = 0.109 - 0.022\alpha - 0.36\alpha^2 + 0.447\alpha^3 - 0.191\alpha^4 + 0.027\alpha^5$	0.997	0.00046	2.78	$HC\% = -0.819 + 0.122\alpha + 2.315\alpha^1 - 3.305\alpha^2 + 2.474\alpha^3 - 0.911\alpha^4 + 0.130\alpha^5$	0.999	0.00026	2.72
$CO\% = -0.049 + 0.012\alpha + 0.642\alpha^2 - 1.157\alpha^3 + 0.79\alpha^4 - 0.174\alpha^5$	0.999	0.0022	2.74	$CO\% = -3.085 + 0.42\alpha + 8.941\alpha^1 - 12.45\alpha^2 + 8.995\alpha^3 - 3.148\alpha^4 + 0.429\alpha^5$	0.999	0.00093	0.99
$D = -660.655 + 101.527\alpha + 1860.082\alpha^1 - 2518.28\alpha^2 + 1805.238\alpha^3 - 647.541\alpha^4 + 91.688\alpha^5$	0.999	0.0007	0.002	$D = 449.390 - 65.367\alpha - 1116.05\alpha^1 + 1466.88\alpha^2 - 1032.19\alpha^3 + 372.488\alpha^4 - 53.859\alpha^5$	0.999	0.0051	0.021

to be continued

1	2	3	4	5	6	7	8
$CO_2\% = -100.571 + 17.241\alpha$ $+ 269.066\alpha^1 - 346.145\alpha^2$ $+ 240.4655\alpha^3 - 85.761\alpha^4$ $+ 12.236\alpha^5$	0.999	0.0003	0.005	$CO_2\% = 14.986 - 0.812\alpha$ $- 26.966\alpha^1 + 43.353\alpha^2$ $- 33.709\alpha^3 + 12.443\alpha^4$ $- 1.839\alpha^5$	0.999	0.000031	0.00053
$HC\% = 0.109 - 0.022\alpha - 0.36\alpha^2$ $+ 0.447\alpha^3 - 0.191\alpha^4$ $+ 0.027\alpha^5$	0.997	0.00046	2.78	$HC\% = -0.533 + 0.081\alpha$ $+ 1.564\alpha^1 - 2.326\alpha^2 + 1.798\alpha^3$ $- 0.673\alpha^4 + 0.096\alpha^5$	0.999	0.00031	2.89
$CO\% = -0.049 + 0.012\alpha$ $+ 0.642\alpha^2 - 1.157\alpha^3 + 0.79\alpha^4$ $- 0.174\alpha^5$	0.999	0.0022	2.74	$CO\% = -0.334 - 0.005\alpha$ $+ 1.837\alpha^1 - 3.009\alpha^2 + 2.148\alpha^3$ $- 0.588\alpha^4 + 0.045\alpha^5$	0.999	0.0011	1.45
$D = -660.655 + 101.527\alpha$ $+ 1860.082\alpha^1 - 2518.28\alpha^2$ $+ 1805.238\alpha^3 - 647.541\alpha^4$ $+ 91.688\alpha^5$	0.999	0.0007	0.002	$D = -59.42 + 11.571\alpha$ $+ 242.639\alpha^1 - 346.571\alpha^2$ $+ 254.519\alpha^3 - 89.512\alpha^4$ $+ 12.187\alpha^5$	0.999	0.0048	0.02
$CO_2\% = -100.571 + 17.241\alpha$ $+ 269.066\alpha^1 - 346.145\alpha^2$ $+ 240.4655\alpha^3 - 85.761\alpha^4$ $+ 12.236\alpha^5$	0.999	0.0003	0.005	$CO_2\% = 9.901 - 0.359\alpha$ $- 7.482\alpha^1 + 8.925\alpha^2$ $- 4.344\alpha^3 + 0.536\alpha^4$ $- 0.0023\alpha^5$	0.999	0.0081	0.12

HC% – amount of hydrocarbons (%); CO% – amount of carbon oxide (%); D – smoke on Hartridge; CO<sub>2</sub>% – amount of carbon dioxide (%); α – air-excess coefficient.

soot, carbon oxide and hydrocarbons. The results obtained after processing the experimental data by the statistical method are shown in Table 1. They confirm the supposition that the fuel burns most completely when using the metal salts of nitrated oil hydrocarbons. This is another proof that the metal cations therein facilitate combustion leading to a more complete utilisation of the fuel injected in the combustion chamber. The most complete combustion takes place when the most favourable composition of the fuel-air mixture is used at  $\alpha$  greater than 0.9.

On the grounds of the results obtained it may be supposed that combustion of the fuel injected in the combustion chamber is a process consisting of a several stages. The first stage involves injection of the fuel in the combustion chamber in the form of a torch with optimum length and diameter of the drops. These parameters are regulated both by the construction of the injection nozzles and by the statistically established optimum range of the values for the standard parameters of the fuel, such as kinematic viscosity, relative density and surface tension. The additives used optimise these parameters within the standard and have a positive effect on the process. The second stage involves mixing the fuel drops with the air which is compressed and heated in the combustion chamber. The third step is heating and evaporation of the separate drops and formation of the combustion vapour. At the fourth stage, part of the unstable hydrocarbons, available mostly in the vapour phase, go on heating and as a result they decompose and transform into lower hydrocarbons. The positive role of the additives under study is that they optimise the cetane number of the fuel and allow sufficient time for the second, third and fourth stage to develop. Probably, the essential combustion process begins at the fifth stage when self-ignition of the separate drops takes place. It is in this stage that the role of the additives is very important, because we suppose that they increase the number of the so called self-igniting centres in the fuel-air mixture. This makes it possible to widen the flame wave front which speeds up the spread of combustion throughout the whole mixture. Besides, the additives do not allow the products obtained by decomposition of the unstable hydrocarbons in the previous stage to undergo polycondensation forming the so-called "pre-soot". Even if such products were obtained at the last stage, they would burn completely under the catalytic effect of the metals in the additives. As a result, the amount of the final combustion products – carbon dioxide and water – will be greater.

## CONCLUSIONS

1. The metallo-organic salts synthesised on the basis of nitrated oil hydrocarbons stimulate more complete combustion of diesel fuel.
2. Nitrated oil hydrocarbons speed up the process connected with thermal decomposition of diesel fuel and shorten the period of self-ignition hold-up.
3. The compounds under study added to diesel fuel do not have a substantial influence on its volatility.

4. The suggested empirical dependences help to model the process of combustion in a diesel engine.

#### REFERENCES

1. P. S. PETKOV, S. IVANOV, D. MINKOV, A. IVANOV: Chemmotology of oils. VHTI, 1989.
2. A. A. BRATKOV: Theoretical bases of chemmotology. Chimia, Moscow, 1985 (in Russian).
3. I. MLADENOV, P. PETKOV, D. MINKOV: Influence of additive MMP-75 on working a diesel engine IT9-3M. *Chimia i industria*, 7, 293 (1978) (in Bulgarian).
4. D. KAMENSKI, V. KORNJUSHKO: Matematical modelling and optimization of chemical processes. VHTI, 1982 (in Bulgarian).

*Received 18 December 2000*

*Revised 12 April 2001*