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Title: Mathematical model of industrial waste-derived fuel droplet combustion in high-temperature air

Authors: K. Paushkina, D. Glushkov, M. Glotov

Affiliations: National Research Tomsk Polytechnic University

30, Lenin Avenue, Tomsk, Russia, 634050.

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Keywords:

composite liquid fuel, droplet, ignition, ignition delay time, mathematical modeling

I. Relevance of the research topic

Growth in energy consumption and waste accumulation

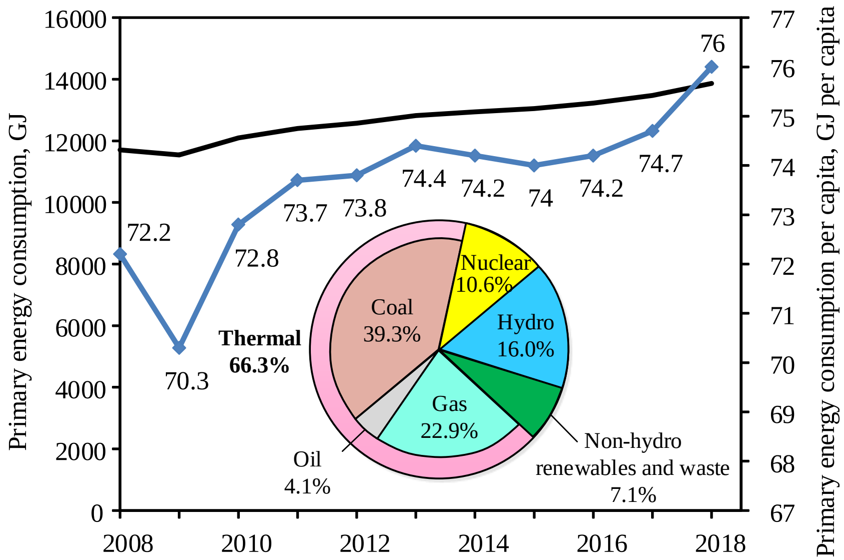

Fig. 1. Energy consumption [1]

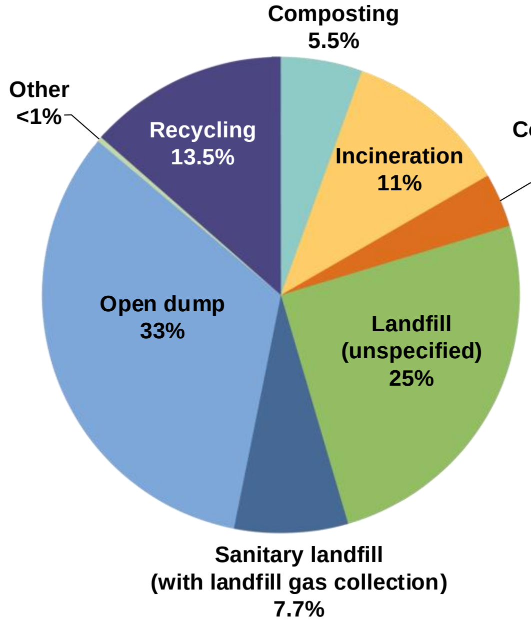

Fig. 2. Global structure of MSW disposal [4]

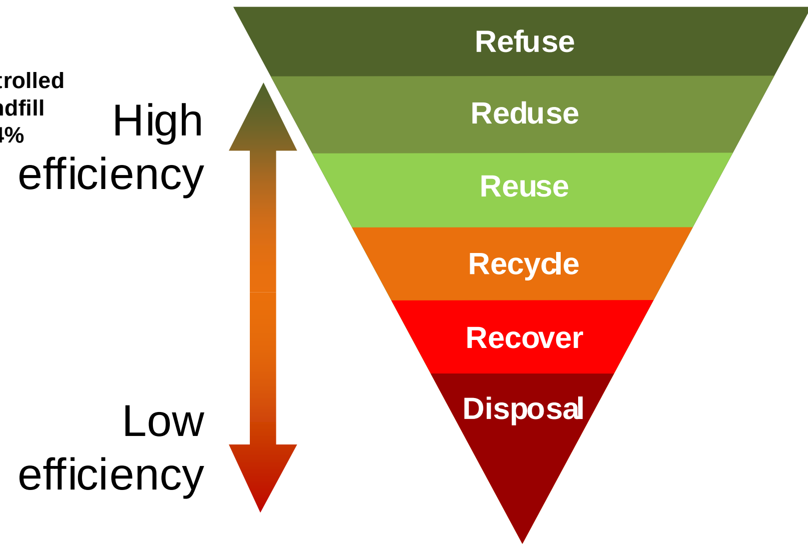

Fig. 3. Waste management methods [4]

Table 1. Worldwide waste statistics

Industrial waste	Used engine oils
7 billion tons are produced annually [2]	**30–40 million tons** are produced annually [3]
Municipal solid waste (MSW)	**Oil sludge**
2.1 billion tons are produced annually (about **70% are stored**) [4]	**60 million tons** are produced annually, **>1 billion tons**’ve been accumulated [3]

MSW contains about **82%** combustible components (cardboard, paper, wood, textiles, rubber, leather, plastic) with a calorific value of **6–13 MJ / kg** [4].

[1] International Energy Agency, 2019. Coal Information. http://www.iea.org.
[2] United Nations Environment Programme, 2015. Global Waste Management Outlook. http://www.uncclearn.org.
[3] Oil Information. International Energy Agency. 2018. http://www.iea.org.
[4] Kaza S et al. What a Waste 2.0: A Global Snapshot of Solid Waste Management to 2050. World Bank; 2018.

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II. Research Objective

Development of a mathematical model of the single composite liquid fuel droplet combustion in an heated to high temperatures air based on the results of experimental studies.

Fig. 4. Videogram of the ignition and combustion of a droplet of a composite liquid fuel at T_g=800 °C [5]

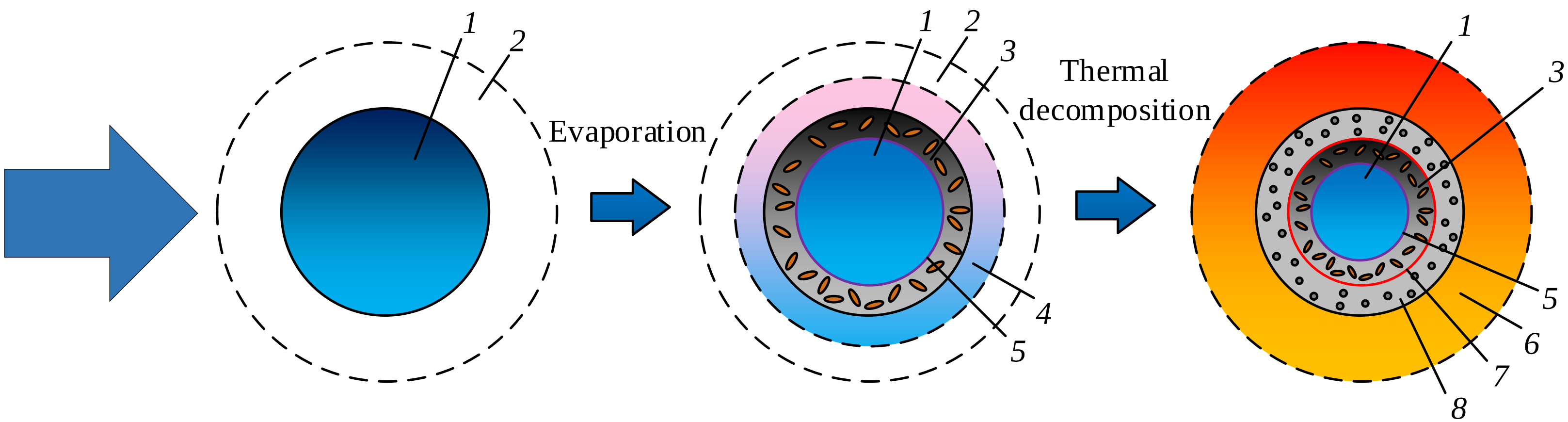

Fig. 5. Scheme of physical model of industrial and municipal waste co-combustion: *1* – initial (saturated) fuel, *2* – heated motionless air, *3* – mixture of FC and MSW, *4* – diffusion zone of flammable gases and water vapors, *5* – evaporation front, *6* – gas phase ignition area, *7* – combustion front, *8* – solid residue [5–8]

[5] Glushkov D.O., **Paushkina K.K.**, Shabardin D.P., Strizhak P.A. // Journal of Cleaner Production 201 (2018) 1029–1042.
[6] Glushkov D.O., Feoktistov D.V., Kuznetsov G.V., Batishcheva K.A., Kudelova T., **Paushkina K.K.** // Fuel 265 (2020) 116915.
[7] Glushkov D.O., **Paushkina K.K.**, Shabardin D.P. // Chemosphere 240 (2020) 124892.
[8] Glushkov D.O., **Paushkina K.K.**, Shabardin D.P., Strizhak P.A., Gutareva N.Yu. // Journal of Environmental Management 231 (2019) 896–904.

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III. Experimental investigation of fuel combustion

Characteristics of fuel components

Fig. 6. Appearance of fuel components

Table 2. Ultimate analysis of fuel components [9,10]

Component	C^{daf} (%)	H^{daf} (%)	N^{daf} (%)	S^{daf} (%)	O^{daf} (%)
FC*	87.2	5.1	2.1	1.1	4.5
Wood	50.3	6.0	0.2	0.1	43.4
Rubber	97.9	1.2	0.3	0.6	–
Plastic	66.7	7.9	–	–	25.4
Cardboard	46.3	6.3	0.3	0.2	46.9

* – dry filter cake.

Table 4. Flash point and ignition temperature of fuel components [9,10]

Component	Flash point (°C)	Ignition temperature (°C)
FC	–	450
Wood	230	340
Rubber	–	350
Plastic	306	415
Cardboard	–	250

Table 3. Proximate analysis of fuel components [9,10]

Component	W^a (%)	A^d (%)	V^{daf} (%)	$Q^a_{s,V}$ (MJ/kg)
FC*	–	26.5	23.1	24.83
Wood	20.0	2.0	–	16.45
Rubber	2.0	1.8	–	33.50
Plastic	2.0	0.2	–	22.00
Cardboard	5.0	3.0	–	17.50

[9] Klepikov D.M., Kudelova (Brozhova) T., **Paushkina K.K.**, Strizhak P.A. // Applied Sciences 10 (19) (2020) Article number 6689.
[10] Glushkov D.O., Kuznetsov G.V., **Paushkina K.K.** // Energies 13 (2020) Article number 259.

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Fuel compositions and setup layouts

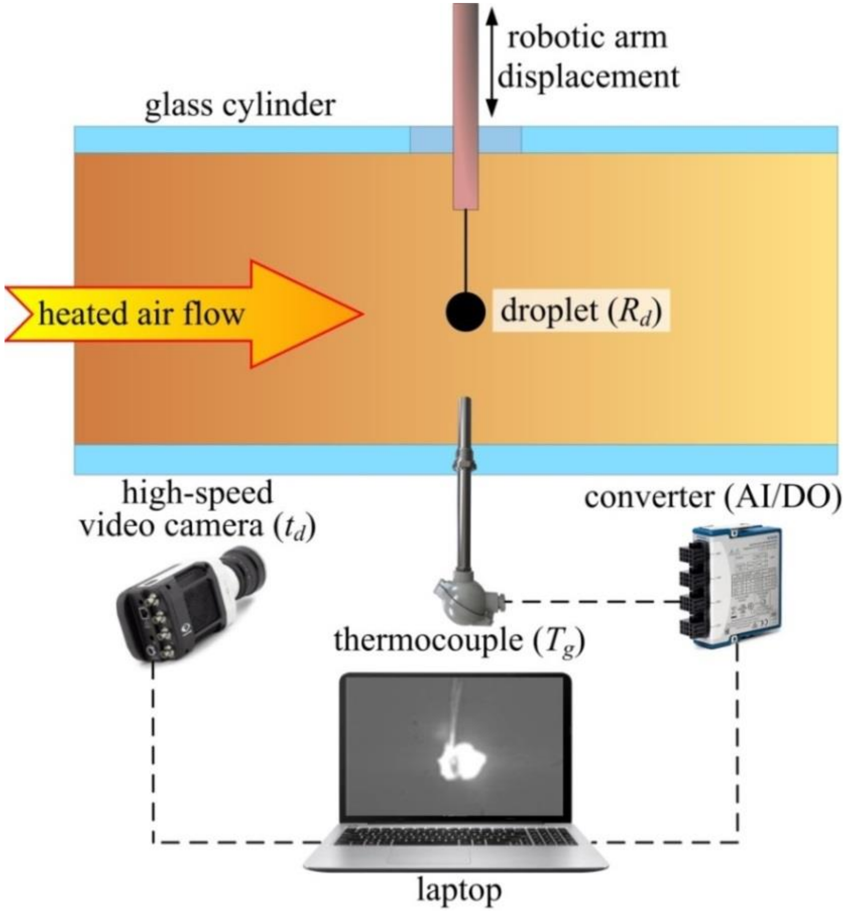

Fig. 7. Schematic of experimental setup [5]: convective heating (V_g≈3 m/s) at T_g=400–700 °C

Table 5. Composite liquid fuel compositions [5]

No.	FC	Wood	Rubber	Plastic	Cardboard	Q (MJ/kg)
1	100%	–	–	–	–	10.78
2	90%	10%	–	–	–	11.29
3	90%	–	10%	–	–	13.05
4	90%	–	–	10%	–	11.88
5	90%	–	–	–	10%	11.43

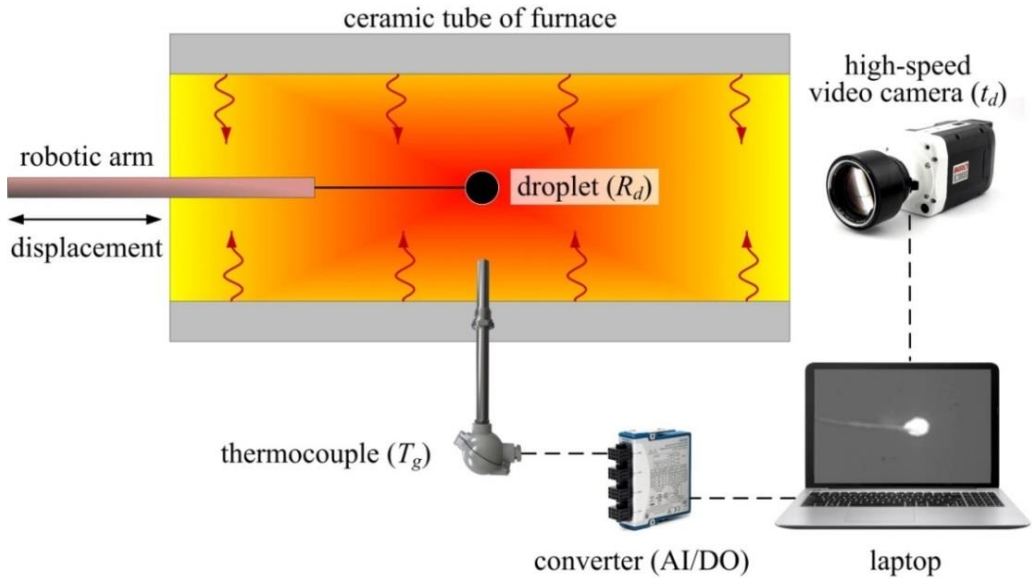

Fig. 8. Schematic of experimental setup [5]: radiant heating (V_g≈0) at T_g=400–1000 °C

[5] Glushkov D.O., **Paushkina K.K.**, Shabardin D.P., Strizhak P.A. // Journal of Cleaner Production 201 (2018) 1029–1042.

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III. Experimental investigation of fuel combustion

Ignition characteristics

Table 6. Averaged experimental ignition delay times of fuel compositions at different ambient temperatures [5]

No. composition	Static air temperature (V_g≈0)						
	450 °C	500 °C	600 °C	700 °C	800 °C	900 °C	1000 °C
1	19.57	16.32	11.39	8.14	5.90	4.13	2.98
2	18.15	15.04	10.47	7.50	5.26	3.77	2.69
3	17.00	14.08	9.67	6.74	4.65	3.29	2.31
4	16.55	13.60	9.19	6.26	4.25	2.98	2.02
5	14.15	11.35	7.30	4.62	2.85	1.73	0.96

No. composition	Air flow temperature (V_g≈3 м/с)					
	450 °C	500 °C	550 °C	600 °C	650 °C	700 °C
1	7.48	6.00	4.86	3.93	3.14	2.56
2	7.03	5.62	4.53	3.65	2.89	2.36
3	6.65	5.38	4.38	3.53	2.81	2.31
4	6.54	5.28	4.26	3.43	2.71	2.19
5	6.37	5.15	4.14	3.34	2.65	2.14

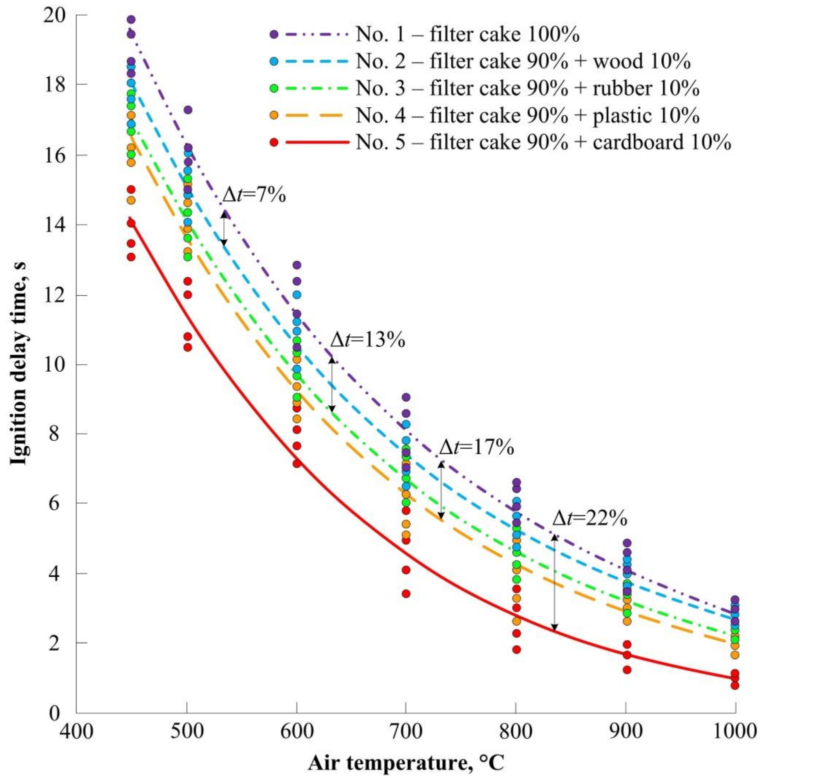

Fig. 9. The dependence of the fuel ignition delay times on the air temperature under radiant heating [5]

[5] Glushkov D.O., **Paushkina K.K.**, Shabardin D.P., Strizhak P.A. // Journal of Cleaner Production 201 (2018) 1029–1042.

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IV. Mathematical model

The gas phase is treated with an Eulerian frame and described by steady-state Reynolds-averaged Navier–Stokes equations (RANS) closed by *k*−*ε* turbulence model equations

$$\nabla \cdot \left(\rho \vec{u} \right) = 0$$

$$\nabla \cdot \left(\rho \vec{u}\vec{u} \right) = -\nabla p + \nabla \cdot \left(\bar{\tau} \right) + \rho \vec{g} + \vec{F}$$

$$\nabla \cdot \left(\vec{u}(\rho H + p) \right) = -\nabla \cdot \left(\sum_i h_i J_i \right)$$

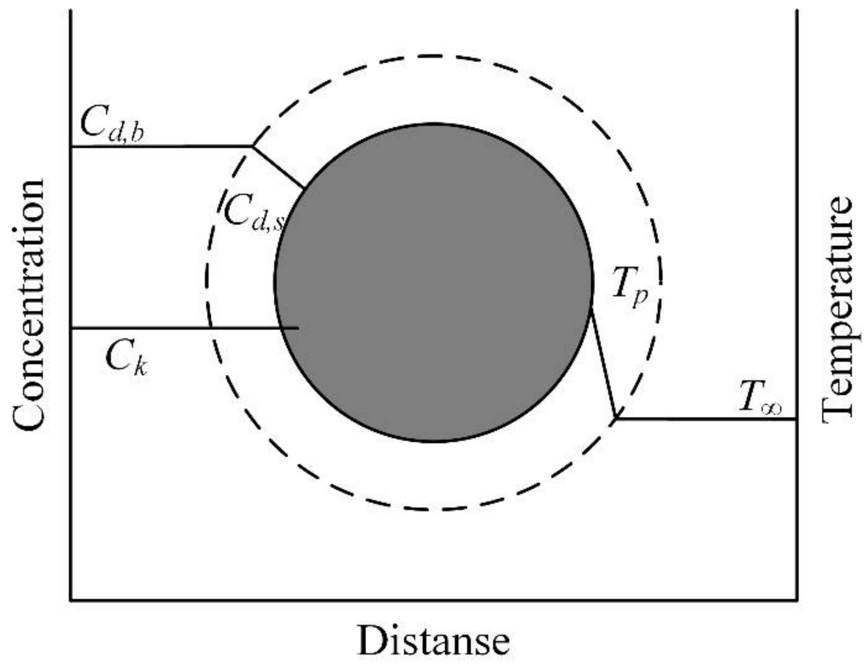
The transport equations for the turbulent kinetic energy *k* and the viscous dissipation *ε* ($C_{\varepsilon 1}$=1.44; $C_{\varepsilon 2}$=1.92; σ_k=1; σ_ε=1.3)

$$div\left(\rho k \vec{u} \right) = div\left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) grad\, k \right] + G_k - \rho\varepsilon$$

$$div\left(\rho \varepsilon \vec{u} \right) = div\left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) grad\, \varepsilon \right] + C_{\varepsilon 1} \frac{\varepsilon}{k} G_k - C_{\varepsilon 2} \rho \frac{\varepsilon^2}{k}$$

The gas species equation

$$\nabla \cdot \left(\rho \vec{u} Y \right) = -\nabla \cdot \vec{J} + R$$



$$\text{particle species} + \text{gas phase species} \rightarrow \text{products}$$

$$\text{Solid fuel} \rightarrow C_\alpha H_\beta O_\gamma N_\delta + C_s$$

Fig. 10. A reacting particle in the Multiple Surface Reactions Model

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IV. Mathematical model

For composite fuels has been developed the discrete particle model (DPM) which follows the Euler–Lagrange approach.

Energy equation includes heat transfer to the particle during devolatilization and char combustion.

$$m_p c_p \frac{dT_p}{dt} = hA_p\left(T_\infty - T_p\right) + \frac{dm_p}{dt} h_{fg} + A_p \varepsilon_p \sigma\left(\theta_R^4 - T_p^4\right)$$

$$m_p c_p \frac{dT_p}{dt} = hA_p\left(T_\infty - T_p\right) - f_h \frac{dm_p}{dt} H_{reac} + A_p \varepsilon_p \sigma\left(\theta_R^4 - T_p^4\right)$$

The particle force balance equation (Newton's second law of motion)

$$\frac{du_p}{dt} = F_D(u - u_p) + \frac{g(\rho_p - \rho)}{\rho_p} + F_a; \qquad F_D = \frac{18\mu}{\rho_p d_p^2} \frac{C_D \operatorname{Re}}{24}.$$

The law of the particle mass change

$$m_p\left(t + \Delta t\right) = m_p\left(t\right) - N_i A_p M_{w,i} \Delta t$$

The law of the particle temperature change

$$T_p\left(t + \Delta t\right) = \alpha_p + \left[T_p\left(t\right) - \alpha_p\right] e^{-\beta_p \Delta t}; \quad \alpha_p = \frac{hA_p T_\infty + \frac{dm_p}{dt} h_{fg} + A_p \varepsilon_p \sigma \theta_R^4}{hA_p + A_p \varepsilon_p \sigma T_p^3}; \quad \beta_p = \frac{A_p\left(h + \varepsilon_p \sigma T_p^3\right)}{m_p c_p}.$$

Typical stages of the thermal decomposition process:

- drying;
- pyrolysis;
- gasification;
- combustion.

Chemical reaction rate (according to Arrhenius law)

$$R_{kin,r} = \frac{A_r T_p^{\beta_r} e^{-\left(E_r / RT_p\right)}}{\left(p_{r,d}\right)^{N_r}} \prod_{n=1}^{n_{\max}} p_n^{N_{r,n}}$$

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IV. Mathematical model

Table 7. Values of kinetic parameters of chemical reactions of composite fuel during heating

Reaction	Pre-exponential factor, s^{-1}	Activation energy, kJ/(mol·K)
Drying (water evaporation)		
$H_2O(l) = H_2O(g)$	$5.13 \cdot 10^{6}$	87.9
Pyrolysis		
Biomass pyrolysis		
lignin=$0.209CO_2+0.396CO+0.109H_2+0.249H_2O+0.037vol$	$2.202 \cdot 10^{12}$	181
hemicellulose=$0.209CO_2+0.396CO+0.109H_2+0.249H_2O+0.037vol$	$2.527 \cdot 10^{11}$	147
cellulose=$0.209CO_2+0.396CO+0.109H_2+0.249H_2O+0.037vol$	$1.379 \cdot 10^{14}$	193
Rubber pyrolysis		
rubber=$0.0009C_2H_4+0.194CH_4+0.0025C_3H_6+0.0018C_4H_6+0.0008C_2H_2+0.8H_2$	$5.5 \cdot 10^{18}$	181
Polyethylene pyrolysis		
plastic=$0.07C_2H_4+0.05CH_4+0.03C_3H_6+0.02C_2H_6+0.005C_3H_8+0.825H_2$	$15 \cdot 10^{3}$	40
Gasification		
$C+H_2O=CO+H_2$	$2.07 \cdot 10^{7}$	220
$C+CO_2=2CO$	$1.32 \cdot 10^{7}$	259
$C+2H_2=CH_4$	$5 \cdot 10^{6}$	30
$C+2H_2O=CO_2+2H_2$	$2.1 \cdot 10^{6}$	158
$CO_2+H_2= CO+H_2O$	$5 \cdot 10^{6}$	30

Reaction	Pre-exponential factor, s^{-1}	Activation energy, kJ/(mol·K)
Combustion		
$C+O_2=CO_2$	$2 \cdot 10^{12}$	60.6
$C+½O_2=CO$	$2 \cdot 10^{12}$	60.6
$H_2+½O_2=H_2O$	$2.1 \cdot 10^{14}$	129.8
$2CO+O_2=2CO_2$	$1.4 \cdot 10^{13}$	96.8
$CO+H_2O=H_2+CO_2$	$5 \cdot 10^{6}$	30
$CO+3H_2=CH_4+H_2O$	$5 \cdot 10^{6}$	30
$C+H_2O=0.5CO_2+0.5CH_4$	$5.6 \cdot 10^{12}$	36.2
$CH_4+2O_2= CO_2+2H_2O$	$5.6 \cdot 10^{12}$	103.8
$C_2H_4+O_2=2CO+2H_2$	$1 \cdot 10^{12}$	173
$2C_3H_6+9O_2=6CO_2+6H_2O$	$1.51 \cdot 10^{15}$	85.6
$2C_2H_6+7O_2=4CO_2+6H_2O$	$1.1 \cdot 10^{12}$	125.52
$2C_3H_8+10O_2=6CO_2+8H_2O$	$8.6 \cdot 10^{11}$	125.52
$C_4H_6+3O_2=4CO+2H_2O+H_2$	$8.8 \cdot 10^{11}$	126.37
$C_4H_8+½O_2=C_2H_4+H_2O$	$6 \cdot 10^{12}$	502
$C_4H_8+6O_2=4CO_2+4H_2O$	$3 \cdot 10^{7}$	10.4
$C_4H_6+11/2O_2=4CO_2+3H_2O$	$3 \cdot 10^{7}$	10.4
$C_2H_2+O_2=2CO+H_2$	$6 \cdot 10^{13}$	50

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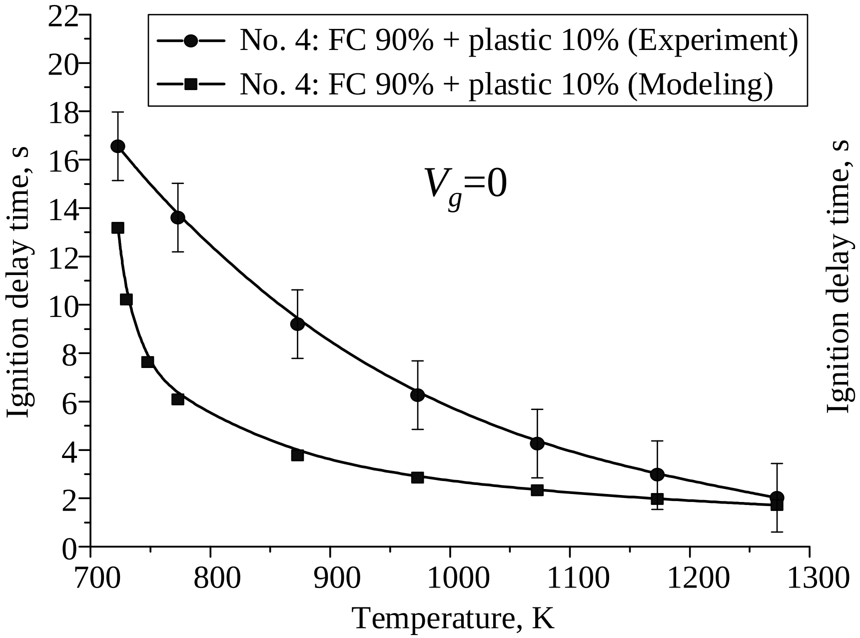
V. Simulation results

The ignition delay times of a droplet (d_p=1 mm) of each fuel composition in a fixed air (V_g=0) when its temperature was varied in the range of 450–1000 °C (723–1273 K) and in the air flow (V_g=3 m/s) heated to temperatures of 450–700 °C (723–973 K) were calculated (in ANSYS Fluent) .



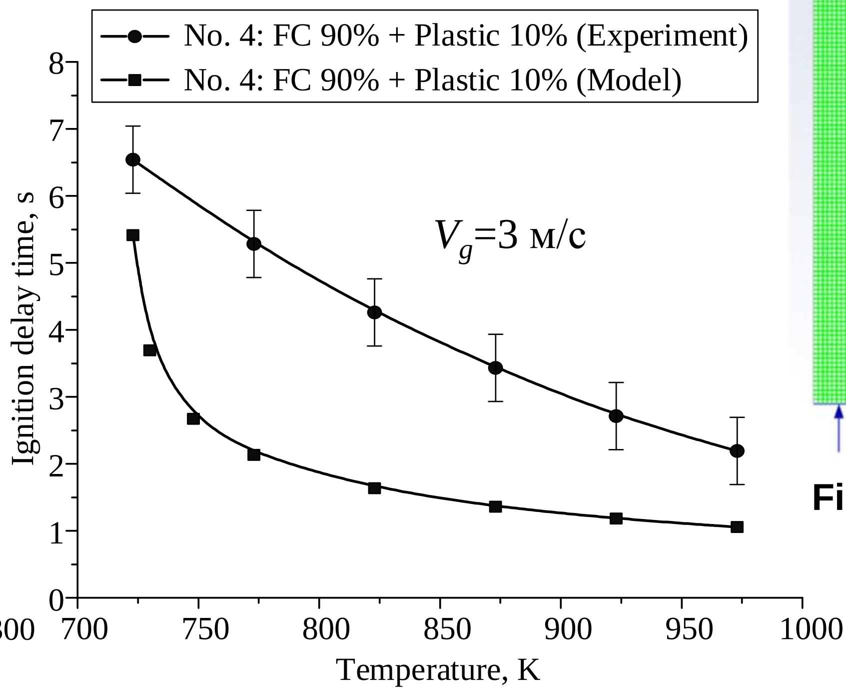


Fig. 11. Comparison of the dependences of the ignition delay times of composition No. 4 (FC 90% + plastic 10%) calculated during the simulation on the air temperature with the experimental data

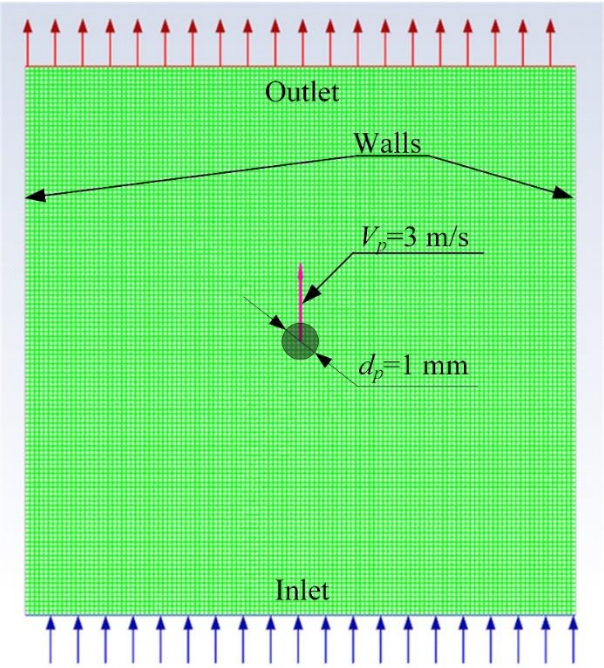


Fig. 12. Driving solutions heat and mass transfer problems in the system of the droplet – gas environment

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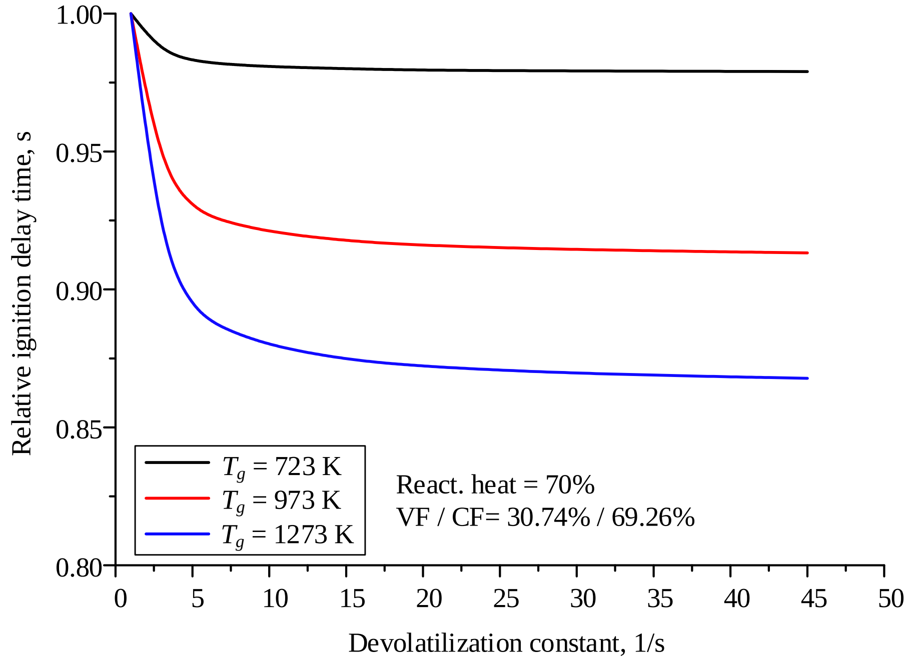
V. Simulation results

Model sensitivity

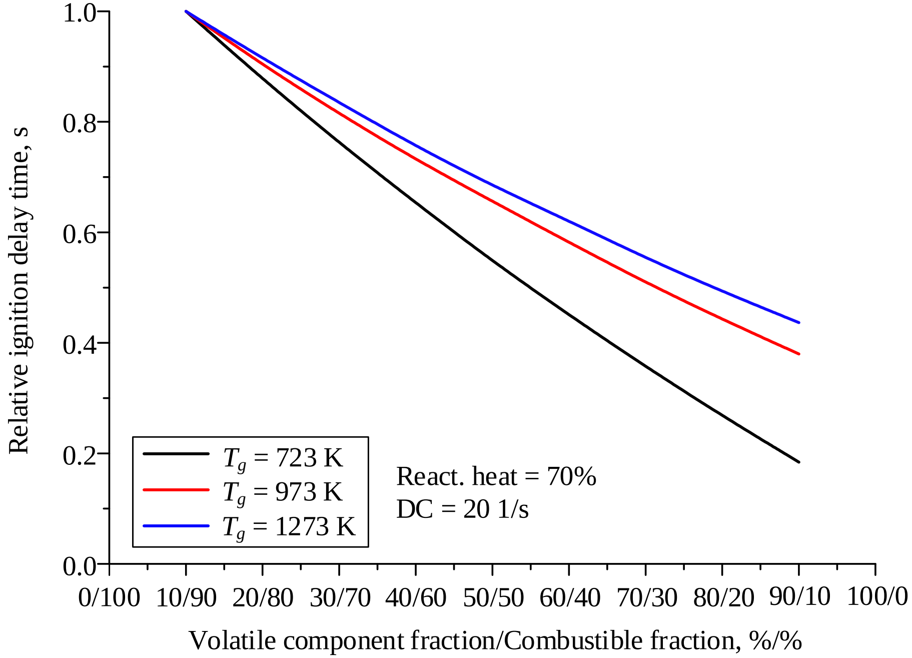
Fig. 13. Dependences of ignition delay times of composite No. 4 (FC 90% + plastic 10%) at various temperatures under radiant heating conditions from:

a) the devolatilization constant of combusting particle;
b) the reaction heat fraction absorbed by solid of combusting particle;
c) the ratio of volatile and combustible fractions in the composition.

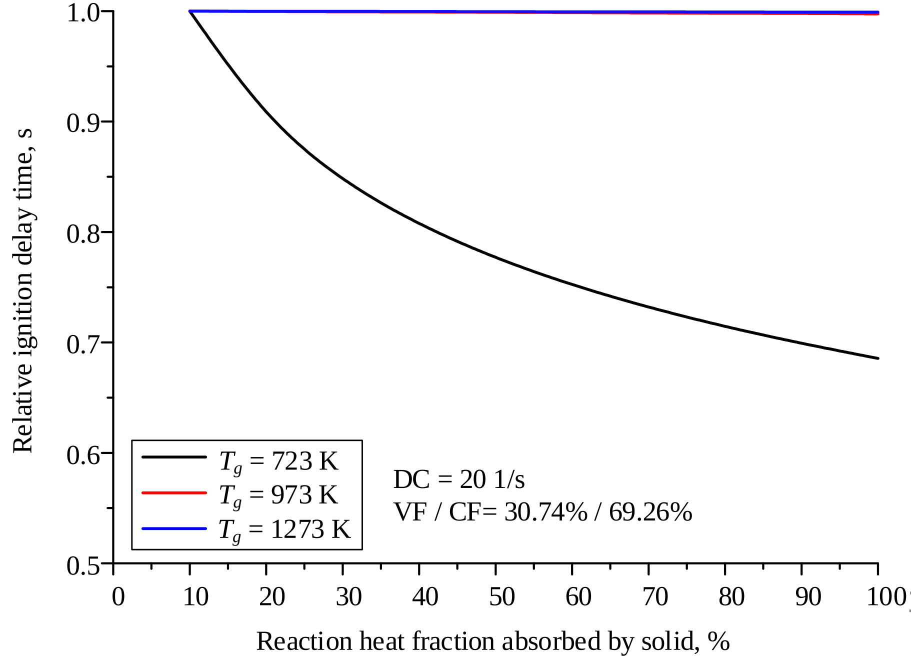
a)



c)



b)



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Conclusions

1. The regularities and necessary conditions for drops ignition of composite fuels based on filter cake with the addition of the typical MSW (wood, food waste, plastic, cardboard) were established experimentally under heating conditions corresponding to the conditions of fuel burning in boiler furnaces. It has been found that 450 °C is the minimum air temperature required for the stable ignition of composite liquid fuel droplet. Depending on the mechanism of heat exchange with the environment at an identical air temperature, the ignition delay times differ by 2–3 times.

2. The mechanism of ignition and combustion of single drops of composite liquid fuel based on FC with the addition of fine particles of typical MSW (wood, rubber, plastic, cardboard) as combustible components has been established. The main stages have been highlighted for mutually dependent physical and chemical processes: inert heating of a droplet; moisture evaporation from the subsurface layer; thermal decomposition of flammable components (coal and MSW); combustible gases mixing with the oxidizer; gaseous mixture ignition and burnout; heating of the solid residue; the heterogeneous ignition and combustion of the solid residue.

3. Based on the experimental studies, an original mathematical model of ignition and combustion of a drop of composite liquid fuel was developed in the commercial software Ansys Fluent. The model describes in detail the physicochemical processes occurring during heating under conditions of radiant and convective heating, and provides reliable prediction of the characteristics of ignition and combustion.

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Thank you for your attention!

Tomsk Polytechnic University
30, Lenin Avenue, Tomsk, Russia, 634050
Kristina Paushkina e-mail: kkp1@tpu.ru
URL: http://hmtslab.tpu.ru/