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Explosion hazards of triple hydrocarbon-hydrogen – air mixtures

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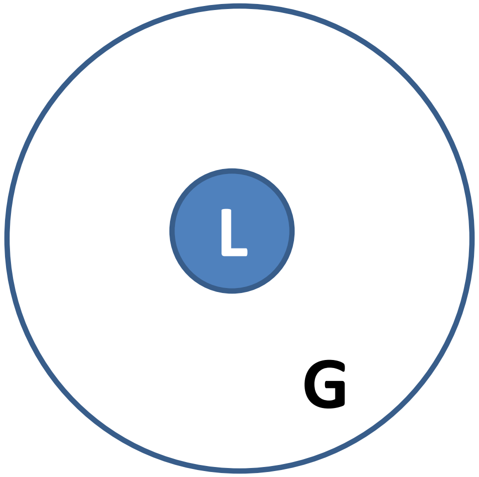
Background

- **Cheng R.K., Oppenheim A.K.** Autoignition in methane-hydrogen mixtures // Combustion and flame. – 1984. – 58. – P. 125.
- **S. Thiessen, E. Khalil,G. Karim**, The autoignition in air of some binary fuel mixtures containing hydrogen// International journal of hydrogen energy.– 2010.– V.35.–P.10013.
- **Karim G.A.** Combustion in gas fueled compression: ignition engines of the dual fuel type // Journal of gas turbine and power. – 2003. – V. 215. – P. 827.
- **Lyn McWilliam**, Combined hydrogen diesel combustion: an experimental investigation into the effects of hydrogen addition on the exhaust gas emissions, particulate matter size distribution and chemical composition / A thesis submitted for the degree of Doctor of Philosophy. 2008. – P. 1.

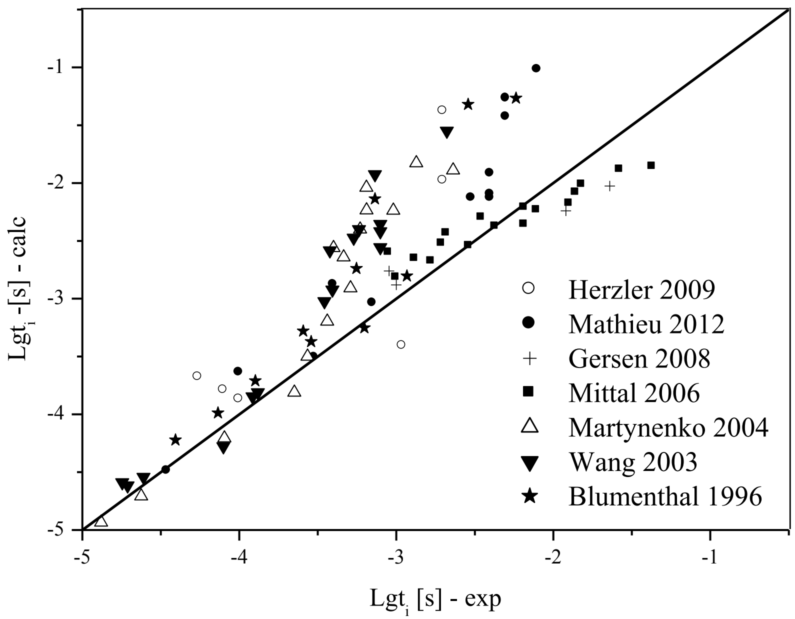
- **No found** investigetions accorded to influence of hydrogen on selfignition and combustion of heterogeneous hyrdocarbon droplets in air.

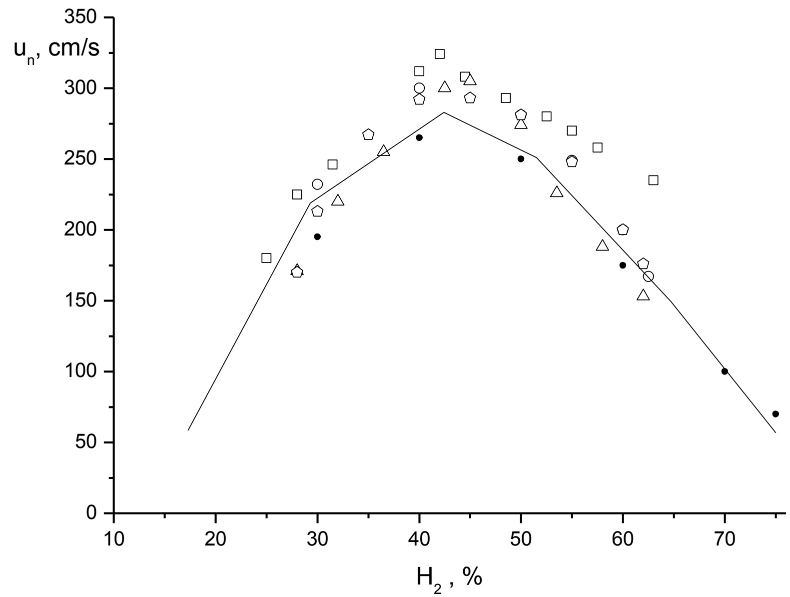
Governing equations

- System of equations for gas and liquid phases:
  - Continuous equation
  - Energy conversation equations
- Applying additional conditions
  - Multi-components diffusion
  - Evaporation and heat expansion



Checking hydrogen-air mixtures



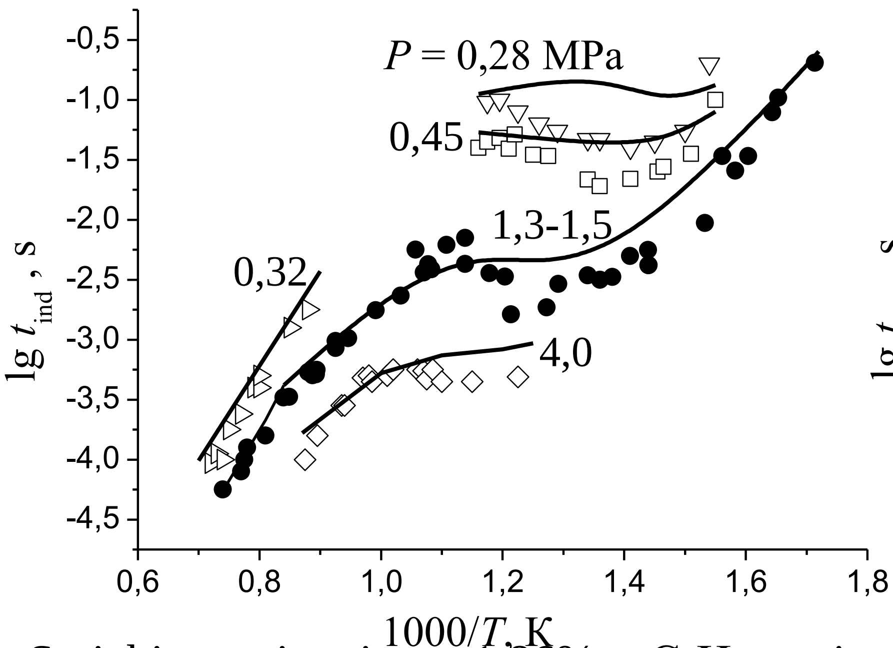


Selfignition

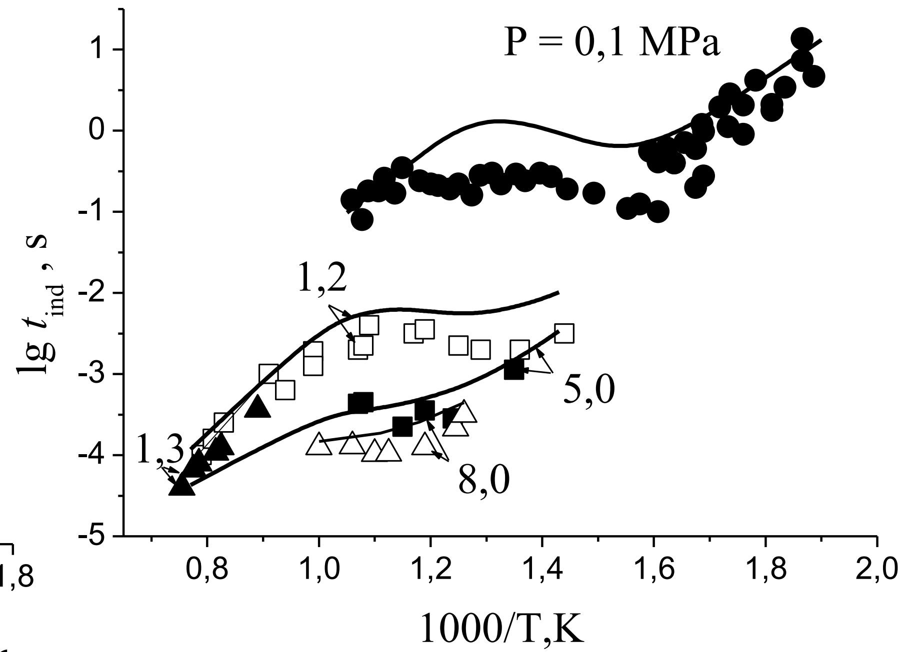
Flame velocity

Kinetic scheme

- 108 species, 1083 reversible reactions

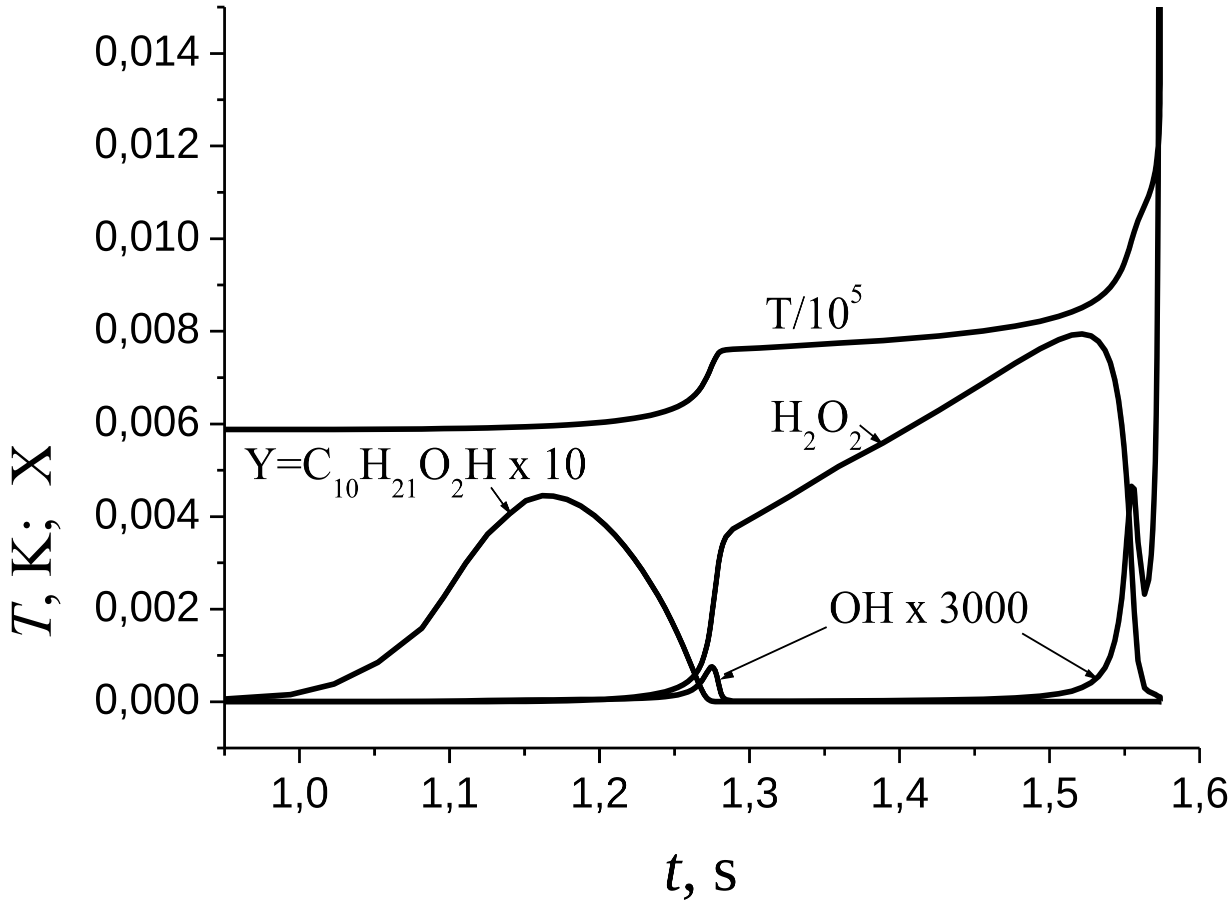


Stoichiometric mixture1,86%$_{vol}$ C_7H_{16} – air at pressures P_0 = 0,28–4,0 MPa: curves – calculations, points – experiments (*Rogener H.* 1949, *Taylor C.F.* 1950, *Ciezki H.* 1987, *Poppe Ch.* 1993,*Ciezki H.* 1993, *Minetti R.* 1995, *Gauthier B.M.* 2004)



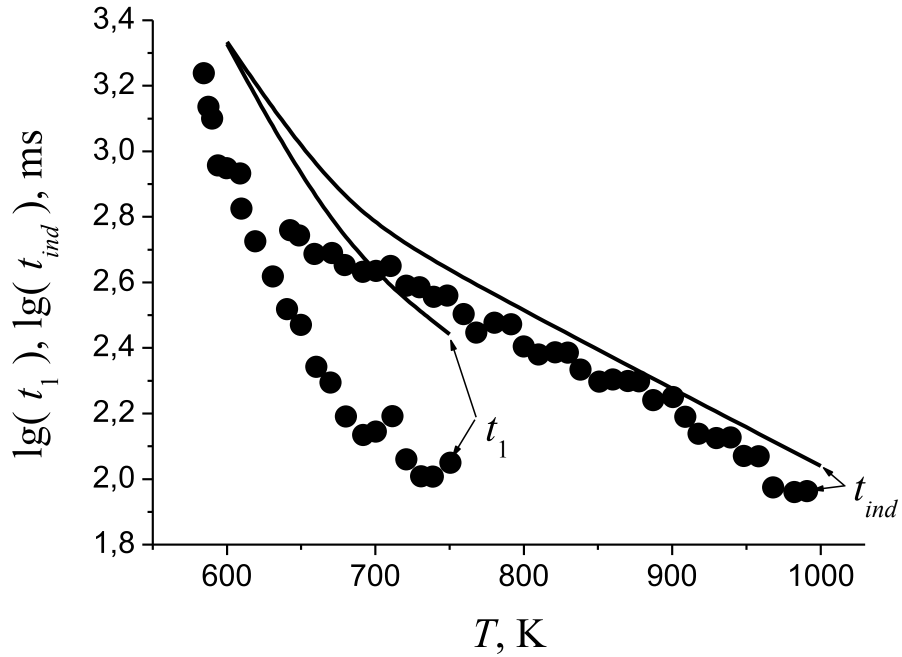
Stoichiometric n-decane-air mixture. Curves – calculations, points – experiments (*Pfahl U.* 1996, *Zhukov V.P.* 2008, *Troshin K.Ya.* 2008)

Kinetic scheme



Stoichiometric n-decane-air mixture. Initial conditions: T_0 = 588 K, P_0 = 0,1 MPa.

Self-ignition single droplet



Single n-heptane droplet in air: initial droplet diameter d_0 = 0,70 mm, initial pressure P_0 =0,1 MPa. Points – experiment (*Moriue O.* 2000), lines – calculations.

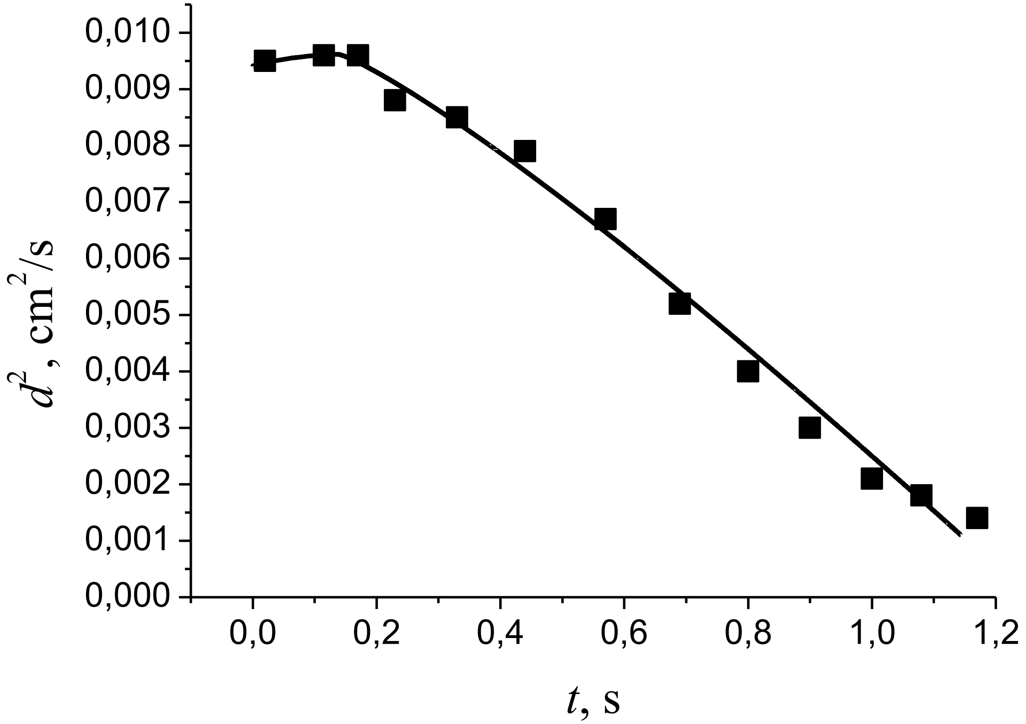
Selignition single n-heptane droplets at pressure P = 0,1 MPa. Experiments*Takei M.* 1993, *Niioka T.* 1994.

$d_{0,}$ μm	T_0, K	t_{ind}, s	
		Exp.	Calc.
700	1000	0.30	0.18
1000	960	0.58	0.27

Droplet combustion

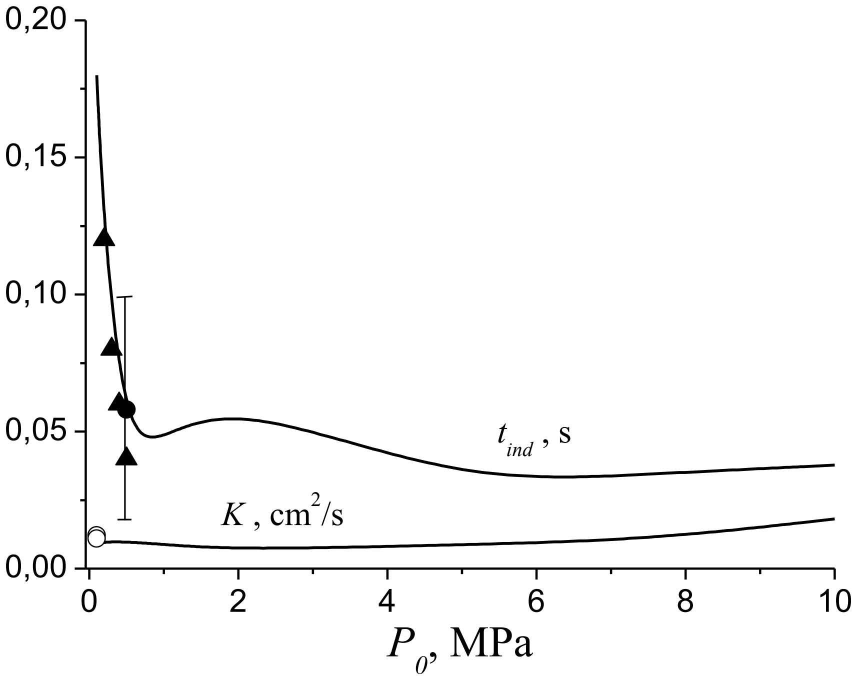
$$d^2 = d_0^2 - K \cdot t$$

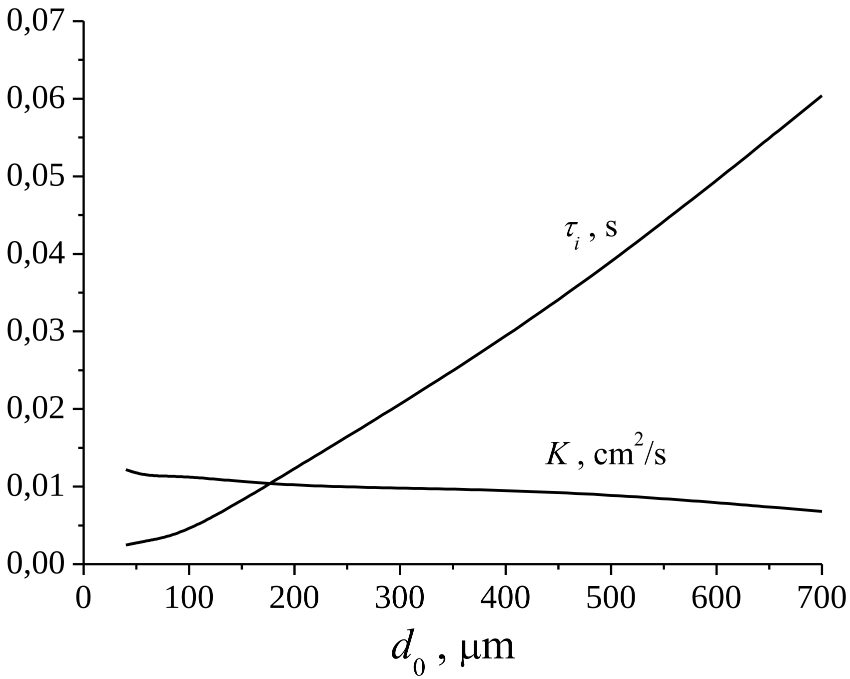
K – combustion velocity constant



Initial conditions: d_0 = 0.91 mm, T_0 = 1093*K*, P_0 = 0,1 MPa. Points - experiment (*Moriue O*. 2000), line – calculation.

Droplet combustion

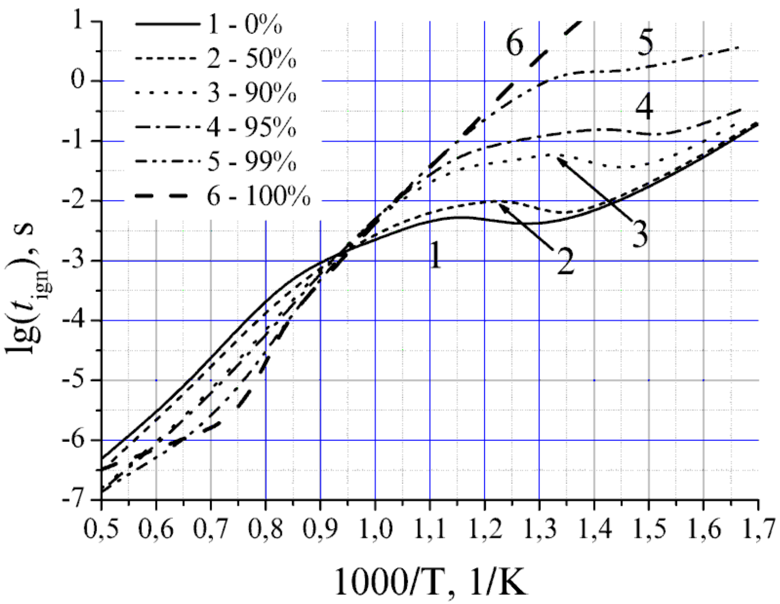




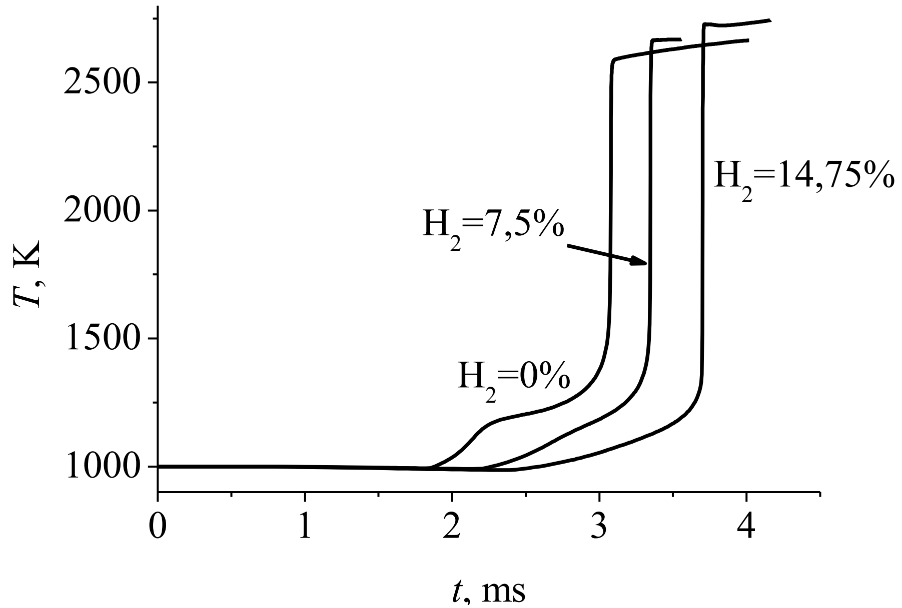
n-heptane droplet system in air: d_0 = 700 mcm, T_{g0} =1000 К и Φ = 1 Curves – calculation, points – experiments (*Tanabe M.* 1995, *Tanabe M*. 1996, *Kobayasi K*. 1955)

n-heptane droplet system in air. Initial conditions: T_{g0} = 1000 K, P_0 = 2,0 MPa and Φ = 1

Influence of H_2 on selfignition

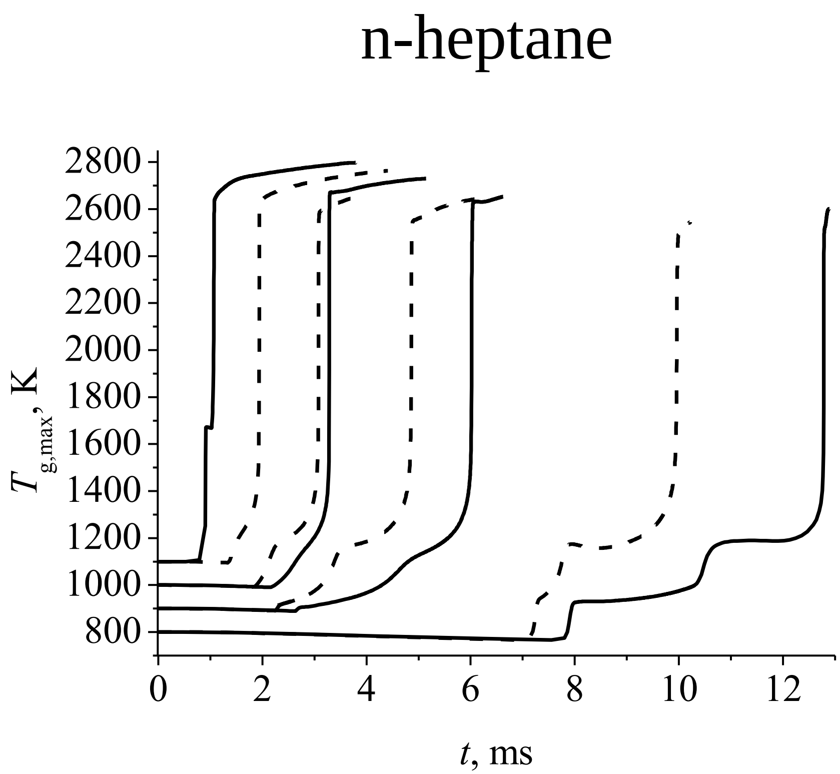


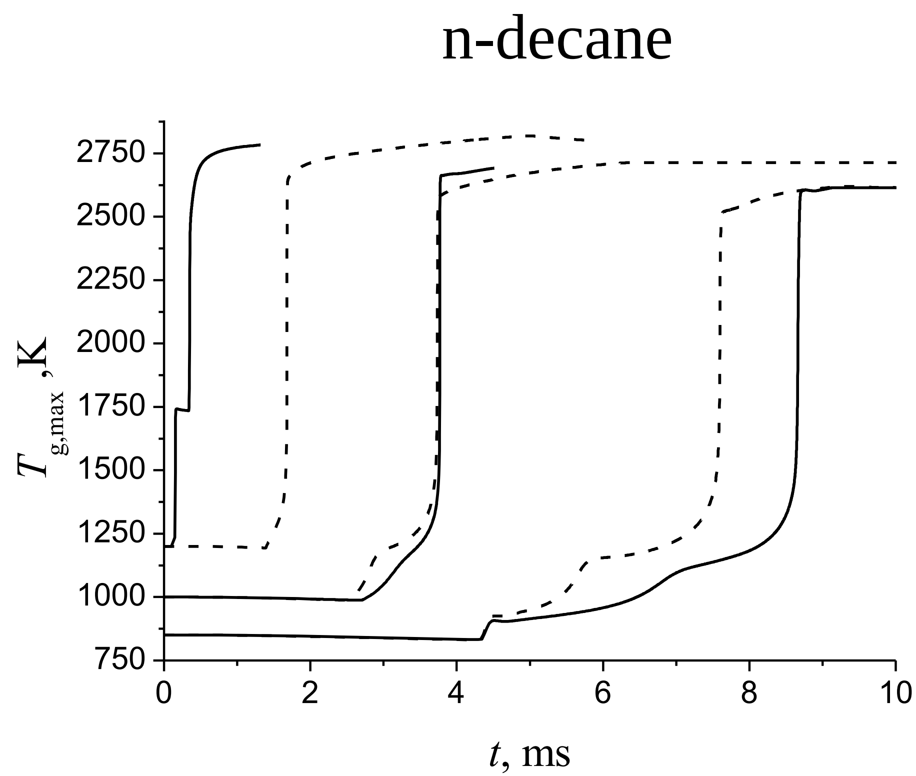
Homogeneous stoichiometric n-heptane – air mixture. Initial pressure P_0=1,5 MPa



Air droplet n-heptane droplets mixture: d_0=60 mcm, T_0 = 1000 K, P_0= 2,0 MPa, Φ=1, H_2 = 0,0%, 7,5% and 14,75%

Influence of H_2 on selfignition



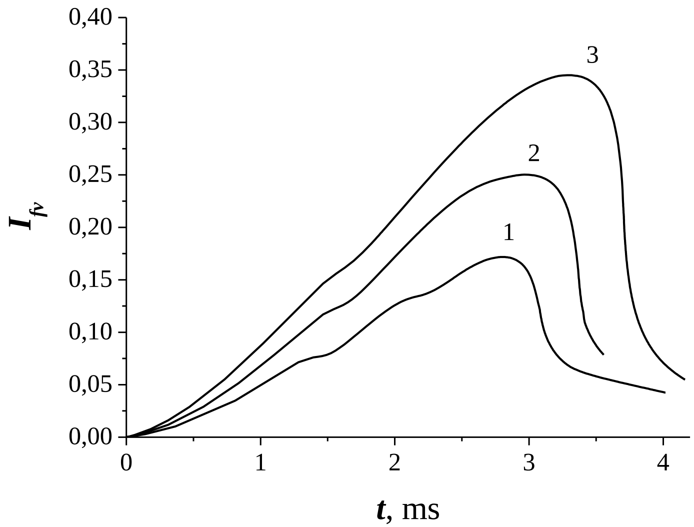


d_0 = 60 mcm, Φ = 1, P_0 = 2 MPa.

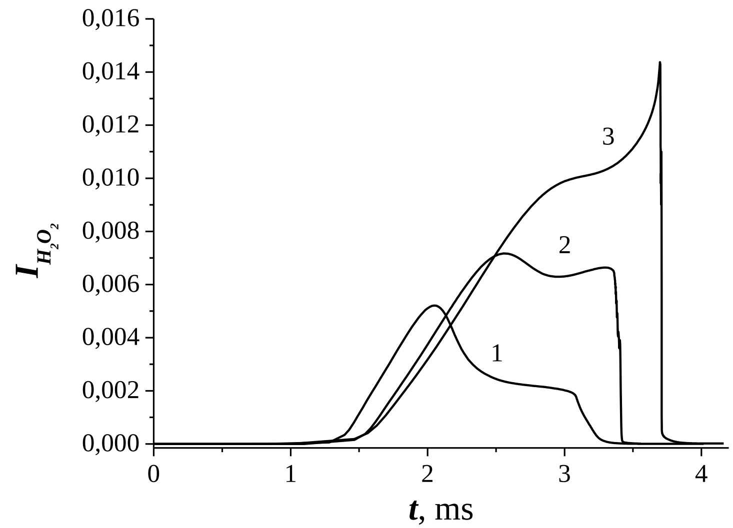
Solid curves – mixture with 7,5% H_2 addition,

dot lines – with 0% H_2

Influence of H_2 on selfignition



(a)

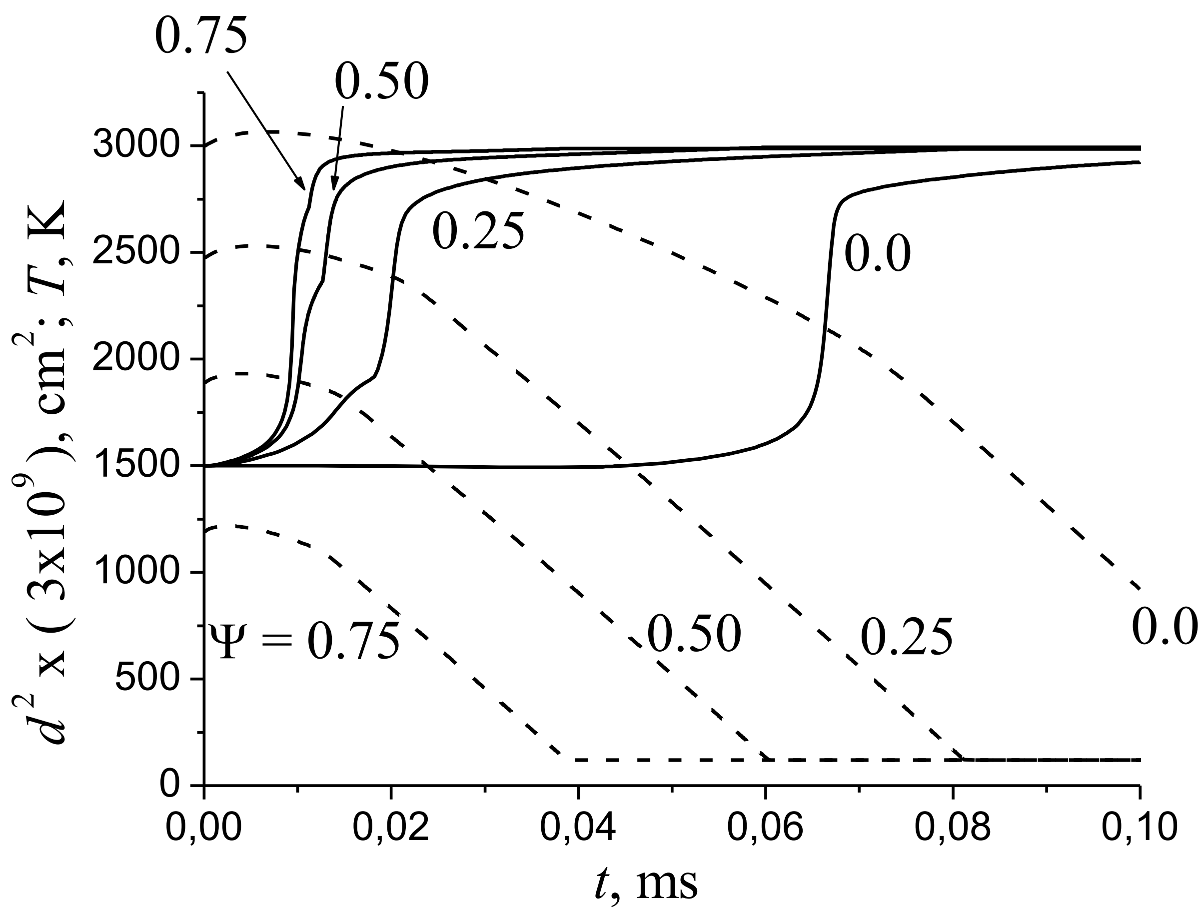


(b)

Predicted time histories of the normalized mass contents of n-heptane vapor (a) and hydrogen peroxide (b) around a drop in uniform stoichiometric n-heptane drop suspension at different initial volumetric hydrogen content: 1 – 0%, 2 – 7.5%, and 3 – 14.5%; drop diameter 60 , P_0 = 2 MPa.

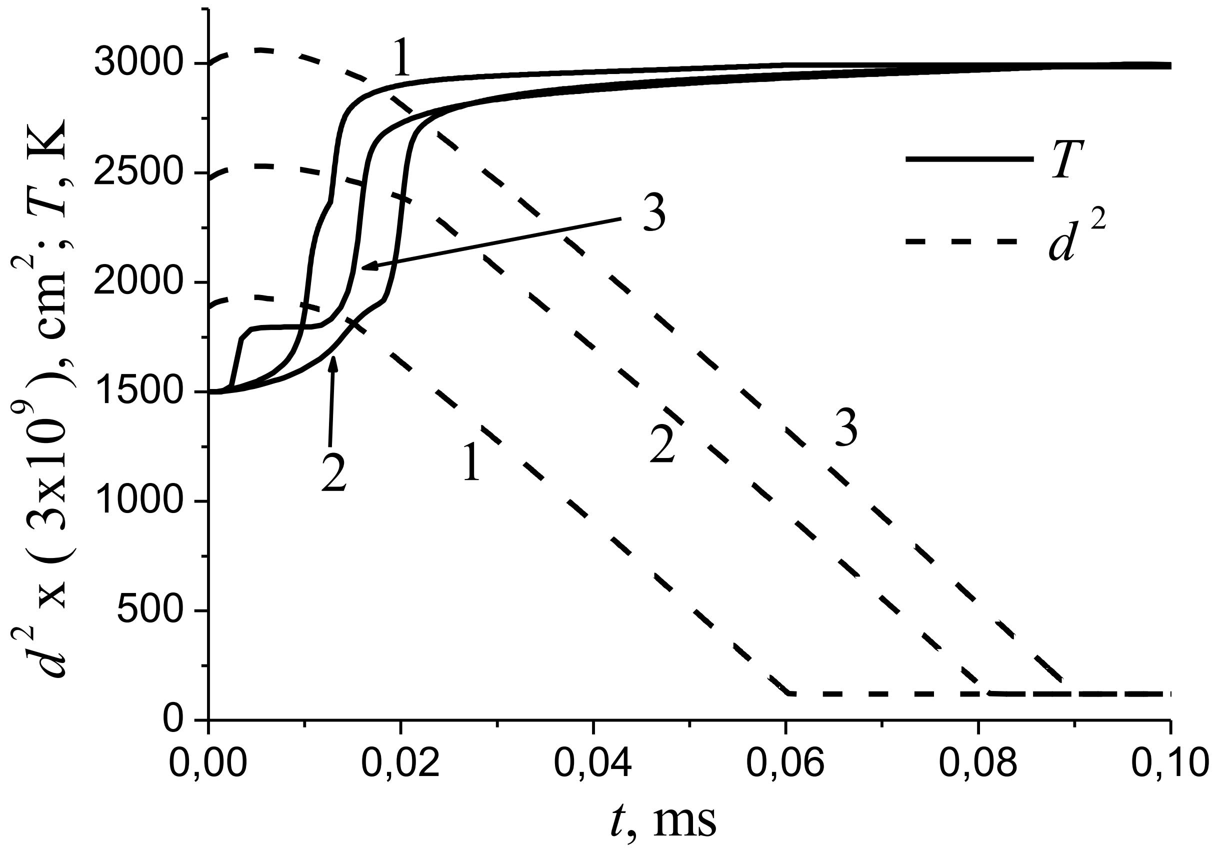
Detonation ability

- Characteristic time t^* = 100 mcs
- Initial conditions P_0 = 3,0 MPa, T_0 = 1500 K, d_0 = 10 mcm



Detonation ability

- 1 – H_2 =0,0%$_{vol}$, ψ = 0,50;
- 2 – H_2 =0,0% $_{vol}$, ψ = 0,25;
- 3 – H_2 =4,3% $_{vol}$, ψ = 0,0



Conclusions

- We study self-ignition of gas and droplet hydrocarbon–hydrogen–air mixtures.
- Detailed reaction mechanism of n-decane oxidation is used.
- At temperature less than 1050 K hydrogen inhibits self-ignition of hydrocarbons.
- At temperature higher than 1050 K hydrogen promotes self-ignition of hydrocarbons.
- These findings are important for hydrogen safety issues and applications.
- Quantity estimations of detonation ability are defined in heterogeneous mixture with different pre-evaporated fuel levels and hydrogen additions.