DETONATION HAZARD of COMBUSTIBLE MIXTURES.
OZONE, HYDROGEN PEROXIDE

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Abstract. The basic parameters of multifront detonation waves are determined with the help of computer code «SAFETY» for hydrogen peroxide and ozone at its mix with oxygen or air and at variations of initial pressure P_0 and temperature T_0.

Keywords: initiation, critical energy, combustion, multifront detonation, hazard, cell size, critical diameter

Introduction.

The basic parameters of multifront detonation waves (DW) such as velocity, pressure, temperature, cell size, critical initiation energy for plane, cylindrical and spherical case, critical diameters for diffraction and self-sustaining propagation in free and limiting gaseous charge, etc... are calculated with the help of computer code «SAFETY» (Chem. Phys. Reports, 1997, Vol. 16(9), p.1659-1666) for hydrogen peroxide and ozone at its mix with oxygen or air and at variations of initial pressure P_0 and temperature T_0. The basic parameters are velocities, pressure, temperature, cell size, critical initiation energy, etc... The chemical substances were assumed as ideal gases and with chemical equilibrium in final state, and in gaseous or vapor form in initial state.

Results.

*OZONE***.** Pure ozone as monofuel is characterized by higher detonation hazard in comparison with ozone-oxygen or ozone-air mixtures. Example: at $P_0 = 10^5$ Pa and $T_0 = 298$ K the detonation velocity D_0 equals 1915 m/s, product temperature T - 3469 K, pressure ratio p - 33.1, chemical energy-release on unit mass Q = 587 cal/g, dimensionless energy-release $q = Q/c_0^2 = 37.9$ (c_0 - initial sound speed) , cell size *a* = 0.34 mm, critical initiation energies are equal $E_1 = 0.52$ J/cm^2, $E_2 = 0.082$ J/cm and $E_3 = 0.22$ J for plane, cylindrical and spherical cases.

At decreasing of initial pressure or ozone concentration the DW velocity, temperature, pressure ratio, energy-release... are decreased too, while cell size, critical initiation energies, critical diameter... are increased. Ozone-oxygen and ozone-air mixtures have approximately similar dependence of the main DW parameters on fuel concentration.

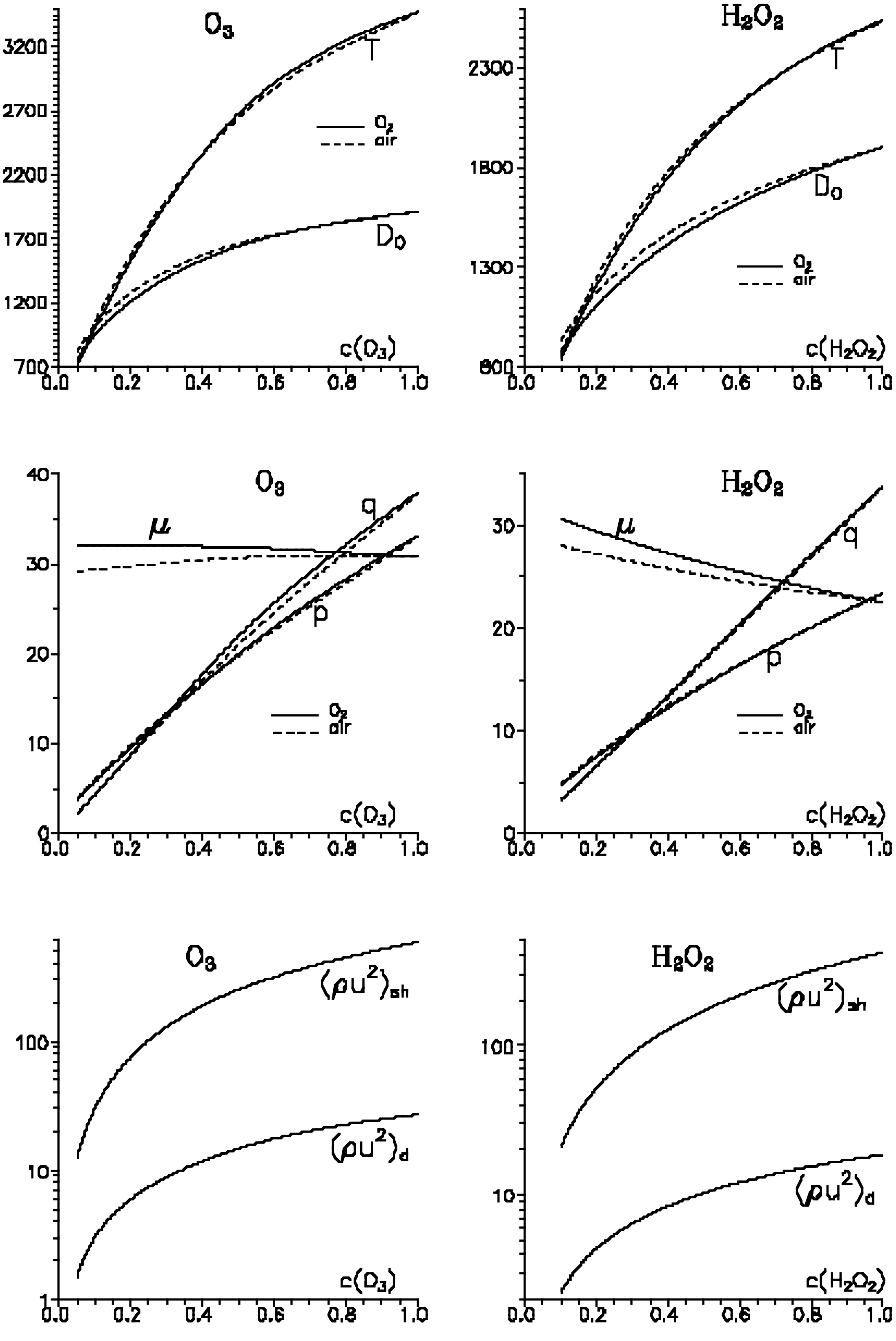
*HYDROGEN PEROXIDE***.** Pure hydrogen peroxide (HP) is characterized by lower detonation hazard but analogous behavior as ozone: higher detonation hazard in comparison with mixtures HP-oxygen or HP-air mixtures.

Example 1: for gaseous HP at $P_0 = 10^5$ Pa and $T_0 = 298$ K the detonation velocity equals 1904 m/s, product temperature - 2539 K, pressure ratio - 23.4, chemical energy-release on unit mass Q = 720 cal/g, dimensionless energy-release q = 33.8, cell size *a* = 6.7 mm, critical initiation energies are equal $E_1 = 19.4$ J/cm^2, $E_2 = 64$ J/cm and $E_3 = 8500$ J for plane, cylindrical and spherical cases.

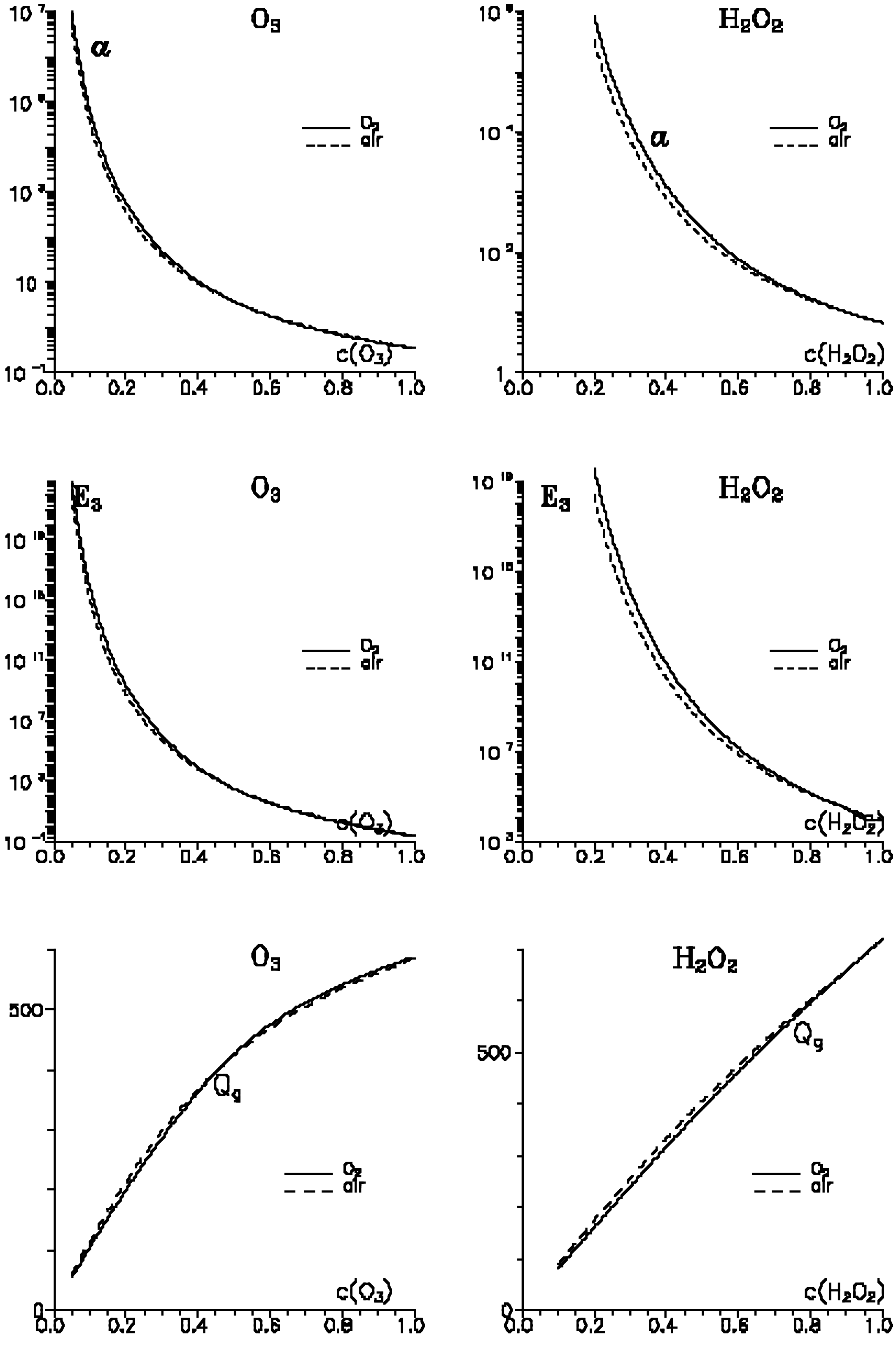
Example 2: at $P_0 = 10^5$ Pa and $T_0 = 423$ K (temperature of liquid-vapor phase transition) the detonation velocity equals 1910 m/s, product temperature - 2591 K, pressure product ratio - 16.8, chemical energy-release on unit mass Q = 705 cal/g, dimensionless energy-release $q = Q/c_0^2 = 23.8$, cell size *a* = 4.1 mm, critical initiation energies are equal $E_1 = 9.9$ J/cm^2, $E_2 = 18$ J/cm and $E_3 = 1500$ J for plane, cylindrical and spherical cases.

At decreasing of initial pressure or hydrogen peroxide concentration the DW velocity, temperature, pressure ratio, energy-release... are decreased too, while cell size, critical initiation energies, critical diameter... are increased. As for ozone HP-oxygen and HP-air mixtures have approximately similar dependence of the main DW parameters on fuel concentration.

If HP assumes in vapor form in initial mixture then the calculated results are the next: the detonation velocity equals 1533 m/s, product temperature - 1685 K, pressure ratio - 14.9, chemical energy-release on unit mass Q = 765 cal/g, dimensionless energy-release q = 36, cell size *a* = 1620 mm, critical initiation energies are equal $E_1 = 2650$ J/cm^2, $E_2 = 2\ 10^6$ J/cm and $E_3 = 5.6\ 10^{10}$ J for plane, cylindrical and spherical symmetry. In this


O_3
3200
2700
2200
1700
1200
700
T
D_0
O_2
air
$c(O_3)$
0.0
0.2
0.4
0.6
0.8
1.0
H_2O_2
2300
1800
1300
800
T
D_0
O_2
air
$c(H_2O_2)$
0.0
0.2
0.4
0.6
0.8
1.0
40
30
20
10
0
O_3
μ
q
p
O_2
air
$c(O_3)$
0.0
0.2
0.4
0.6
0.8
1.0
30
20
10
0
H_2O_2
μ
q
p
O_2
air
$c(H_2O_2)$
0.0
0.2
0.4
0.6
0.8
1.0
100
10
1
O_3
$\langle\rho u^2\rangle_{sh}$
$\langle\rho u^2\rangle_d$
$c(O_3)$
0.0
0.2
0.4
0.6
0.8
1.0
100
10
H_2O_2
$\langle\rho u^2\rangle_{sh}$
$\langle\rho u^2\rangle_d$
$c(H_2O_2)$
0.0
0.2
0.4
0.6
0.8
1.0

Figs. 1-3.


O3
α
O2
air
c(O3)
10^7
10^5
10^3
10
10^-1
0.0
0.2
0.4
0.6
0.8
1.0
H2O2
α
O2
air
c(H2O2)
10^6
10^4
10^2
1
E3
10^19
10^15
10^11
10^7
10^3
Q_g
500
0

Figs. 4-6.

case the part of chemical energy-release energy expends on phase change of liquid HP to gaseous. The energy values demonstrate that liquid HP may be classified as hard-detonation substance, but gaseous HP is more dangerous (and may be compared with many fuel-air mixtures).

Some calculated results are demonstrated on Figs. 1-6: detonation velocity D_0 m/s and product temperature T K; pressure ratio $p=P/P_0$, dimensionless energy-release q and product mole mass μ g/mole; dynamic pressure ρu^2 atm of DW products (detonation product - index d) and chemical spike (behind shock wave - index sh); cell size *a* mm, critical energy for spherical initiation E_3 J; energy release Q cal/g; *c*(fuel) - molar concentration of fuel in fuel-oxygen (solid lines) or fuel-air (dashed lines) mixtures.

Dependence of critical diameters for diffraction, self-sustaining propagation in free and limiting gaseous charge are similar to cell size line qualitatively. Analogous situation observes among E_3 and E_1 or E_2 - lines.

Conclusion.

The calculated results correspond adequately to available (not numerous) experimental data (for example, Getzinger R.W., Bowen J.R., Oppenheim A.K., Boudart M. Steady detonations in gaseous ozone//10-th Symp. (Int.) on Comb., The Combustion Institute, 1965, pp.779-784).