

**Lutradyn**

# **14<sup>th</sup> Workshop on Pyrotechnic Combustion Mechanisms**

**Combustion & Detonation of  
Energetic Materials  
Round Robin Test Program**

## **Participants**

**EKVI-Code**, B. Noläng, University of Upsalla, Sweden  
**EXPLO-5 Code**, M. Sućeska, University of Zagreb, Croatia  
**FACT-Sage** , K. Hack, GTT Technologies, Germany  
**ICT Code**, S. Kelzenberg, Fraunhofer ICT, Pfinztal, Germany  
**IVTAN THERMO Code**, G. Belov, Russia  
**NASA-CEA**, E.-C. Koch, Lutradyn, Germany  
**REAL**, G. Belov, Russia  
**THOR Code**, A. Campos, University of Coimbra, Portugal

Dear Colleagues,

Thank you again for your kind willingness to present at the

**14<sup>th</sup> Workshop on Pyrotechnic Combustion Mechanisms**

on June 25, 2018.

The Workshop will start with a get together the day before (Sunday June 24) around 18:00 with a “warm up” for the presenters to meet and talk.

The workshop starts on Monday 25, at 8:30 with sessions presenting the various codes by their developers or advanced users.

After a (lunch) break the Workshop looks into the results of the Round Robin which is followed by a final discussion.

For the Round Robin we kindly ask you to conduct the following calculations and submit the results in the required form (ascii text files) no later than June 17, 2018, to:

[e-c.koch@lutradyn.com](mailto:e-c.koch@lutradyn.com) and [sebastian.knapp@ict.fraunhofer.de](mailto:sebastian.knapp@ict.fraunhofer.de)

We look forward to seeing you in Kaiserslautern!

Best regards

Ernst-Christian Koch	–	Sebastian Knapp
Lutradyn		Fraunhofer ICT
Kaiserslautern/Germany		Pfinztal/Germany
Workshop Co-Chairs		

## Thermodynamic and compositional data

Name	Formula	Density (g cm <sup>-3</sup> )	$\Delta_f H$ (kJ mol <sup>-1</sup> )
Aluminum	Al	2.699	0
Boron carbide	B <sub>4</sub> C	2.52	-62.68
Copper oxide	CuO	6.3	-156.1
Hexafluoropropene-	(C <sub>3</sub> F <sub>6</sub> ) <sub>n</sub> (C <sub>2</sub> H <sub>2</sub> F <sub>2</sub> ) <sub>m</sub>	1.775	-2784
Vinylidene fluoride-copolymer, <i>Viton</i> <sup>®</sup> A	n/m = 1/3.5		
Octogen (HMX)	C <sub>4</sub> H <sub>8</sub> N <sub>8</sub> O <sub>8</sub>	1.906	84.01
Phosphorus, red (P <sub>R</sub> )	P	2.2	0
Polytetrafluorethylene (PTFE)	(C <sub>2</sub> F <sub>4</sub> ) <sub>n</sub>	2.25	-809
Potassium perchlorate	KClO <sub>4</sub>	2.52	-432.79
Potassium nitrate	KNO <sub>3</sub>	2.109	-494.63
Silicon	Si	2.329	0
Silver iodate	AgIO <sub>3</sub>	5.890	-164. 24

## Test case 1, TC-1

High Explosive, PBXN-5

95 wt-% Octogen

05 wt-% Viton<sup>®</sup>A

### Detonation at TMD<sup>(1)</sup>:

- $P_{CJ}^{(2)}$  [GPa]
- $V_D^{(3)}$  [ $m\ s^{-1}$ ]
- $T_{CJ}^{(4)}$  [K]
- $V/V_0^{(5)}$  [ $kJ\ cm^{-3}$ ]
- Gas volume [ $dm^3\ kg^{-1}$ ]
- Composition of detonation products at 298 K (25 °C) (no reaction with ambient air) [wt-%]

### Deflagration at $P = 0.1\ MPa, 1\ MPa$

- Composition of deflagration products at 298 K (25 °C) (no reaction with ambient air) [wt-%]
- Adiabatic deflagration temperature,  $T_{ad}$  (no reaction with ambient air) [K]

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<sup>1</sup> Theoretical Maximum Density

<sup>2</sup> Detonation Velocity

<sup>3</sup> Detonation-Pressure

<sup>4</sup> Detonation Temperature

<sup>5</sup> Cylinder Expansion Energy

## Test case 2, TC-2

Aluminized High Explosive, PBX-Alf

60 wt-% Octogen  
10 wt-% Aluminum  
20 wt-% PTFE  
10 wt-% Viton<sup>®</sup>A

### Detonation at TMD:

- $P_{CJ}$ [GPa]
- $V_D$ [m s<sup>-1</sup>]
- $T_{CJ}$ [K]
- $V/V_0$  [kJ cm<sup>-3</sup>]
- Gasvolume [dm<sup>3</sup> kg<sup>-1</sup>]
- Composition of detonation products at 298 K (25 °C) (no reaction with ambient air) [wt-%]

### Deflagration at P = 0.1 MPa, 1 MPa

- Composition of deflagration products at 298 K (25 °C) (no reaction with ambient air) [wt-%]
- Adiabatic deflagration temperature,  $T_{ad}$  (no reaction with ambient air) [K]

## Test case 3, TC-3

High Blast Explosive, PBX-PF

68 wt-% Octogen

20 wt-% P<sub>R</sub>

12 wt-% Viton<sup>®</sup>A

### Detonation at TMD:

- P<sub>CJ</sub> [GPa]
- V<sub>D</sub> [m s<sup>-1</sup>]
- T<sub>CJ</sub> [K]
- V/V<sub>0</sub> [kJ cm<sup>-3</sup>]
- Gasvolume [dm<sup>3</sup> kg<sup>-1</sup>]
- Composition of detonation products at 298 °C (no reaction with ambient air) [wt-%]

### Deflagration at P= 0.1 MPa, 1 MPa

- Composition of deflagration products at 298 K (25 °C) (no reaction with ambient air) [wt-%]
- Adiabatic deflagration temperature, T<sub>ad</sub> (no reaction with ambient air) [K]

## Test case 4, TC-4

ADW-Pyrolant

65 wt-% AgIO<sub>3</sub>

15 wt-% Viton<sup>®</sup>A

20 wt-% Si

### Deflagration at P = 0.1 MPa, 1 MPa

- Composition of the equilibrium composition at T<sub>ad</sub>. (no reaction with ambient air)
- Composition of deflagration products at 298 K (25 °C) (no reaction with ambient air) [wt-%]
- Adiabatic deflagration temperature, T<sub>ad</sub> (no reaction with ambient air) [K]

## Test case 5, TC-5

Screening Smoke

60 wt-% P<sub>R</sub>

05 wt-% Viton<sup>®</sup>A

15 wt-% Si

20 wt-% KNO<sub>3</sub>

Deflagration at P = 0.1 MPa, 1 MPa

- Composition of the equilibrium composition at T<sub>ad</sub>. (no reaction with ambient air)
- Composition of deflagration products at 298 K (25 °C) (no reaction with ambient air) [wt-%]
- Adiabatic deflagration temperature, T<sub>ad</sub> (no reaction with ambient air) [K]



## Test case 6, TC-6

Green Flare

57 wt-% KClO<sub>4</sub>

38 wt-% B<sub>4</sub>C

05 wt-% Viton<sup>®</sup>A

Deflagration at P = 0.01MPa, 0.1 MPa, 1 MPa

- Composition of the equilibrium composition at T<sub>ad</sub>. (no reaction with ambient air)
- Composition of deflagration products at 298 K (25 °C) (no reaction with ambient air) [wt-%]
- Adiabatic deflagration temperature, T<sub>ad</sub> (no reaction with ambient air) [K]

## Test case 7, TC-7

Thermite

Fuel: Al

Oxidant: CuO

Deflagration at  $P = 0.01\text{MPa}$ ,  $0.1\text{ MPa}$ ,  $1\text{ MPa}$

- Determine the range of stoichiometries for which a solution can be obtained
- Composition of the equilibrium composition at  $T_{\text{ad}}$ . (no reaction with ambient air) versus stoichiometry
- Composition of deflagration products at  $298\text{ K}$  ( $25\text{ }^\circ\text{C}$ ) (no reaction with ambient air) [wt-%] versus stoichiometry
- Adiabatic deflagration temperature,  $T_{\text{ad}}$  (no reaction with ambient air) [K] versus stoichiometry