Simulation of the heating up of the propellant charge body of a high precision machine gun during firing

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Presentation on the
8th International Heat Flow Calorimetry Symposium on Energetic Materials (HFC-S EM)
October 29 – 31, 2012
Wokefield Park, Mortimer
Reading, West Berkshire, UK
Motivations and Objectives

- Company Diehl introduced a new concept of the ammunition loading for a machine gun
- Separate loading of the projectile and the caseless propellant body
- Company Diehl asked ICT for support to protect the charge body against thermal threats

- Development of a thermal insulation for the charge body based on hard energetic PUR foam
- Estimation of time to ignition of the propellant body if placed in a hot burning chamber
Visualization of the two chambers and view on the caseless propellant body

New concept of a high precision machine gun, 12.7mm
Uses separated loading of projectile and caseless charge
Caseless charge is a consolidated body made from glued ball powder
Thermally insulated by PUR foam with 50 mass-% HMX by a coating of the body and by four spacers
The caseless propellant body

The propellant body is a cylindrical body made of glued double base ball powder (ÁkII stabilized) containing nitroglycerine.

For protection against direct flame ignition it has a coating.

Further four spacers have been applied in 90° distance on the outside.

The coating and the spacers are made of hard polyurethane foam filled with 50 mass-% HMX.

The foam and its application have been worked out at Fraunhofer ICT in the group of Dr. Böhnlein-Mauß.
Principle functioning of the machine gun - 1

Start position, just before loading cycle

Above the double projectile chamber, below the double charge chamber
Loading the projectile (above) and the charge (below) simultaneously in the two different chambers.

After the loading, the two double chambers counter rotate by 90° into the firing position, where loaded projectile chamber and loaded charge chamber are in line.
Firing position,
the breech of the charge chamber is closed.

After firing, the two double chambers counter rotate further by 90° back to the deloading and loading position.
Before loading again, the two chambers from the beforehand firing position are checked by the deloading device.

If the shot would have been unsuccessful, these chambers will be cleared before their next loading.
Simulation of the cook-off behaviour of PUR foam spacer, PUR foam coating and propellant body PB.
General heat balance equation and special cases

\[ c_p \cdot \rho \cdot \frac{dT(t, \bar{r})}{dt} = \rho \cdot \frac{dQ(T(t, \bar{r}))}{dt} + \text{div}(\lambda \cdot \text{grad}T(t, \bar{r})) - \frac{h \cdot S}{V} (T(t, \bar{r}) - T_w) \]

- Temp. change of the sample
- Heat generation in the sample
- Heat conduction in the sample
- Heat transfer between sample and environment

Heat generation equals heat conduction in material

**Frank-Kamenetzki (FK case)**

To be used for solids with low to medium heat conductivity
Approximative for unstirred liquids and gases
!! Assumes infinite fast heat transfer at the outside of body to the environment !!

Heat generation equals heat transfer to environment

**Semenov (Se case)**

To be used for well stirred reaction vessel, equal temperature inside the liquid material

Both special cases consider only the stationary situation (means dependence from space only),
**no time dependence, no influence of consumption of material**
Frank-Kamenetzki evaluation - improved expression

Boundary condition:

\[ \left( \frac{dT}{dr} \right)_{r=r_0} = -h \cdot (T_s - T_w) \]

\[ \frac{1}{\delta c_v} = \frac{1}{\delta c_c} + 2 \cdot e \cdot \frac{\lambda}{2 \cdot r_0 \cdot h} \cdot \frac{V}{S \cdot r_0} \]

\[ \frac{\delta c_v}{r_0^2} = \frac{\rho}{\lambda} \cdot \frac{E_a Q}{R T_w^2} \cdot Z_Q \cdot \exp(-E_a Q / R T_w C) \]
Determination of \( T_w C \) at given \( r_0 \)

\[ \frac{\delta c_v}{r_0^2} = \frac{\rho}{\lambda} \cdot \frac{E_a Q}{R T_w^2} \cdot Z_Q \cdot \exp(-E_a Q / R T_w) \]
Determination of \( r_0 C \) at given \( T_w \)

\( \delta c_c \)  
FKP\(_C\) at constant surface temp. of self heating substance, shape dependent [-]

\( \delta c_v \)  
FKP\(_C\) at variable surface temp. of self heating substance, shape dependent [-]

\( r_0 \)  
characteristic length of the geometry of self heating substance

\( T_s \)  
temperature at surface of self heating substance; if \( h = \infty \) then \( T_s = T_w \)

\( V \)  
volume of the geometry of self heating substance

\( S \)  
surface of the geometry of self heating substance

\( e \)  
Euler number, \( e=2.71828 \)

\( h \)  
heat transfer coefficient [energy/time/surface/K]

\( Nu \)  
Nusselt number \( Nu=2 \cdot r_0 \cdot h / \lambda \)
Principle of Finite Elements (FE) solution of General Heat Balance Equation

\[
\rho_s c_{p,s} \frac{\partial T_s}{\partial t} + \bar{u}_s \cdot \nabla T_s = \lambda_s \nabla^2 T_s + \rho_s c_{p,s} \Delta T_{ad} \frac{d\alpha}{dt}
\]

\(\dot{Q}_x = -k A \frac{\partial T}{\partial x}\)

\(\dot{Q}_y + \Delta y\)

\(\dot{Q}_z + \Delta z\)

Temperature

DSC & Kinetics

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Pre-requisites needed to perform the simulation

- Thermal decomposition behaviour, which is determined by DSC in closed, pressure resistant crucibles
  for PUR foam PU8
  for the propellant body
- Parameterization of the DSC measurements to be usable in the FE calculations
- Heat conductivity of the PUR foam (formulation PU8)
- Heat conductivity of the propellant body PB
- Specific heat capacity for PUR foam PU8
- Specific heat capacity for propellant body PB
- Mass density for PUR foam PU8
- Mass density for propellant body PB
- Heat conductivity, specific heat capacity, mass density for the steel of the burning chamber and of the air enclosed in the central bore of the PB
- Geometrical dimensions of the arrangement, rotational symmetry is given
- Heat transfer coefficient between outside air, acts here also as heat reservoir, and the steel body
Sample bodies to determine hat conductivity with the HotDisk™ method

Example of PB test body, view from above.

Example of PB test body, view from side.

Example of PU8 test body, view from side.

48 to 50 mm

Used sensor diameter: 19 mm
Determined temperature rises for the two samples in HotDisk™ measurement

**Temperature Increase $\Delta T$ in Sensor Spiral**

**Measurement Data**

- **PUR Foam PU8**
  - Heat power: 0.08 W
  - Measurement time: 320 s
  - Sensor radius: 9.87 mm
  - $\lambda = 0.169$ W/m/K
  - $c_p = 1.094$ J/g/K

- **Propellant Body**
  - Heat power: 0.08 W
  - Measurement time: 640 s
  - Sensor radius: 9.87 mm
  - $\lambda = 0.175$ W/m/K
  - $c_p = 1.147$ J/g/K

Graph shows temperature increase $\Delta T$ in sensor spiral with regard to start temperature as a function of measurement time [s].
**Thermal data of polyurethane foam spacer**

DSC data of the spacer foam PU8. Measured (coloured) and modelled (black) heat flow curves at the heating rates 0.5, 1, 2, 3 °C/min.

Result of the Friedman analysis (=differential iso-conversional data analysis) of the DSC data of the spacer foam PU8. Activation energy and pre-exponential factor as function of conversion of the exothermal decomposition reaction.
Thermal data of propellant body

DSC data of the ball powder based propellant body. Measured (coloured) and modelled (black) heat flow curves at the heating rates 0.25, 0.5, 1 °C/min.

Result of the Friedman analysis (=differential iso-conversional data analysis) of the DSC data of the propellant body. Activation energy and pre-exponential factor as function of conversion of the exothermal decomposition reaction.
Layer scheme used in simulation

Layer scheme of the calculations with FE programme package.
Layer no. 2, 3 and 4 are energetic.
A cylindrical geometrical arrangement was used.

<table>
<thead>
<tr>
<th>Layer material</th>
<th>Layer thickness [mm]</th>
<th>Layer No.</th>
<th>Thermal decomposi-</th>
<th>Initial temp. [°C]</th>
<th>Heat transfer number h [W/cm²/K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat reservoir (air)</td>
<td></td>
<td>0</td>
<td>-</td>
<td>300</td>
<td>50</td>
</tr>
<tr>
<td>Steel</td>
<td>10</td>
<td>1</td>
<td>-</td>
<td>300</td>
<td>-</td>
</tr>
<tr>
<td>PU8 spacer</td>
<td>1.1</td>
<td>2</td>
<td>x</td>
<td>20</td>
<td>-</td>
</tr>
<tr>
<td>PU8 coating of PB</td>
<td>0.1</td>
<td>3</td>
<td>x</td>
<td>20</td>
<td>-</td>
</tr>
<tr>
<td>Propellant body (PB)</td>
<td>8.8</td>
<td>4</td>
<td>x</td>
<td>20</td>
<td>-</td>
</tr>
<tr>
<td>Central bore of PB</td>
<td>2.5</td>
<td>5</td>
<td>-</td>
<td>20</td>
<td>-</td>
</tr>
</tbody>
</table>

The AKTS software was used: the Thermokinetics and the Safety module
Graphical presentation of the layer system used. Layer thicknesses are given in Table 7. The diagram shows a calculation at 300°C.
To be noted is the starting peak of the temperature in layer 2, the PU8 spacer.
Temperature – time course in layer 1 and layer 2 at outside-T = 300°C

Temperature distribution in layer 1, steel of burning chamber

Temperature distribution in layer 2, PU8 spacer

On the side of heat reservoir
On the side of the PU8 spacer
On the side to steel of burning chamber
On the side to PU8 coating of the charge

Temperature distribution in layer 1, steel of burning chamber

Temperature distribution in layer 2, PU8 spacer
Temperature – time course in layer 3 and layer 4 at outside $T = 300^\circ C$

Temperature distribution in layer 3, PU8 coating on PB

Temperature distribution in layer 4, the PB

Temperature distribution in layer 3, PU8 coating on the PB

Temperature distribution in layer 4, the PB

On the side to PU8 spacer

On the side to propellant body PB

On the side to the bore of the PB
Criteria for the ignition of PU-foam and propellant body PB

Two criteria for ignition have been applied:

- the occurrence of the peak in the rising temperature in any layer
- the temperature reaches 190°C in the propellant body
- the temperature reaches 210°C in the foam
Calculated times to ignition of the propellant charge with PUR spacers

Layer system 3
steel / ePU8 spacer / ePU8 coating / PB / air
temperature T is preset isothermally
times \( t_{Aig} \) up to autoignition \( Aig \)

Aig point: raising peak of temperature in material
Aig point: at 190°C in PB, at 210°C in PU8
Comparison of calculated and measured time to ignition

![Graph showing comparison of calculated and measured time to ignition](image)

- ePU8-ePU8-ePB
- iPU8-iPU8-ePB
- Steel direct on ePB
- Simulation; Aig at 190°C in PB; at 210°C in PU8
- Simulation; Aig at raising peak
- Steel direct on ePB ePB without PU8-coating

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Arrhenius plot of times to autoignition $t_{\text{Aig}}$ in the upper temperature range

All energetic.

Arrhenius plot of times to autoignition $t_{\text{Aig}}$ in the upper temperature range,
The ignition starts in the energetic PU8 foam.

$E_a = 143 \text{ kJ/mol}$
Arrhenius plot of times to autoignition $t_{Aig}$ in the lower temperature range.

All energetic.

Arrhenius plot of times to autoignition $t_{Aig}$ in the lower temperature range.

The ignition starts in the NC-based PB.

The activation energy is remarkably low:

$E_a = 41 \text{ kJ/mol}$
**Arrhenius plots of the times to autoignition** $t_{Aig}$ - inert spacer and coating - energetic PB.

PU is inert

At high temperatures the activation energy is small indicating only a weak temperature dependence of $t_{Aig}$. At low temperatures the activation energy becomes great, indicating long times $t_{Aig}$ and strong temperature dependence.

<table>
<thead>
<tr>
<th>Temperature Range</th>
<th>Activation Energy $E_a$ (kJ/mol)</th>
<th>$\lg(Z [1/s])$</th>
<th>$R^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>260°C to 420°C</td>
<td>26.6</td>
<td>0.766</td>
<td>0.9958</td>
</tr>
<tr>
<td>160°C to 260°C</td>
<td>45.8</td>
<td>2.664</td>
<td>0.9962</td>
</tr>
<tr>
<td>130°C to 140°C</td>
<td>245.3</td>
<td>27.696</td>
<td>1</td>
</tr>
</tbody>
</table>

- $\ln(1/t_{Aig})$ vs. $1/T$ [K]
- $\ln(1/taig)$ vs. $260-420°C$
- $E_a = 26.6$ kJ/mol
- $\lg(Z [1/s]) = 0.766$
- $R^2 = 0.9958$

- $\ln(1/taig)$ vs. $160-260°C$
- $E_a = 45.8$ kJ/mol
- $\lg(Z [1/s]) = 2.664$
- $R^2 = 0.9962$

- $\ln(1/taig)$ vs. $130-140°C$
- $E_a = 245.3$ kJ/mol
- $\lg(Z [1/s]) = 27.696$
- $R^2 = 1$
Summary and conclusions

- Suitable foam was found by ICT to protect the caseless propellant body (PB)
- The foaming technology was developed by ICT
- ICT calculated the times to ignition of the foamed PB caused by hot burning chamber wall
- The thermal decomposition properties of PB and foam as well as heat conductivity and specific heat have been determined at ICT
- After the calculations company Diehl performed an experimental determination of the cook-off times of the propellant body
- The agreement between calculations and experimental determination is very good.

- In the temperature range 250°C to 350°C a bifurcation of the time to ignition occurs
  This effect may be seen as a type of ‘ignition instability’ of the material meant in the way that it has two possibilities to ignite – in foam or in PB
- This bifurcation is verified experimentally also by a greater scattering than outside this temperature range
Recourse to the 7th HFC-Symposium on Energetic Materials
Typical conversion-time-temperature graph with DSC and TGA

Substance conversion $\alpha$ [-]

$\alpha$-range = 0 to 1

Typical error in conversion: 4 to 10%

Typical sample amount: 0.5 to 1.5 mg

Measurement time [h]

30 min to 3 hours

Measurement temperature [°C]

20 to 300°C

In use situation

In service time period: 0 to 15 years

In service temp. range: -30°C to +80°C

In service conversion range: 0 to max. 0.05
**Typical conversion-time-temperature graph with HFMC and ML (g amounts)**

- **Substance conversion** $\alpha$ [-]
- **Measurement time** [d]
- **Measurement temperature** [°C]
- **α-range** = 0 to 0.1
- **In use situation**
  - In service time period: 0 to 15 years
  - In service temp. range: -30°C to +80°C
  - In service conversion range: 0 to max. 0.05

- **Typical error in conversion**: 0.1 to 1%
- **Typical sample amount**: 1 to 2 g

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Conclusion (from the 2010 presentation on 7th HFC-S on EM)

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**Sensitivity and speed in experimental data acquisition**

To acquire data near the in-service temperatures needs time. The principle of equivalent load should be fulfilled.

Standard thermoanalytical equipment as DSC and TGA can provide with a set of experimental data in just one day.

But their accuracy is much lower than the one of the high sensitivity microcalorimeters. With DSC the error in reaction heat is often in the range or is even larger than the heat produced during full in-service time. This gives in prediction errors up to 200 % and more.

*for the low temperature prediction !!*

**In contrast:**

**DSC data are suitable to predict high temperature processes.**
Acknowledgement

Company Diehl BGT Defence is thanked for financing the project and for the permission to present the results.
Thank you for your attention

Questions?