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Explosives for civil uses - High explosives - Part 15: Calculation of thermodynamic properties

Explosivstoffe für zivile Zwecke - Sprengstoffe - Teil 15: Berechnung der thermodynamischen Eigenschaften

Explosifs a usage civil - Explosifs - Partie 15 : Calcul des propriétés thermodynamiques

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Explosives for civil uses - High explosives - Part 15: Calculation of thermodynamic properties

Explosifs à usage civil - Explosifs - Partie 15 : Calcul des propriétés thermodynamiques

Explosivstoffe für zivile Zwecke - Sprengstoffe - Teil 15: Berechnung der thermodynamischen Eigenschaften

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COMITÉ EUROPÉEN DE NORMALISATION
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Contents

Foreword

This document (EN 13631-15:2005) has been prepared by Technical Committee CEN/TC 321 "Explosives for civil uses", the secretariat of which is held by AENOR.

This European Standard shall be given the status of a national standard, either by publication of an identical text or by endorsement, at the latest by November 2005, and conflicting national standards shall be withdrawn at the latest by November 2005.

This document has been prepared under a mandate given to CEN by the European Commission and the European Free Trade Association, and supports essential requirements of EU Directive(s).

For relationship with EU Directive(s), see informative Annex ZA, which is an integral part of this document.

This European Standard is one of a series of standards on *Explosives for civil uses– High explosives.* The other parts of this series are:

Part 1: Requirements.

Part 2: Determination of thermal stability of explosives.

Part 3: Determination of sensitiveness to friction of explosives.

Part 4: Determination of sensitiveness to impact of explosives.

Part 5: Determination of resistance to water.

Part 6: Determination of resistance to hydrostatic pressure.

Part 7: Determination of safety and reliability at extreme temperatures.

Part 10: Method for the verification of the means of initiation.

Part 11: Determination of transmission of detonation.

Part 12: Specifications of boosters with different initiating capability.

Part 13: Determination of density.

Part 14: Determination of velocity of detonation.

Part 16: Detection and measurement of toxic gases.

This document includes a Bibliography.

According to the CEN/CENELEC Internal Regulations, the national standards organizations of the following countries are bound to implement this European Standard: Austria, Belgium, Cyprus, Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, Netherlands, Norway, Poland, Portugal, Slovakia, Slovenia, Spain, Sweden, Switzerland and United Kingdom.

Introduction

Some properties of the explosives used to define their energetic performance on an *a priori* basis are obtained by means of a thermodynamic calculation. The outcome of such calculation, based on the composition and density of the explosive, is dependent on the detonation state considered, the thermodynamic data used and the calculation method itself.

The simplest thermodynamic calculation of explosives is the one for a constant-volume reaction, usually referred to as constant-volume explosion state. Other calculations such as the Chapman-Jouguet (CJ) detonation state are also commonly used, leading to important dynamic values such as detonation pressure and velocity. However, these calculated values are not meaningful in practice for non-ideal industrial explosives. For this reason, only the simple values of energy and amount of gases produced are considered in this European Standard.

1 Scope

This European Standard specifies a method to calculate the detonation characteristics at the constant-volume explosion state and some parameters derived thereof.

2 Normative references

The following referenced documents are indispensable for the application of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

EN 13857-1:2003; *Explosives for civil uses - Part 1:Terminology*

3 Terms and definitions

For the purposes of this European Standard, the terms and definitions given in EN 13857-1:2003 and the following apply.

3.1
constant-volume explosion state
detonation point of theoretical nature in which the specific volume of the detonation products is that of the unreacted explosive

3.2
heat of explosion
energy released in the chemical reaction of the explosive when the composition of the reaction products is that of the constant-volume explosion state. It is usually given per mass of explosive

3.3
gas volume
volume occupied by the detonation product gases, as calculated from the chemical equilibrium composition in the constant-volume explosion state, at a specified condition of temperature and pressure. It is usually given per mass of explosive

3.4
specific force
result of the calculation: nRT, n being the number of moles of detonation product gases per mass, R the universal gas constant and T the temperature of explosion. It would be equal to the pressure exerted by the detonation gases if the specific volume were unity and the gases behaved as ideal. It is also called in some places specific energy

4 Calculation procedure

4.1 Thermodynamic Data and Functions

4.1.1 General

The thermodynamic properties needed relate to both explosive components and detonation products.

4.1.2 Explosive components

For each component the following data are required:

- Molecular or empirical formula.

- Energy of formation.

Table 1 shows these values for some explosives components. Whenever the explosive composition include any component not included in such table, the relevant values should be obtained elsewhere, e.g., from a thermochemical data source. In this case, the values used and the source should be reported.

Table 1 - Explosives components

Name	Abbreviation	Molecular or empirical formula	ΔE_f^{298} kJ/kg	Reference
Aluminium	Al	Al	0	
Ammonium chloride		ClH_4N	–5 739	Meyer
Ammonium nitrate	AN	$H_4N_2O_3$	–4 428	Meyer
Ammonium perchlorate	AP	ClH_4NO_4	–2 412	Meyer
Calcium carbonate		$CCaO_3$	–12 022	Meyer
Calcium nitrate		CaN_2O_6	–5 657	Meyer
Calcium stearate		$C_{36}H_{70}CaO_4$	–4 416	Meyer
Carbon, Graphite		C	0	
Cellulose		$C_6H_{10}O_5$	–5 670	USAMC
Dinitrotoluene 2,4	DNT 2,4	$C_7H_6N_2O_4$	–292,8	Meyer
Dinitrotoluene 2,6	DNT 2,6	$C_7H_6N_2O_4$	–159,5	Meyer
Ethylene diamine dinitrate	EDDN	$C_2H_{10}N_4O_6$	–3 378	Meyer
Glycol		$C_2H_6O_2$	–7 177	Meyer
Guar gum		$C_{37,26}H_{55,89}O_{31,05}$	–6 900	Meyer
Hexanitrostilbene	HNS	$C_{14}H_6N_6O_{12}$	239,8	Meyer
Hexogene, Cyclonite	RDX	$C_3H_6N_6O_6$	401,8	Meyer
Methylamine nitrate	MAN	$CH_6N_2O_3$	–3 604	Meyer
Nitrocellulose 11,5 % N	NC11,5	$C_{6000}H_{7890}N_{2111}O_{9222}$	–2 793	Meyer
Nitrocellulose 12,0 % N	NC12,0	$C_{6000}H_{7739}N_{2261}O_{9520}$	–2 663	Meyer
Nitrocellulose 12,5 % N	NC12,5	$C_{6000}H_{7579}N_{2416}O_{9833}$	–2 534	Meyer
Nitroglycerine	NG	$C_3H_5N_3O_9$	–1 540	Meyer
Nitroglycol	EGDN	$C_2H_4N_2O_6$	–1 499	Meyer

Nitroguanidine	NQ	$CH_4N_4O_2$	–773,0	Meyer
Nitromethane	NM	CH_3NO_2	–1 731	Meyer
Octogen	HMX	$C_4H_8N_8O_8$	353,6	Meyer
Oil; fuel oil, diesel oil		$C_{16}H_{34}$	-1 828	Lide
Paraffin, solid; wax		$C_{71}H_{148}$	–2 094	Meyer
Pentaerithrytol tetranitrate	PETN	$C_5H_8N_4O_{12}$	–1 611	Meyer
Polyisobutylene	PIB	CH_2	–1 386	Meyer
Potassium chlorate		$ClKO_3$	–3 205	Lide
Potassium nitrate		KNO_3	–4 841	Meyer
Potassium sulfate		K_2O_4S	–8 222	Lide
Sodium chlorate		$ClNaO_3$	–3 390	Lide
Sodium chloride		ClNa	–7 013	Chase
Sodium nitrate		$NNaO_3$	–5 447	Meyer
Sodium perchlorate		$ClNaO_4$	–3 080	Lide
Trinitrophenil methyl nitramine	Tetryl	$C_7H_5N_5O_8$	147,6	Meyer
Trinitrotoluene	TNT	$C_7H_5N_3O_6$	–219,0	Meyer
Urea		CH_4N_2O	–5 403	Meyer
Water (liquid)		H_2O	–15 660	Chase
Wood dust, plant meal		$C_{41,7}H_{60,4}O_{27,4}$	–4 564	Meyer
NOTE References are listed in the Bibliography. In many cases, internal energies of formation have been worked out from enthalpy of formation values.				

4.1.3 Detonation products

Detonation calculations require, in all cases, the following knowledge on detonation products:

- Formula.

- Internal energy or enthalpy of formation at a reference temperature, e.g. 298 K (ΔE_f^{298}, ΔH_f^{298}); Table 2 shows these data for some detonation products. Data for other products may be obtained elsewhere. In this case, values used and the source should be reported.

Table 2 - Detonation products

Name	Formula	ΔE_f^{298} kJ/mole	ΔH_f^{298} kJ/mole	Reference
Ammonia	H_3N	–43,42	–45,90	Chase
Aluminium oxide (l)	Al_2O_3 (l)	–1 617	–1 621	Chase
Aluminium oxide (s)	Al_2O_3 (s)	–1 672	–1 676	Chase
Calcium chloride (l)	$CaCl_2$ (l)	–771,6	–774,1	Chase
Calcium chloride (g)	$CaCl_2$ (g)	–471,5	–471,5	Chase
Calcium oxide (s)	CaO (s)	–633,8	–635,1	Chase
Carbon (s)	C	0	0	
Carbon dioxide	CO_2	–393,8	–393,8	Meyer
Carbon monoxide	CO	–111,9	–110,6	Meyer
Chlorine	Cl_2	0	0	
Hydrogen	H_2	0	0	
Hydrogen chloride	ClH	–92,4	–92,4	Meyer
Iron (III) oxide (s)	Fe_2O_3 (s)	–821,8	–825,5	Chase
Magnesium oxide (g)	MgO (g)	56,9	58,2	Chase
Magnesium oxide (l)	MgO (l)	–531,4	–532,6	Chase
Magnesium oxide (s)	MgO (s)	–600,0	–601,2	Chase
Methane	CH_4	–72,4	–74,9	Chase
Nitrogen	N_2	0	0	
Nitrogen monoxide	NO	90,3	90,3	Meyer
Oxygen	O_2	0	0	
Potassium carbonate (l)	CK_2O_3 (l)	–1 127	–1 131	Chase
Potassium carbonate (s)	CK_2O_3 (s)	–1 146	–1 150	Chase
Potassium chloride (g)	ClK (g)	–215,9	–214,7	Chase
Potassium chloride (l)	ClK (l)	–420,6	–421,8	Chase
Potassium chloride (s)	ClK (s)	–435,4	–436,7	Chase
Silicon dioxide (l)	O_2Si (l)	–900,2	–902,7	Chase

Silicon dioxide (s)	O_2Si (s)	–908,4	–910.9	Chase
Sodium carbonate (l)	CNa_2O_3 (l)	–1 105	–1 109	Chase
Sodium carbonate (s)	CNa_2O_3 (s)	–1 127	–1 131	Chase
Sodium chloride (g)	ClNa (g)	–182,7	–181,4	Chase
Sodium chloride (l)	ClNa (l)	–384,7	–385,9	Chase
Sodium sulfate (s)	Na_2O_4S (s)	– 1 382	-1 387	Lide
Water (g)	H_2O (g)	–240,6	–241,8	Chase
NOTE 1 (g), (l) and (s) indicate gaseous, liquid and solid state respectively. Where no state is indicated, data are for the gas. NOTE 2 References are listed in the Bibliography. In many cases, internal energies of formation have been worked out from enthalpy of formation values.				

- Internal energy or enthalpy as a function of temperature[1].

As a minimum, the detonation products listed in Table 2 should be considered, as required, depending on the composition elements. Others may also be included. The detonation products used should be reported.

For the calculation of the equilibrium composition by means of minimization of the free energy of the products, the following is also required to build a chemical potential:

- Entropy constant, or entropy at one temperature.

With these basic data, the following ideal thermodynamic functions can be formed; reference state is taken that of the elements in their stable state at 298 K and atmospheric pressure:

Internal energy

For gases,

$$E_i(T) = \Delta E_{fi}^{298} + (E^T - E^{298})_i = \Delta E_{fi}^{298} + (H^T - H^{298})_i - \mathrm{R}(T - 298)$$

T being absolute temperature. For condensed species,

$$E_i(T) = \Delta H_{fi}^{298} + (H^T - H^{298})_i$$

Chemical potential:

$$\mu_i^o(T) = \Delta H_{fi}^{298} + (H^T - H^{298})_i - TS_i$$

[1] These can be obtained from Chase (1998), Meyer et al. (2002) and other sources. Polynomial fits are customarily used. The source of the data used should be reported.