NO SPRAY.

Combustion Phenomena Evaluation by Means of Fifth Order Logarithmic Polynomials

3/3

Lanzafame Rosario and Messina Michele*
rlanzafa@diim.unict.it
mmessina@diim.unict.it

* Corresponding author

University of Catania
DIIM - Dipartimento di Ingegneria Industriale e Meccanica
Viale A. Doria, 6 – 95125 Catania – Italy
Phone: +39 95 738 24 14/26
Fax: +39 95 337994

ABSTRACT

A new set of mathematical functions, that is able to describe gases' thermodynamic properties, has been developed. These functions have the form of a fifth order logarithmic polynomial (VoLP). They could be utilized for combustion processes, with "frozen composition" and "composition in equilibrium" evaluation. The VoLPs present several advantages: they are able to cover a wide range of temperatures with only a single mathematical function; they have an elevate accuracy and they present the possibility to extrapolate experimental data beyond the experimental temperature range. The VoLP coefficients have been evaluated through the least squares fit on the basis of experimental measurements (taken from scientific literature). The set of VoLPs gives the possibility to study the combustion phenomena and allows to describe specific heat at constant pressure, enthalpy, entropy and equilibrium constants for gases dissociation.

KEYWORDS: Combustion, Thermochemical dissociation, Gases Thermodynamic Properties, Fifth order Logarithmic Polynomials, Internal Combustion Engine.

NOMENCLATURE

a_i	coefficients of $\tilde{c}_p(T)$
$b_0,\ldots,b_5$	$\tilde{h}(T)$ coefficients
b_6	constant of integration
c_0	constant of integration
$c_1,..,c_6$	$\tilde{s}(T,p)$ coefficients
$\tilde{c}_p$	molar specific heat at constant pressure [J mol^{-1} K^{-1}]
c_p	specific heat at constant pressure [J kg^{-1} K^{-1}]
$\tilde{g}$	Gibbs function [J mol^{-1}]
g_j	Gibbs function coefficients
$\tilde{h}_0$	molar enthalpy at $T=T_0$
$\tilde{h}$	molar enthalpy [J mol^{-1}]
h	enthalpy [J kg^{-1}]
ICE	Internal Combustion Engine
K_p	equilibrium constant
n.gases	number of gases present in the mixture
M	molecular weight
p_0	reference pressure 101325 Pa
p	pressure [Pa]
$\tilde{R}$	universal gas constant 8.314472 [J mol^{-1}K^{-1}]
R^2	correlation factor
$\tilde{s}_0$	molar entropy for $p=p_0$ and $T=T_0$
$\tilde{s}$	molar entropy [J mol^{-1} K^{-1}]
s	entropy [J kg^{-1} K^{-1}]
T_0	reference temperature 298.15 K
T	temperature [K]
VoLP	V order Logarithmic Polynomial
x	molar fraction
Φ	fuel to air equivalence ratio
ν_i	dissociation reaction stoichiometric coefficient
$\Delta\tilde{s}_{mix}$	entropy of mixing

1. INTRODUCTION

New polynomial functions have been investigated for the determination of gases' thermodynamic properties. These functions have been implemented to evaluate "frozen composition", "composition in equilibrium" and the dissociation equilibrium constants.

The polynomials have been calculated for isobaric specific heat, enthalpy, entropy and equilibrium constants. The polynomials coefficients for the isobaric specific heat have been computed for each single gas through the least squares method, and the coefficients for enthalpy and entropy are expressed as a combination of the previous ones.

The polynomial functions have the functional form of a V order Logarithmic Polynomial (VoLP), and can be used in temperature ranges of practical interest (ICE applications, Turbogas applications, etc).

VoLPs coefficients have been obtained by matching the thermodynamic properties data taken from [1, 7, 8, 9 and 10].

The isobaric specific heats have been calculated depending to temperature, and they have been compared with the experimental ones, in order to evaluate the relative errors.

The VoLPs pointed out an elevate interpolation accuracy, the possibility to utilize a single VoLP for a wide temperature range, and the possibility to extrapolate data beyond the experimental temperature range.

Utilizing the VoLPs for the equilibrium constants, it is possible to evaluate the molar fraction of the gases constituting the products of combustion, and the thermodynamic properties of the mixture.

In this formulation the mixing entropy has been taken into account for a correct evaluation of the mixture entropy, besides it is possible to take into account the heat occulted during the dissociation phenomenon and the great influence of thermochemical dissociation on mixture specific heat.