Aerospace Science and Technology 66 (2017) 177–192

Contents lists available at ScienceDirect

Aerospace Science and Technology

www.elsevier.com/locate/aescte

Thermodynamic properties of carbon–phenolic gas mixtures

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ARTICLE INFO

Article history:
Received 5 October 2016
Received in revised form 15 February 2017
Accepted 17 February 2017
Available online 10 March 2017

Keywords:
Thermodynamics
Ablation
Pyrolysis
Carbon–phenolic
Thermal protection materials
Re-entry vehicles

ABSTRACT

Accurate thermodynamic properties for species found in carbon–phenolic gas mixtures are essential in predicting material response and heating of carbon–phenolic heat shields of planetary entry vehicles. A review of available thermodynamic data for species found in mixtures of carbon–phenolic pyrolysis and ablation gases and atmospheres rich with C, H, O, and N such as those of Earth, Mars, Titan, and Venus, is performed. Over 1200 unique chemical species are identified from four widely used thermodynamic databases and a systematic procedure is described for combining these data into a comprehensive model. The detailed dataset is then compared with the Chemical Equilibrium with Applications thermodynamic database developed by NASA in order to quantify the differences in equilibrium thermodynamic properties obtained with the two databases. In addition, a consistent reduction methodology using the mixture thermodynamic properties as an objective function is developed to generate reduced species sets for a variety of temperature, pressure, and elemental composition spaces. It is found that 32 and 23 species are required to model carbon–phenolic pyrolysis gases mixed with air and CO_2, respectively, to maintain a maximum error in thermodynamic quantities below 10%.

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1. Introduction

In the wake of the Apollo program and multiple atmospheric entries on other planets and moons, the next two space exploration challenges, in terms of aerothermodynamics, are robotic sample return missions and the human exploration of Mars. Many achievements in atmospheric entry science have been made since the 1960s, but prediction of the heat flux at the surface of the spacecraft remains an imperfect art.

Ablative thermal protection systems (TPS), like those recently used on the successful Mars Science Laboratory (MSL) and Stardust missions, dissipate the extreme convective and radiative heat fluxes imposed on hypersonic entry vehicles through thermal decomposition of the thermal protection material (TPM). Ablative TPMs have also been used in the design of solid rocket nozzles to protect the nozzle walls from the high temperature gaseous combustion products. A specific class of lightweight, composite ablators were developed at NASA Ames Research Center (ARC) in the 1990s in an effort to improve on the existing TPMs [1,2]. In general, these materials are composed of low density, fibrous carbon substrates impregnated with an organic, polymeric resin. Examples designed for high-enthalpy atmospheric entry include phenolic impregnated carbon ablator (PICA, developed at NASA ARC in the 1990s and first used on the Stardust forebody heat shield, launched in 1999) [1–3], ASTERM (a PICA-like material under development by Astrium through ESA, starting in the early 2000s) [4], and PICA-X[3] (a PICA-like material developed by NASA for SpaceX). Sharpe and Wright [5] provide a review of materials used for applications in extreme environments from the 1960s until the present.

The accurate characterization and modeling of these TPMs is crucial for the safe design of TPSs and rocket nozzles. Although this

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[3] PICA Heat shield, http://www.spacex.com/news/2013/04/04/pica-heat-shield, accessed May 4, 2016.

http://dx.doi.org/10.1016/j.ast.2017.02.025
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Nomenclature

$\mathcal{A}$	ordered species set with decreasing Θ
a	sound speed, m s^{-1}
B	stoichiometry matrix
B'	nondimensional mass flux
C_M	Stanton number
C_p	molar specific heat at constant pressure, J mol^{-1} K^{-1}
c_p	specific heat at constant pressure per mass, J kg^{-1} K^{-1}
c_v	specific heat at constant volume per mass, J kg^{-1} K^{-1}
e	energy per mass, J kg^{-1}
G	Gibbs free energy, J mol^{-1}
H	molar enthalpy, J mol^{-1}
h	enthalpy per mass, J kg^{-1}
M	molecular weight, kg mol^{-1}
$\dot{m}$	mass flux, kg s^{-1} m^{-2}
N	moles, mol
P	(T, p, x^e) point
p	pressure, Pa
$\mathcal{R}$	reduction space
R_j	species gas constant, R_u/M_j
R_u	universal gas constant, 8.314 J mol^{-1} K^{-1}
S	entropy, J mol^{-1} K^{-1}
s	entropy, J kg^{-1} K^{-1}
$\dot{s}$	recession rate, m s^{-1}
T	temperature, K
Θ	thermodynamic error function
u	velocity, m s^{-1}
x	mole fraction
y	mass fraction
χ	char yield
$\mathcal{E}$	set of element indices
γ	specific heat ratio, c_p/c_v
γ_s	isentropic exponent
ρ	density, kg^{-1} m^{-3}
$\mathcal{S}$	set of species indices

Subscripts

c	char
e	boundary layer edge
g	pyrolysis gas
i, k	element
j	species
r	reduction space
s	species subset
w	wall

Superscripts

e	elemental quantity
resin	resin quantity
s	computed using species in $\mathcal{S}_s$
$\circ$	evaluated at standard-state p

Acronyms

ATcT	Active Thermochemical Tables
CEA	Chemical Equilibrium with Applications
JANAF	Joint-Army-Navy-Air Force
NASA	National Aeronautics and Space Administration
NIST	National Institute of Standards and Technology
PAH	Polycyclic Aromatic Hydrocarbons
PICA	Phenolic Impregnated Carbon Ablator
TN	Thermochemical Network
TPS	Thermal Protection System

has been an active field of research since the 1960s [6–19], state of the art modeling tools used for high-enthalpy aerothermodynamic predictions leave room for improvement, and prediction uncertainties remain as high as 60% for laminar convective heating [20–23]. These uncertainties force TPS designers to include significant safety factors when determining the TPS thickness, adding unnecessary mass to the vehicle design which in turn increases propellant mass and decreases mass available for scientific payloads.

Ablation phenomena have been described previously in great detail, and many of the modeling issues and uncertainties that are associated with ablation have been reviewed in previous works [24–33] and are summarized below. In general, the virgin TPM is primarily affected by two physical phenomena. The first, known as pyrolysis, refers to the thermal decomposition of a phenolic resin. At high temperatures, phenolic resin is progressively carbonized into a lower density carbon, known as char. Approximately 50% of the resins' original mass is converted to the gas phase [16,34]. Pyrolysis gases are then transported out of the heatshield by diffusion and convection through the porous carbon fiber substrate. The chemical composition of the high temperature pyrolysis gas evolves as it flows through the porous carbon fiber structure, and will eventually mix and continue to react with the surface ablation products and the atmospheric gases.

The second phenomenon, surface ablation, refers to mass removal in a thin volumetric layer of carbon fibers near the surface of the heatshield through heterogeneous chemical processes, including oxidation, nitridation, and sublimation. Surface ablation occurs in both non-charring materials, such as carbon/carbon ablators, and in charring ablators, such as carbon–phenolics. Charring ablators will be focused on in this work.

Determining the chemical composition of the gas close to the surface of an ablative heatshield is necessary to accurately predict the surface heat flux. Many material response codes assume that the gas mixture near the surface of the heatshield is in thermodynamic equilibrium (see [35] for a summary of ablation code capabilities), and this paper will remain consistent with that assumption. An analysis of finite-rate kinetics related to the gas mixture is outside of the scope of this work. Equilibrium compositions are dependent entirely on the underlying thermodynamic data for the species considered. To the authors' knowledge, a detailed review of thermodynamic data for carbon–phenolic gases has never been performed and no consensus exists concerning which species should be considered in these mixtures.

The primary goals of this work are to a) provide a detailed review of available thermodynamic data for species relevant to the simulation of the material response of carbon–phenolic TPMs, subjected to high-enthalpy flows, b) compile a detailed thermodynamic database based on this review, and c) develop reduced species sets suitable for the accurate calculation of mixture thermodynamic properties over the range of temperatures, pressures, and elemental compositions of interest to TPS designers. The paper is organized in several parts. In the following section, a review of experimental and theoretical elemental compositions relevant to carbon–phenolic TPMs is performed in order to define the elemental composition space of interest in this work. Next, a review of thermodynamic data sources is presented along with a methodology for combining each data source to form an extensive thermodynamic database for carbon phenolic-gases, placing an emphasis on the consistency and quality of the data. The database is then compared to the commonly used CEA [36] database and the rel-

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