Experimental Thermal and Fluid Science 35 (2011) 1588–1599

Contents lists available at ScienceDirect

Experimental Thermal and Fluid Science

journal homepage: www.elsevier.com/locate/etfs

Uncertainty quantification of a graphite nitridation experiment using a Bayesian approach

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ARTICLE INFO

Article history:
Received 16 March 2011
Received in revised form 20 July 2011
Accepted 26 July 2011
Available online 3 August 2011

Keywords:
Uncertainty quantification
Parameter estimation
Bayesian method
Graphite nitridation experiment

ABSTRACT

In this paper, a stochastic system based Bayesian approach is applied to estimate different model parameters and hence quantify the uncertainty of a graphite nitridation experiment. The Bayesian approach is robust due to its ability to characterize modeling uncertainties associated with the underlying system and is rigorous due to its exclusive foundation on the axioms of probability theory. We choose an experiment by Zhang et al. [1] whose main objective is to measure the reaction efficiency for the active nitridation of graphite by atomic nitrogen. To obtain the primary physical quantity of interest, we need to model and estimate the uncertainty of a number of other physical processes associated with the experimental setup. We use the Bayesian method to obtain posterior probability distributions of all the parameters relevant to the experiment while taking into account uncertainties in the inputs and the modeling errors. We use a recently developed stochastic simulation algorithm which allows for efficient sampling in the high-dimensional parameter space. We show that the predicted reaction efficiency of the graphite nitridation and its uncertainty is $\sim 3.1 \pm 1.0 \times 10^{-3}$ that is slightly larger than the ones deterministically obtained by Zhang et al. [1].

1. Introduction

Experiments are performed to test physical theories or to estimate parameters of widely used theoretical models. An experimentalist usually prescribes the measurement uncertainties while reporting the results. The theorists or the users of theoretical models need to estimate parameters appearing in their models using the experimental data (i.e., a calibration process). There are various methods of parameter estimation that can be found in many textbooks on data analysis, under the category of inverse problems (for example [2] and many others). Inverse problems can be very ill-conditioned and in many cases special numerical techniques are required. In this work, we focus on the Bayesian method that is a robust method when there are uncertainties due to the experimental measurements as well as uncertainties in the model used to reduce the measured data [3]. We consider an experiment for the nitridation of graphite conducted by Zhang et al. [1]. The quantity that needs to be calibrated is the reaction probability of the graphite–nitrogen atom surface reaction. This reaction is of great importance for modeling the thermo-chemical ablation of thermal protective systems used in earth re-entry space vehicles [4] and for assessment of the safety of the heat shield material [5]. As a result several experimental efforts have been undertaken to measure the reaction efficiency for this system. In [6], the reaction of dissociated nitrogen with resistively heated graphite was studied in an evacuated quartz bulb. The reaction probability was measured at various temperatures ranging from 1500 to 2500 K. Park and Bogdanoff [7] used a shock tube facility to dissociate nitrogen and measured reaction efficiency from nitridation of a graphite wire suspended in the shock tube. Suzuki et al. [8,9] used an Inductively Coupled Plasma (ICP) torch to measure the total mass loss from the exposed area of the surface. The incoming mass flux of N atoms was measured using numerical analysis of a two-dimensional jet flow. The results obtained from these experiments differ substantially. The results reported in [7] are three orders of magnitude higher than the other results that also differ significantly. This could be attributed to different grades of graphite being used as well as errors in the data reduction model that maps the parameters to the experimentally observed mass loss rate. We note that the physical model that relates the mass loss rate due to nitridation with the surface temperature and wall concentration is relatively simple. However due to the complexity of the experimental setups, detailed models need to be employed to compute the temperature of the graphite and the wall

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doi:10.1016/j.expthermflusci.2011.07.010