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Quentin Faure Internship Report

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Idaho National Laboratory
Idaho Falls, Idaho 83415

http://www.inl.gov

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1 Introduction

During the internship, the student has studied and modeled hydrogen diffusion, desorption, and adsorption in ZrH and YH using Bison. The student will move towards coupling the model developed in Bison for hydrogen migration to the neutronic response obtained from Griffin for the unit cell of a prototypical microreactor. Due to the length of the report being short, only a small part of the YH modeling is being presented here.

2 Theory and Results

Three driving forces determine the hydrogen current within the YH_x bulk: (1) Fickian diffusion, redistributing hydrogen from regions of high concentration to regions of low concentration, (2) thermal diffusion (the Soret effect), redistributing the hydrogen from higher temperature zones to lower temperature zones, and (3) the stress gradients redistributing the hydrogen from high compression to high tensile regions. Since the stress-induced diffusion can usually be neglected due to its lower order of magnitude compared to Fickian and Soret diffusion [1], the hydrogen redistribution can be translated mathematically into the following equation [2]:

$$\frac{\partial c_H}{\partial t} = \nabla \cdot \left[-D \left(\nabla c_H + \frac{Q c_H}{RT^2} \nabla T \right) \right], \tag{1}$$

$$D = 3.00.10^{-1} exp\left(\frac{-160000}{RT} \right). \tag{2}$$

where c_H denotes the hydrogen molar concentration, D is the diffusion coefficient of hydrogen in Y, R the gas constant, T the temperature, Q is the heat of transport. For Y, the diffusion coefficient can be described by the following Arrhenius law.

During desorption or adsorption, at the surface, the flux of hydrogen is:

$$\vec{J_i} \cdot \hat{n} = k \times (c_H^{Surface} - C_{eq}). \tag{3}$$

A model for the mass heat transfer, here denoted as k, was developed to match the experimental curves in Ref. [3].

$$k = \left[k_0 + k_1 exp(-k_2 \frac{C_H}{C_{eq}})\right] exp(-\frac{E_a}{RT}). \tag{4}$$

The latter showed agreement within 6% between Bison results and the experiment. The values for k_0, k_1, k_2, and E_a are: 24.9526 m/s, 10.1951 m/s, 5, and 147668 j/mol, respectively. These values were computed by minimizing the L2 norm of the error between BISON results and experimental values. Figure 1 shows the adsorption curves obtained with this model as well as the experimental values.

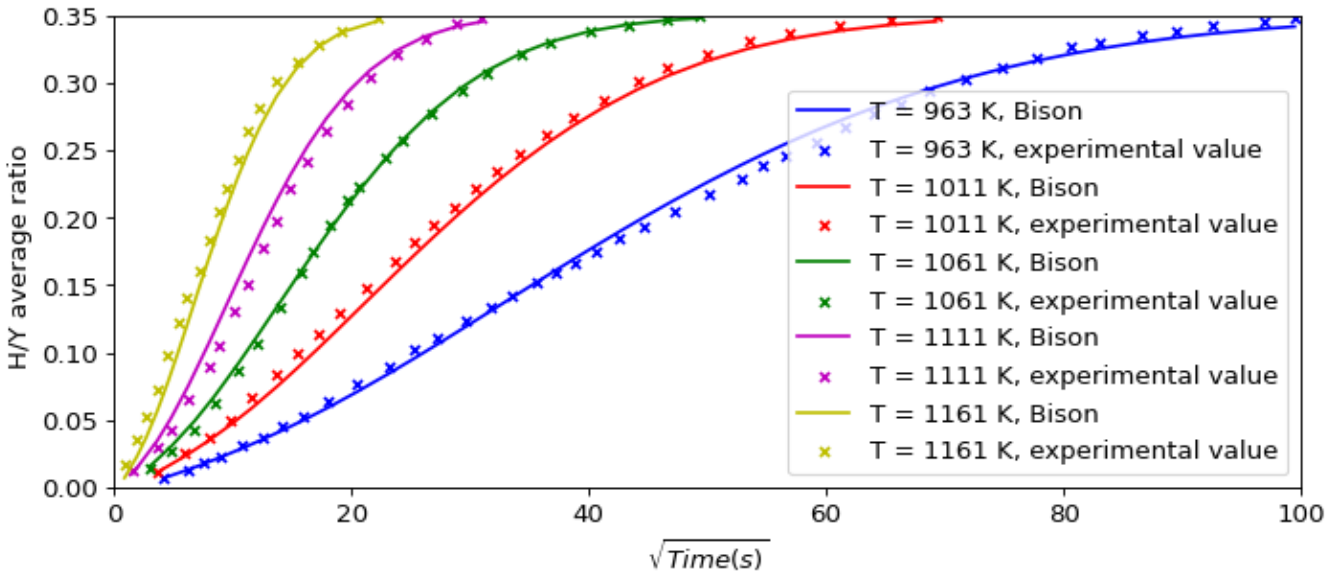

Figure 1. Temporal H/Y evolution for different temperatures

3 Reference

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