# Quantitative Modeling for Gas Bubble Evolution in Nuclear Fuel and Pitting Corrosion

**†San-Qiang Shi[1], Zhihua Xiao[1], and Talha Q ANSARI[1]**

[1]Department of Mechanical Engineering. The Hong Kong Polytechnic University, Hong Kong, China

†Corresponding author: mmsqshi@polyu.edu.hk

## Abstract

A quantitative phase-field model was developed to predict the evolution of gas bubbles in nuclear fuels. The model takes into account temperature, gas bubble internal pressure, interfacial energy between bubble and matrix, and elastic strain energy within the material. The model can handle real equilibrium concentrations of vacancies and gas atoms, which is in the order of 10-10 to 10-11 at 1500K. Case studies include time-dependent bubble size evolution as a function of temperature, vacancy and gas generation rates; interaction between gas bubbles and distribution of gas bubble sizes, etc.

A quantitative model for pitting corrosion in stainless steel was develop. The mass transport in the electrolyte and electrochemical reactions in the electrolyte/electrode interface are taken into consideration in the model in order to simulate metal corrosion in a corrosive environment. The governing equations for the mass transport and phase order parameter are solved in such a way that the free energy of the system is reduced as a result of diffusion and migration process while the distribution of electrostatic potential is governed by Poisson's equation. A calibration study is performed to relate the kinetic interface parameter with the corrosion current density which results in a direct relation between overpotential and kinetic interface parameter. A comparative study is performed to validate the model against the experimental results.

The work was supported by Research Grants Council of Hong Kong (PolyU 152140/14E, PolyU 152636/16E) and a grant from NSFC (No. 51672232).

Keywords: **Computer modeling, Environmental degradation of materials**