**8th. World Congress on Computational Mechanics (WCCM8)**
**5th. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)**
**June 30 – July 5, 2008**
**Venice, Italy**

# THERMODYNAMIC MODELS AND SIMULATIONS OF ADVANCED NUCLEAR FUELS

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**Key Words:** *Thermodynamics, Models and Simulations, Transport, Nuclear Energy*

## ABSTRACT

Nuclear fuels and structural materials are subject to severe radiation environments and their properties change significantly with time and irradiation level. The major factors that influence the thermal, chemical and mechanical properties of nuclear fuels are temperature, stoichiometry, and microstructure (especially porosity and point defects). In particular, the accumulation of fission products and the formation of gas bubbles can decrease the heat transfer, leading to overheating of the fuel element. This presentation reviews recent results on the effect of irradiation on properties such as thermal conductivity, oxygen diffusivity, and thermal expansion. The scientific methods used in this approach cover a large spectrum of time and space scales, from electronic structure, atomistic levels, through meso-scale, all the way to continuum [1]. The simulations include coupled heat transport, diffusion, and thermal expansion, gas bubble formation and temperature evolution [2], as well as predictions of point defect concentrations, stoichiometry, and phase stability [3]. The multi-scale approach is illustrated using results on oxide fuels with metal cladding [4]. The presentation ends with a discussion of the major challenges in the area of materials models and simulations for nuclear energy applications.

## REFERENCES

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