FUEL PERFORMANCE AND THERMOCHEMISTRY MODELING OF CANDU NUCLEAR FUEL

Progress in developing a self standing integrated code

M.H.A. Piro
Department of Chemistry and Chemical Engineering,
Royal Military College of Canada, Kingston, Ontario, Canada
Supervisors: B.J. Lewis and W.T. Thompson

Abstract

A numerical model is in the process of being created to simulate the behaviour of CANDU nuclear fuel under normal operating conditions. A finite volume code is being written in FORTRAN that is capable of predicting heat transfer, fission gas release, grain growth and structural deformation due to: thermal expansion, creep, irradiation-induced densification, fission product swelling and external coolant pressure. A thermodynamic model is also under development that is capable of estimating the equilibrium composition of multi-phase and multi-component systems. The coupling of both fuel performance and thermochemistry codes will provide an ideal platform for modeling nuclear fuels under normal and accident conditions.

1. Introduction

The necessity of accurately predicting the behaviour of nuclear fuel is driven by both economic and safety concerns of the regulator, industry and that of the general public. The ability to model fuel behaviour allows the designer to engineer a reactor that maximizes thermal power while maintaining a high level of safety. However, the prediction of such complicated phenomena that is associated with the operation of nuclear fuel demands substantial research efforts.

The current focus of this particular work is on the numerical modeling of CANDU fuel performance under normal operating conditions; although the investigation of defective fuels remains a possibility in future research. There is a need to provide a platform for testing on which different models related to fuel behaviour could be tested to better understand their importance on fuel performance without having to implement such models in commercial codes which is an expensive and difficult process. The majority of physical models that have been implemented in this numerical simulation have been reproduced from the work done by Morgan at the Royal Military College of Canada (RMC) [1]. Results produced by the Morgan model were in very good agreement with ELESTRES, a fuel performance code used in the Canadian nuclear industry and was developed by Atomic Energy of Canada Limited (AECL). Despite Morgan being able to produce excellent results, the model was not numerically stable which necessitated the need to investigate alternative computational platforms.

Initial efforts of this project were to create a fuel performance code using ANSYS-Multiphysics, which included ANSYS-Mechanical coupled with CFX. The ANSYS workbench was found to be very robust, but had limited capabilities that made it inadequate for this particular problem. Research efforts were then redirected towards the creation of a custom finite volume code written in FORTRAN, which places the capabilities of the software in the programmer's ability to write appropriate code. The benefit of having greater control over modeling techniques is accompanied by the requirement to verify the solver.

2. Fuel performance model development

The goal of this work is to reproduce the fuel performance model created by Morgan on a more robust platform and to then improve upon it with the use of more sophisticated models and greater numerical capabilities. This model solves for heat transfer, structural deformation and fission gas release of CANDU nuclear fuel under normal operating conditions. This section briefly describes the physical models that have been implemented and identifies the literature that has been used.

2.1 Heat transfer

The transport of heat through the uranium dioxide fuel is represented by the following expression, which includes thermal generation due to fissioning, which assumes that 200 MeV is generated per fission event [2].

$$\frac{\partial\left(\rho C_p T\right)}{\partial t} = \nabla\cdot\left(k\nabla T\right) + \frac{P_{lin}}{\pi a_{pel}^2}\left(\frac{\kappa a_{pel}}{2I_1(\kappa a_{pel})}\right) I_0(\kappa r) \qquad (1)$$

where T [K] is the temperature, P_{lin} [W m^{-1}] is the linear power rating of the fuel, κ [m^{-1}] is the inverse neutron diffusion length, a_{pel} [m] is the initial radius of the fuel pellet and I_0 and I_1 are the zeroth and first order modified Bessel functions of the first kind, respectively. Fuel density accounts for such effects as thermal expansion, densification and fission product swelling, which will be further discussed in Section 2.2. Specific heat capacity of the fuel is temperature dependent and is given by [3]:

$$\begin{aligned} C_P = {} & 5.21743*10^{1} + 8.7951*10^{-2}T - 8.4241*10^{-5}T^2 \\ & + 3.1542*10^{-8}T^3 - 2.6334*10^{-12}T^4 - 7.1391*10^{5}T^{-2} \end{aligned} \qquad (2)$$

Thermal conductivity of the fuel is an important quantity to accurately approximate as it has the greatest influence in calculating the temperature distribution within the pellet. The evolution of this expression has allowed for multiple functions to be incorporated in addition to temperature. The most recent correlation from MATPRO-1996 for approximating thermal conductivity, k [W m^{-1} K^{-1}], of uranium dioxide fuel is [4]:

$$k = \left[\frac{D}{1+(6.5-0.00469T')(1-D)}\right]\left[\frac{C_v}{(A+BT'')(1+3\varepsilon_{th})}\right] + 5.2997\times10^{-3}T\mathrm{e}^{\left[\frac{-13358}{T}\right]}\left\{1+0.169\left[\left(\frac{13358}{T}\right)+2\right]^2\right\} \quad (3)$$

Terms in the above equation are summarized in the Nomenclature found in Section 7. This term utilizes a semi-empirical method of approximating the thermal conductivity of the fuel, which was derived using theoretical calculations and empirical correlations to match experimental data. The error in the above correlation is approximated at ± 0.2 [W m^{-1} K^{-1}] [4], which can be quite significant in thermal calculations of CANDU fuel [1].

Heat transfer through the fuel-to-sheath gap is a complicated factor to approximate as many parameters must be taken into consideration. The conductance of solid-solid contact can be quite significant once the sheath comes into contact with the fuel pellet, and is included in the first term of (4). The second term in (4) accounts for heat transfer through the gas in the gap, which includes a weighted average of thermal conductivities of individual gaseous species. The contribution of heat transfer through radiation is represented by the final term in (4), which is for the most part only important at high temperatures.

$$h_T = \left(\frac{k_{hm}}{a_0 R^{0.5}}\frac{P_{\mathrm{int}}^{0.5}}{H}\right) + \left(\frac{k_f}{C(R_1+R_2)+t_g+g_{jump}}\right) + \left(\sigma\varepsilon_m\left(T_f^2+T_S^2\right)\left(T_f+T_S\right)\right) \quad (4)$$

2.2 Structural deformation

Although the fuel pellet and sheath will only deform by a small proportion relative to their original dimensions, the gap between the pellet and the sheath will change by an appreciable amount. The gap distance does have a directly pronounced effect on the estimated heat transfer coefficient between the sheath and the fuel pellet [1].

Thermal expansion has a great effect on the deformation of the pellet and is also accounted for in density calculations. Fink proposed the following correlation of linear expansion of UO_2 [3]:

For $273\,\mathrm{K} \le T \le 923\,\mathrm{K}$:

$$\frac{L(T)}{L_{273}} = 9.973\times10^{-1} + 9.082\times10^{-6}T - 2.705\times10^{-10}T^2 + 4.391\times10^{-13}T^3 \quad (5)$$

For $923\,\mathrm{K} < T \le 3120\,\mathrm{K}$:

$$\frac{L(T)}{L_{273}} = 9.672\times10^{-1} + 1.179\times10^{-5}T - 2.429\times10^{-9}T^2 + 1.219\times10^{-12}T^3 \quad (6)$$

Similarly, thermal strain of the sheath in the radial direction is given by:

For $T < 1050\ \text{K}$:

$$\varepsilon_{th}^{r} = -2.073\times10^{-3} + 6.721\times10^{-6}T \quad (7)$$

For $1050\ \text{K} \le T < 1270\ \text{K}$:

$$\varepsilon_{th}^{r} = 1.486\times10^{-2} - 9.398\times10^{-6}T \quad (8)$$

For $T \ge 1270\ \text{K}$:

$$\varepsilon_{th}^{r} = -9.450\times10^{-3} + 9.7\times10^{-6}T \quad (9)$$

Irradiation also has an effect on the structural characteristics of the fuel. The process of densification describes the effect of shrunken or destroyed pores within the fuel due to fission spikes [5]. Hastings proposed a correlation describing F as the contribution of porosity removed from the pellet due to densification [6]:

For $F \le 0.67$:

$$F = -0.43\times[1+\exp(-0.71Bu)] + 0.71\times10^{-3}[1-\exp(-0.6Bu)]T \quad (10)$$

For $F > 0.67$:

$$F = 0.67 \quad (11)$$

Both solid and gaseous fission products are formed during the process of irradiation, which causes the fuel to swell. To avoid any potential confusion, the gaseous fission product swelling terms in (12) used to describe structural deformation and density of the UO_2 fuel is independent of the fission gas release model described in Section 2.3. MATPRO offers a correlation to approximate this complex mechanism to match experimental data as a function of temperature, density and burnup [4]:

$$\frac{\partial(\Delta V_{GFP}/V)}{\partial t} = 9.42\times10^{-36}(2800-T)^{11.73}e^{[-0.0162(2800-T)]}e^{[-8.0\times10^{-27}\,Bu\rho]}\rho\frac{\partial Bu}{\partial t} \quad (12)$$

Accumulation of solid fission products produces an additional swelling effect that is not temperature dependent, but is rather entirely dependent upon burnup. Olander suggests that the volumetric change in UO_2 contributed by solid fission product swelling is 0.32% per atom percent burnup [7]:

$$\frac{\Delta V_{SFP}}{V} = 0.0032\left(\frac{Bu}{225}\right) \quad (13)$$

The effect of creep in the fuel pellet is also considered using a correlation from MATPRO-1996, which incorporates the rate of fissioning, temperature, internal stresses, the theoretical density factor, grain size and the time since the last power ramp. The creep strain rate is given by [4]:

$$\dot{\varepsilon}_{creep} = \left(\frac{(0.3919 + 1.3100 \times 10^{-19} \dot{\phi}) \sigma_1 \exp\left(\frac{9.00 \times 10^4}{RT} \right)}{(D - 87.7) G n^2} + \frac{2.0391 \times 10^{-25} \sigma^{4.5} \exp\left(\frac{1.314 \times 10^5}{RT} \right)}{D - 90.5} \right.$$

$$\left. + 3.72264 \times 10^{-35} \dot{\phi} \sigma^{4.5} \exp\left(\frac{2.6167 \times 10^3}{RT} \right) \right) \times \left(2.5 \exp(-1.40 \times 10^{-6} t) + 1 \right) \quad (14)$$

The creep strain rate of the sheath accounts for many factors, including: dislocation glide, grain boundary sliding and the transformation from the alpha phase to the beta phase [8].

$$\dot{\varepsilon}_{creep} = C_d \exp\left(-\frac{34726}{T} \right) \sigma_*^{5.3} + F_{gb} \left(\frac{\sigma_a}{G * d} \right)^2 \exp\left(-\frac{9431}{T} \right) + 2.4 \times 10^{-3} f_a \dot{\phi} \sigma_a \quad (15)$$

2.3 Fission gas release mechanism

Knowledge of the behaviour of fission gases is critical to the operation of nuclear fuels under normal operating conditions. Heat transfer through the fuel-to-sheath gap is largely dependent upon the concentration of fission gases and the total fluid pressure in the gap. Fission gases are generated within a fuel grain, released to the grain surface and then released to the fuel-to-sheath gap once saturation is reached within a fuel pellet. A fission gas diffusion model was implemented in the code which approximates the radial diffusion of these gases within an idealized spherical fuel grain using a Booth model [9]:

$$\frac{\partial \psi}{\partial t} = D_{eff} \nabla^2 \psi + S_\psi \quad (16)$$

Where ψ [atoms μm^{-3}] is the total concentration of fission gas atoms, D_{eff} [$\mu m^2\ s^{-1}$] is the effective diffusive term and S_ψ [atoms $\mu m^{-3}\ s^{-1}$] is the generation of fission gases within the fuel grain. The generation of fission product gases is dependent upon the rate of fissioning and it is assumed that 25 stable gas atoms are formed for every 100 fission events [10].

The effective diffusive term is comprised of several terms that are individually more prevalent in particular temperature ranges. Diffusion is dominated by the rate of fissioning at temperatures below 1100 K, which is described by Turnbull as an athermal tail [11]. Diffusion is mostly determined by the presence of vacancies and intersititials at intermediate temperatures in the range of 1100 – 1700 K [12]. Above temperatures of 1700 K, diffusion is entirely temperature dependent [12]. Additional effects such as intragranular trapping and irradiation resolution are also incorporated in the effective diffusive term.

Fission product gases accumulate at the grain boundary from diffusion from within the grain and form bubbles. The release of the gases to the grain surface is defined by a

Booth flux, given by the following equation. Both the diffusion of fission gas atoms in (16) and the Booth flux require knowledge of the grain size, Gn [μm], which is discussed in section 2.4.

$$J_{Booth} = -\pi Gn^2 D_{eff} \left. \frac{\partial \psi}{\partial r} \right|_{r=\frac{Gn}{2}} \tag{17}$$

As fission gases accumulate on the grain boundary, the bubbles that are formed continue to grow until the grain surface eventually reaches saturation. A saturation concentration of fission gases on the grain boundary, N_s [atoms μm^{-2}], is estimated by White [13]:

$$N_s = \frac{4 r_f f(\theta) f_B}{3kT \sin^2 \theta} \left(P_{ext} + \frac{2\gamma}{r_f} \right) \tag{18}$$

All of the variables in the above equation are taken as constants except for temperature. Therefore, the concentration of fission gases on the grain boundary is inversely proportional to temperature. Any excess gas from a particular saturation value will be released to the fuel-to-sheath gap, which then affects fluid pressure and the heat transfer coefficient given in [4].

2.4 Grain growth

The size of fuel grains influences the calculation of many terms in this model, including the thermal conductivity of the fuel in (3), creep (14) and more importantly the release of fission gases. Predictions of the growth of fuel grains are based on the work of Ainscough et al. and Khoruzhii et al. by the following expression [14, 15]:

$$\frac{dGn}{dt} = k \left(\frac{1}{Gn} - \frac{1}{Gn_{\max}} - \frac{1}{Gn_{ir}} \right) \tag{19}$$

Where k [μm^2 s^{-1}] is a temperature dependent rate constant, Gn [μm] is the size of the fuel grain, $Gn_{\max}$ [μm] is the maximum fuel grain size and Gn_{ir} [μm] is a term that reflects the adverse effect of grain growth that is associated with irradiation intensity [15].

3. Thermochemistry model development

A thermochemistry model is also currently being developed that will be capable of predicting the equilibrium composition of multiphase and multicomponent systems. The model utilizes a Gibbs energy minimization technique that calculates equilibrium concentrations from the first principles of thermodynamics. Very realistic estimates can therefore be made.

A computer code has been written in FORTRAN that systematically alters the molar concentrations of numerous species of interest to yield a solution that has the lowest Gibb's energy for a particular temperature and pressure [16]. The intent of this work is to be able to directly implement this thermochemistry model in the fuel performance code discussed in Section 2 without any approximations or limitations associated with data transfer between database operations.

The capability of predicting chemical equilibrium compositions of nuclear materials within a fuel performance code can be a powerful tool to have. For instance, the incorporation of the Uranium-Oxygen-Fission product system in this thermochemistry model can predict the partial pressures of numerous fission product gases that are released to the fuel-to-sheath gap. Results produced by Thompson et al. are shown in Figure 1 which lists the predicted fission product inventory of irradiated CANDU fuel at 175 MWh/kgU burnup [17]. Figure 1 includes the gaseous phase (containing fission gases and oxygen) and several solid phases (which are also comprised of solid fission products). The code that is under development for this work has the potential to perform such calculations.

Thermochemistry modeling is also very important in simulating accident conditions involved with defective fuels. A breach in the sheath allows coolant to come into contact with the pellet, permitting oxidation of the fuel and of the sheath, not to mention any subsequent reactions with gaseous species that were present in the fuel-to-sheath gap. Any harmful materials that were housed in the fuel-to-sheath gap are allowed to escape into the primary heat transport system.

Additionally, the thermal performance of the element suffers due to the substitution of helium gas with water vapour and hydrogen in the fuel-to-sheath gap [18]. Heat transfer within the pellet is also degraded due to lower thermal conductivity of the fuel as it oxidizes with surrounding water making it hyperstoichiometric [18]. The melting temperature of the non-stoichiometric fuel may be lower than pure UO_2, resulting in even greater complications that must be given careful attention. In addition, elevated mobility of fission product gases within hyperstoichiometric fuel may also lead to higher release rates of fission gases within fuel grains.

The thermochemistry code discussed here will be capable of predicting equilibrium concentrations of a Uranium-Oxygen binary system for a range of O/U ratios for a large range of temperatures, and will be able to reproduce the phase diagram illustrated in Figure 2. The direct implementation of this thermochemical model in the fuel performance code discussed earlier allows for the capability of solving phenomena associated with defective fuel elements.

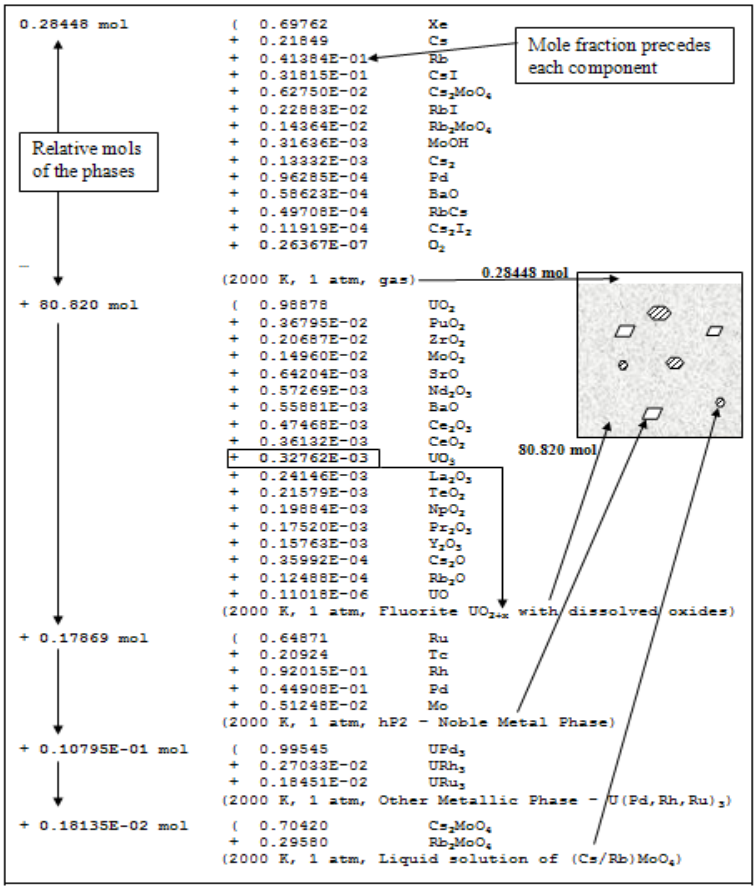

Figure 1 Predicted composition of Uranium-Oxygen-Fission product system of irradiated CANDU fuel [17].

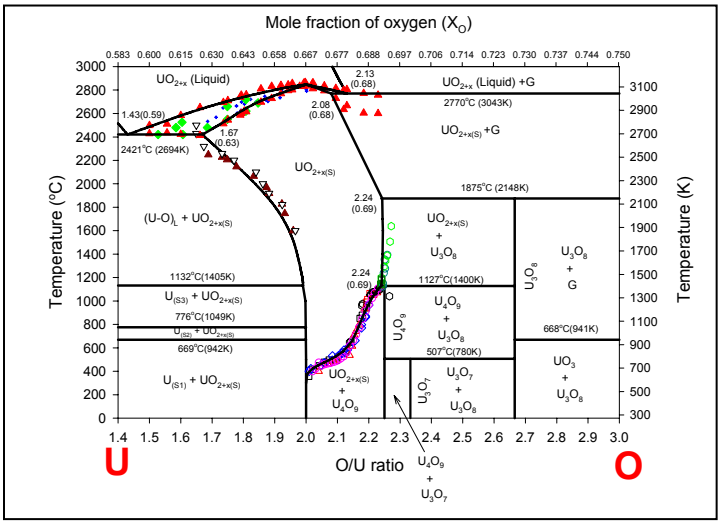

Figure 2 Phase diagram of the Uranium-Oxygen system [19-23].

4. Conclusions

The framework of a coupled fuel performance and thermochemistry model has been presented to predict the behaviour of CANDU nuclear fuel under normal operating conditions. The fuel performance model is capable of predicting heat transfer, structural deformation and fission gas release due to multiple complex phenomena with the use of a custom transient finite volume solver. Thermochemistry calculations allow for the capability of predicting the products of uranium dioxide fuel, water and numerous fission products. This numerical model will provide an ideal platform for further considerations of CANDU fuel.

5. Acknowledgements

The authors would like to acknowledge the outstanding work done by Dan Morgan for the development of a thermomechanical model of CANDU fuel in his master's thesis. The fuel performance model discussed in this paper was based on his work. The current work was sponsored by the CANDU Owners Group (COG) and the Natural Sciences and Engineering Research Council (NSERC).

6. References

[1] Morgan, D., "A Thermomechanical model of CANDU fuel", MSc.Eng. Thesis, Royal Military College of Canada, 2007.

[2] Lassmann K., "The structure of fuel element codes," *Nuclear Engineering and Design*, 57, 1980, pp. 17-39.

[3] Fink J.K., "Thermophysical properties of uranium dioxide," *Journal of Nuclear Materials*, 279, 2000, pp. 1-18.

[4] Hagerman D.T., ed., MATPRO—A Library of Materials Properties for Light-Water-Reactor Accident Analysis, SCDAP/RELAP5/Mod 3.1 Code manual, NUREG/CR-6150 Vol. 4, 1997.

[5] Assmann H., Stehle H., "Thermal and in-reactor densification of UO_2: Mechanisms and experimental results," *Nuclear Engineering and Design*, 45, 1978, pp. 59-67.

[6] Hastings I.J., P.J. Fehrenbach, R.R. Hosbons, "Densification in Irradiated UO_2 Fuel," *Journal of the American Ceramics Society*, 67, 1984, C-24.

[7] Olander D.R., "Fundamental Aspects of Nuclear Reactor Fuel Elements," TID-26711-p1, US. Department of Energy, 1976.

[8] Sills H.E., Holt R.A., "Predicting High-Temperature Transient Deformation from Microstructural Models," Zirconium in the Nuclear Industry (Fourth Conference), ASTM STP 681, *American Society for Testing and Materials*, 1979, pp. 325-341.

[9] Booth A.H., "A method of calculating fission gas diffusion from UO_2 fuel and its application to the X-2-f loop test," AECL 496, 1957.

[10] Hering W., "The KWU fission gas release model for LWR fuel rods," *Journal of Nuclear Materials*, 114, 1983, pp. 41-49.

[11] Turnbull J., Friskney C.A., Findlay J.R., Johnson F.A., Walter J.J., "The diffusion coefficients of gaseous and volatile species during the irradiation of uranium dioxide," *Journal of Nuclear Materials*, 107, 1982, pp. 168-184.

[12] Turnbull J., White R., Wise C., "The diffusion coefficient for fission gas atoms in UO_2," IAEA-TC-659/3.5, 1987, 174-181.

[13] R.J. White, M.O. Tucker, "A new fission-gas release model." *Journal of Nuclear Materials*, 118, 1983, pp. 1-38.

[14] Ainscough J.B., Oldfield B.W., Ware J.O., "Isothermal grain growth kinetics in sintered UO_2 pellets," *Journal of Nuclear Materials*, 49, 1973, pp. 117-128.

[15] Khoruzhii O.V., Kourtchatov S.Yu., Likhanskii V.V., "New model of equiaxed grain growth in irradiated UO_2," *Journal of Nuclear Materials*, 265, 1999, pp. 112-116.

[16] Eriksson G., Thompson W.T., "A procedure to estimate equilibrium concentrations in multicomponent systems and related applications," *CALPHAD*, Vol. 13, Iss. 4, 1989, pp. 389-400.

[17] Thompson W.T., Lewis B.J., Corcoran E.C., Kaye M.H., White S.J., Akbari F., He Z., Verrall R., Higgs J.D., Thompson D.M., Besmann T.M., Vogel S.C., "Thermodynamic treatment of uranium dioxide based nuclear fuel", *International Journal of Materials Reasearch*, 98, 2007, pp. 1004-1011.

[18] Higgs J., "Modelling oxidation behaviour in operating defective nuclear reactor fuel elements," PhD. Thesis, Royal Military College, 2006.

[19] Higgs J.D., Lewis B.J., Thompson W.T., and He Z., "A Conceptual Model for the Fuel Oxidation of Defective Fuel", *9th International Conference on CANDU Fuel: Belleville ON*, 2005.

[20] Akbari F., Welland M.J., Lewis B.J., and Thompson W.T., "Considerations in Modelling the Melting of Fuel Containing Fission Products and Solute Oxides". *9th International Conference on CANDU Fuel: Belleville ON*, 2005.

[21] Lewis B.J., Thompson W.T., Higgs J.D., Akbari F., Kaye M.H., Thurgood C., Serdula J., and Morrison C., "Modelling of Fuel Oxidation Behaviour in Defective Fuel", COG Report - COG-04-2043, 2005.

[22] Higgs J.D., Lewis B.J., Thompson W.T., "A Conceptual Model for the Fuel Oxidation of Defective Fuel", *Journal of Nuclear Materials*. 366, 2007 pp. 99-128.

[23] Lindemer T.B. and Besmann T.M., "Chemical Thermodynamic Representation of $UO_{2\pm x}$," *Journal of Nuclear Materials*, 130, 1985, pp. 473-488.

7. Nomenclature

SYMBOL	DESCRIPTION [UNITS]
ρ	Density [kg m^{-3}]
C_p	Constant pressure specific heat capacity [J mol^{-1} K^{-1}]
T	Temperature [K]
t	Time [s]
k , k_f	Thermal conductivity of fuel and fluid in gap [W m^{-1} K^{-1}]
P_{lin}	Linear power rating [W m^{-1}]
κ	Inverse neutron diffusion length [m^{-1}]
a_{pel} , r	Initial pellet radius and instantaneous raidus [m]
I_0 , I_1	Zeroth and first order modified Bessel function of the 1st kind
D	Dimensionless fraction of theoretical density [kg m^{-3}]
T', T''	Empirically derived temperature corrections [K]
C_v	Phonon contribution to the specific heat [J kg^{-1} K^{-1}]
A	Point defect contribution to the phonon mean path [m s kg^{-1} K^{-1}]
B	Phonon-phonon scattering contribution [m s kg^{-1} K^{-1}]
ε_{th}	Thermal strain [#]
$\frac{L(T)}{L_{273}}$	Linear thermal expansion of fuel [#]
F	Fraction of porosity removed due to densification
Bu	Burnup of fuel [MWh kg^{-1}]
$\frac{\partial(\Delta V_{GFP}/V)}{\partial t}$	Rate of volumetric deformation of fuel due to gaseous fission products [s^{-1}]
$\frac{\Delta V_{SFP}}{V}$	Volumetric deformation of fuel due to solid fission products [#]
h_T	Heat transfer coefficient through gap [W m^{-2} K^{-1}]
k_{hm}	Harmonic mean conductivity[W m^{-1} K^{-1}]

P_{int}	Interfacial pressure [MPa]
a_0	Constant [$m^{0.5}$ $MPa^{-0.5}$]
R , R_1 , R_2	Root mean square surface roughness [m]
H	Meyer hardness [MPa]
C	Constant [#]
t_g	Hot gap width [m]
g_{jump}	Temperature jump distance [m]
σ	Stefan-Boltzmann constant [W m^{-2} K^{-4}]
ε_m	Emissivity [#]
T_f T_S	Fuel and sheath temperatures [K]
$\dot{\beta}$	Rate of fissioning [fissions m^{-3} s^{-1}]
σ_1 , σ	Transition and internal stresses [MPa]
R	Universal gas constant [J mol^{-1} K^{-1}]
Gn	Grain size [μm]
t	Time [s]
C_d	Constant [s^{-1} $MPa^{-5.3}$]
σ_*	Effective stress acting on sheath [MPa]
F_{gb}	Constant [μm^2]
G	Shear modulus of sheath [MPa]
d	Effective grain size [μm]
$\dot{f}_a$	Volume fraction of crystals in alpha phase
ψ	Total concentration of fission gas atoms [atoms μm^{-3}]
D_{eff}	Effective diffusive term of fission gas atoms [μm^2 s^{-1}]
S_ψ	Generation of fission gas atoms with a grain [atoms μm^{-3} s^{-1}]
J_{Booth}	Flux of fission gas atoms to grain surface [atoms $grain^{-1}$ s^{-1}]
N_s	Saturation concentration of atoms on grain surface [atoms μm^{-2}]
r_f	Curvature radius of grain boundary bubbles [m]
$f(\theta)$	Correction for lenticular bubbles [#]
f_B	Fraction of the grain occupied by intergranular bubbles [#]
θ	Half angle between surfaces of bubbles [º]
P_{ext}	External pressure to bubble [MPa]
γ	Surface energy of bubbles [J m^{-2}]
$Gn_{\max}$	Maximum grain size [μm]
Gn_{ir}	Empirical correction for irradiation [μm]