A Model of Fission Gas Release and Swelling in UO_2 for Engineering Fuel Analysis

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Introduction

- We present an engineering model of fission gas behavior that is used to compute FGR and gaseous swelling in multiple fuel performance codes
- As opposed to empirical models often used in engineering codes, the present model is physically based. Advantages include flexibility and potential for multiscale coupling
- Work comprises development, validation, uncertainty and sensitivity analysis
- Originally developed at Politecnico di Milano and JRC-Karlsruhe[1]. Variants are used in the fuel performance codes BISON (INL)[2] and TRANSURANUS (JRC)[3]. It has also been implemented in FRAPCON and FINIX (at VTT)[4,5]

[1] G. Pastore, L. Luzzi, V. Di Marcello, P. Van Uffelen, Nucl. Eng. Des. 256, 75-86, 2013

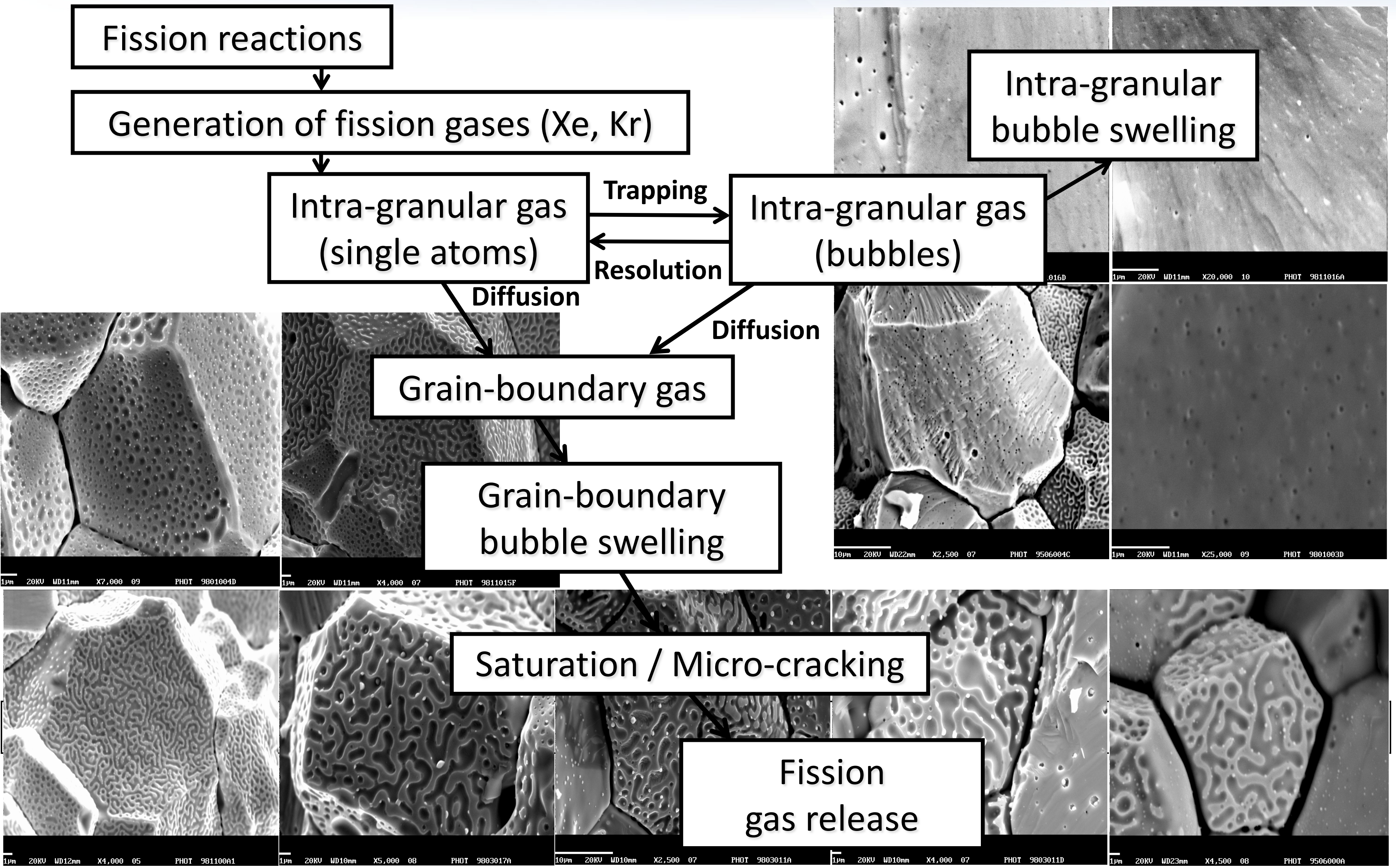
[2] G. Pastore, L.P. Swiler, J.D. Hales, S.R. Novascone, D.M. Perez, B.W. Spencer, L. Luzzi, P. Van Uffelen, R.L. Williamson, J. Nucl. Mater. 456, 398-408, 2015

[3] K. Lassmann, A. Schubert, P. Van Uffelen, C. Györi, J. van de Laar, TRANSURANUS Handbook, ©1975-2014, Institute for Transuranium Elements, Karlsruhe, Germany, 2014.

[4] T. Ikonen, VTT's modifications to the FRAPCON-4.0 code, Tech. Rep. VTT-R-00119-17, Espoo, Finland, 2017

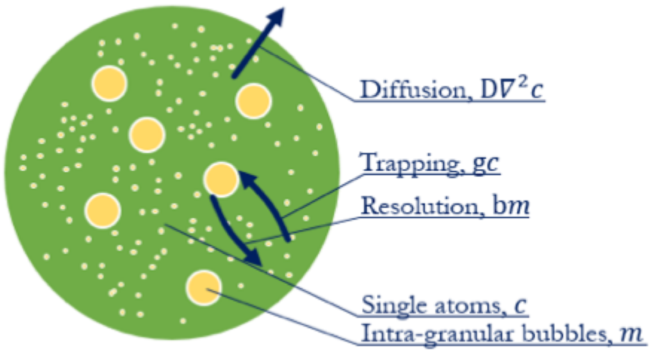
[5] H. Loukusa, J. Peltonen, V. Valtavirta, FINIX - Fuel behavior model and interface for multiphysics applications, Code documentation for version 1.19.1, VTT-R-00052-19, VTT Technical Research Centre of Finland, 2019

Stages of fission gas behavior



Modeling: Intra-granular behavior

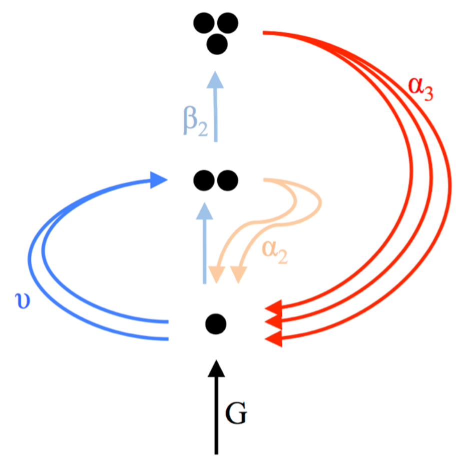
- Compute bubble evolution, swelling and gas diffusion to grain boundaries
- Def. the number density of bubbles, *N*, and the total gas concentration in bubbles, *m*



$$\frac{\partial N}{\partial t} = +\nu - \alpha_{\bar{n}} N$$

$$\frac{\partial m}{\partial t} = +2\nu + \beta_{\bar{n}} N - \alpha_{\bar{n}} m$$

$$\frac{\partial c_1}{\partial t} = +yF + D\nabla^2 c_1 - 2\nu - \beta_{\bar{n}} N + \alpha_{\bar{n}} m$$



$$N = \sum_{n=2}^{\infty} c_n$$

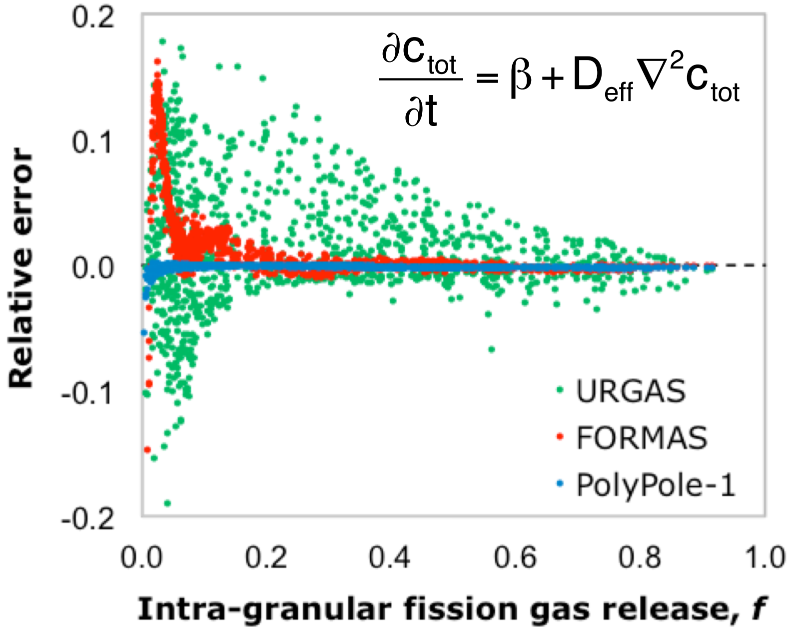
$$m = \sum_{n=2}^{\infty} n c_n$$

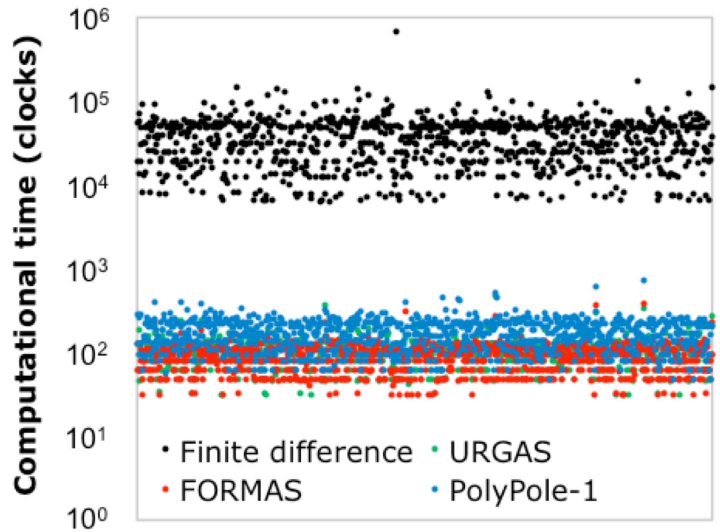
$$\bar{n} = m/N$$

$$R_{\bar{n}} = B\bar{n}^{1/3}$$

D. Pizzocri, G. Pastore, T. Barani, A. Magni, L. Luzzi, P. Van Uffelen, S.A. Pitts, A. Alfonsi, J.D. Hales, A model describing intra-granular fission gas behaviour in oxide fuel for advanced engineering tools, J. Nucl. Mater. 502, 323-330, 2018

Intra-granular diffusion algorithms

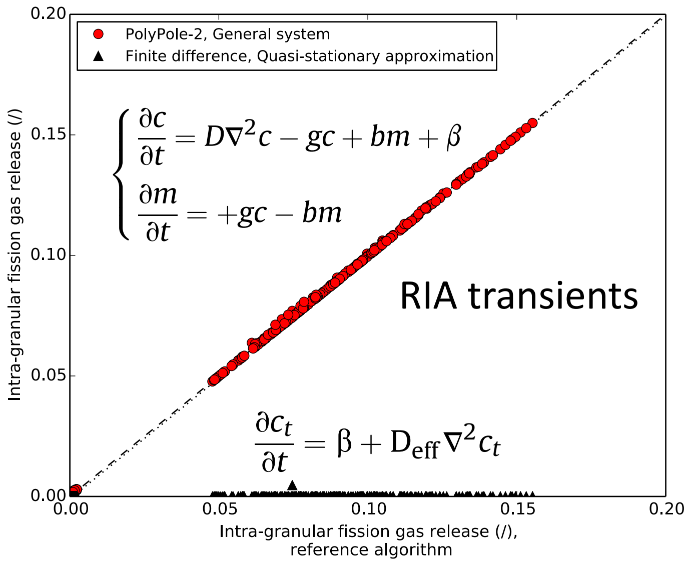


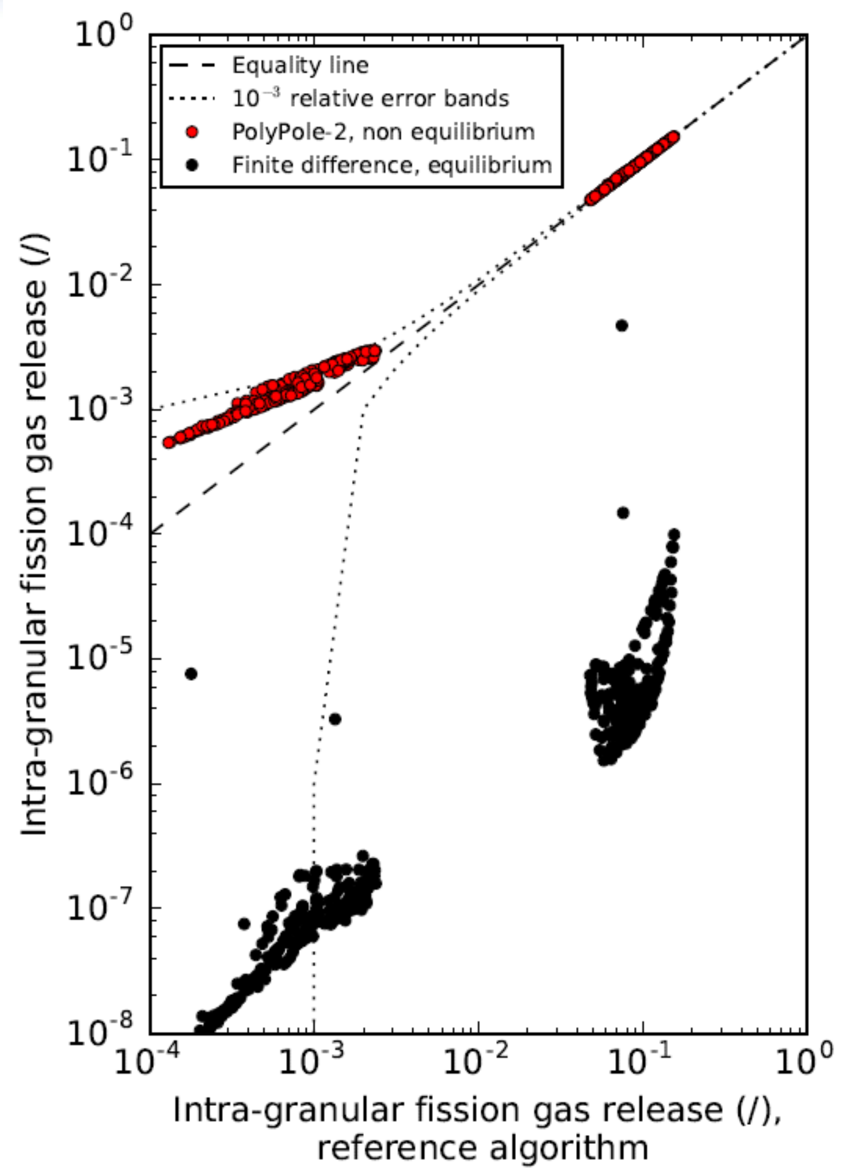


The PolyPole-1 algorithm for the single diffusion equation provides a more accurate solution than other algorithms used in fuel performance codes and is as computationally efficient

D. Pizzocri, C. Rabiti, L. Luzzi, T. Barani, P. Van Uffelen, G. Pastore, PolyPole-1: An accurate numerical algorithm for intra-granular fission gas release, J. Nucl. Mater. 478, 333-342, 2016

Intra-granular diffusion algorithms





The PolyPole-2 algorithm provides an efficient solution of the more general PDE system and overcomes the concept of an effective diffusion coefficient

G. Pastore, D. Pizzocri, C. Rabiti, T. Barani, P. Van Uffelen, L. Luzzi, An effective numerical algorithm for intra-granular fission gas release during non-equilibrium trapping and resolution, J. Nucl. Mater. 509, 687-699, 2018

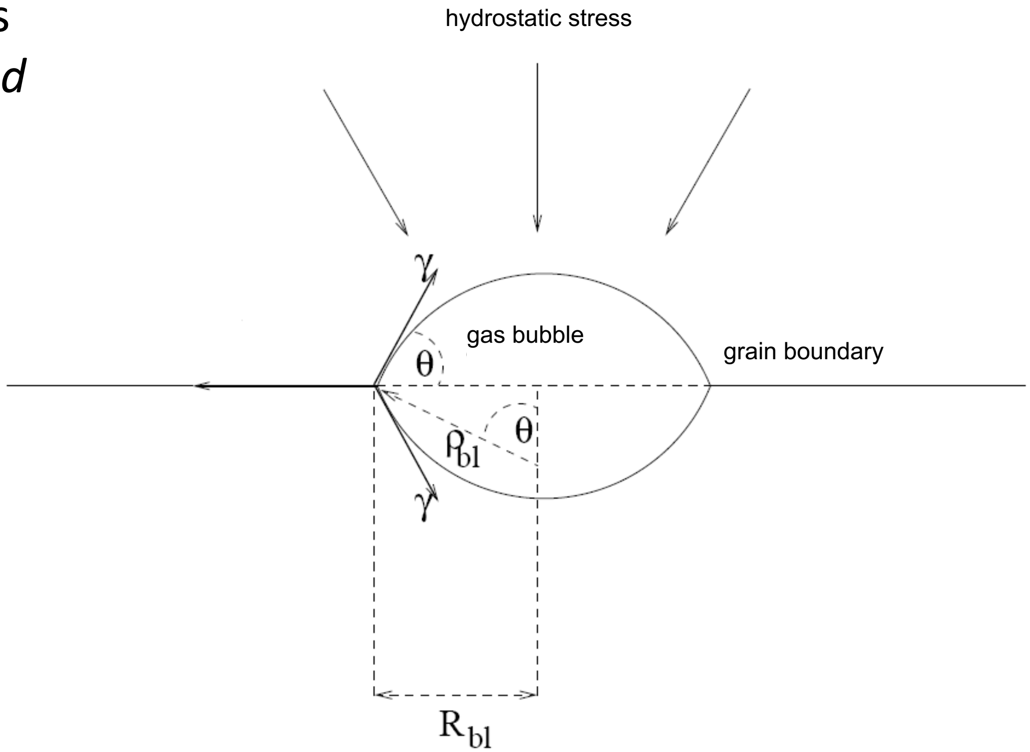
Modeling: Grain-boundary behavior

- Bubble growth with inflow of gas atoms and vacancies (*Speight and Beere, Met. Sci. 9, 1975*)

$$\frac{dn_v}{dt} = \frac{2\pi D_v \delta_{gb}}{kTS}\left(p - p_{eq}\right)$$

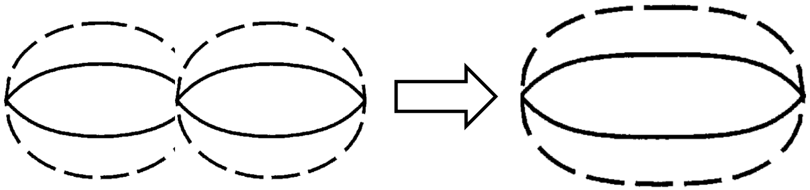
Bubble volume:

$$\frac{dV_b}{dt} = \frac{dn_v}{dt}\Omega + \frac{dn_g}{dt}\omega$$



- Bubble coalescence with geometrical reasoning *(White, JNM 325, 61-77, 2004)*

$$\frac{dN_b}{dt} = -2N_b^2\frac{dA_b}{dt}$$



Modeling: Grain-boundary swelling

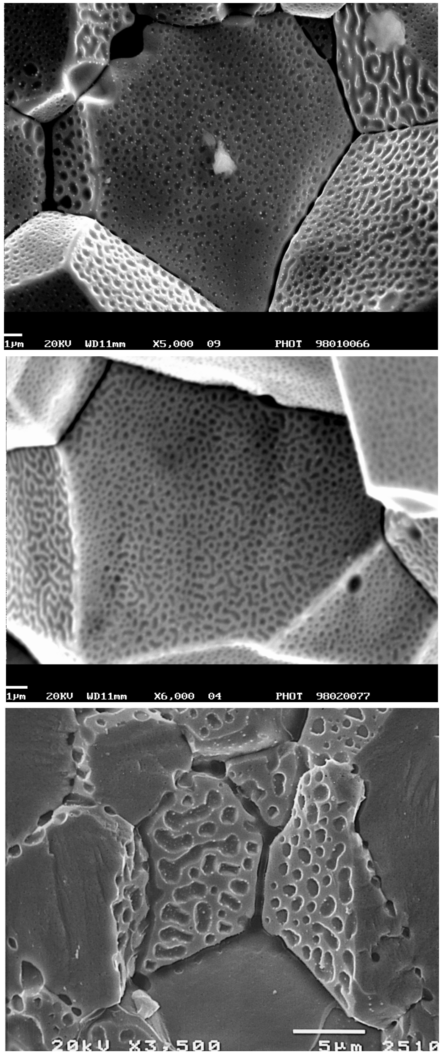
- Fractional volume grain-boundary bubble swelling:

Bubble number per unit surface

Bubble volume

$$\frac{\Delta V}{V} = \frac{1}{2}\frac{N_b}{\frac{1}{3} r_{gr}} V_b$$

Grain volume/surface

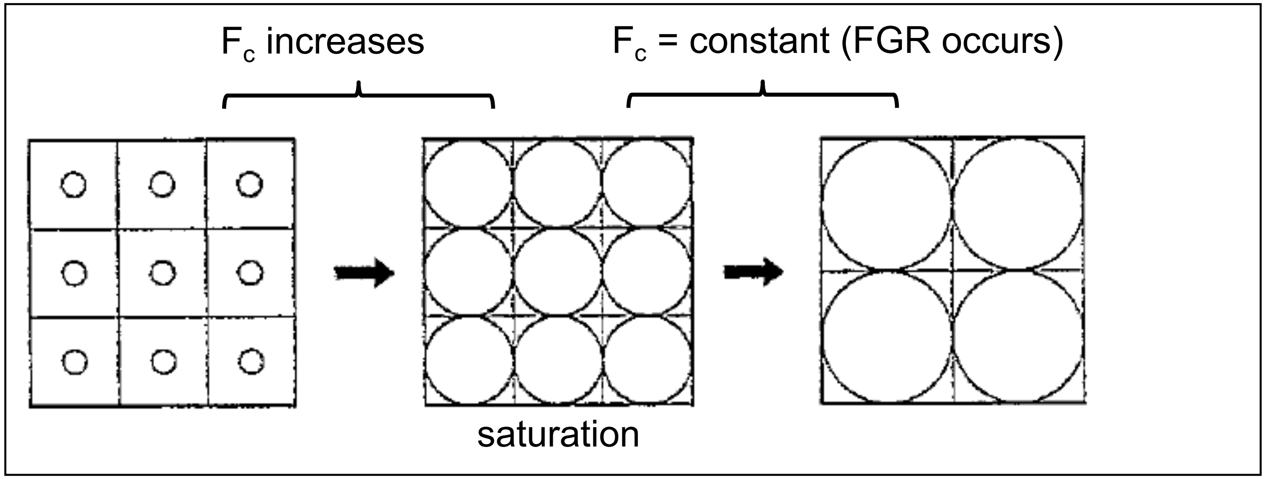


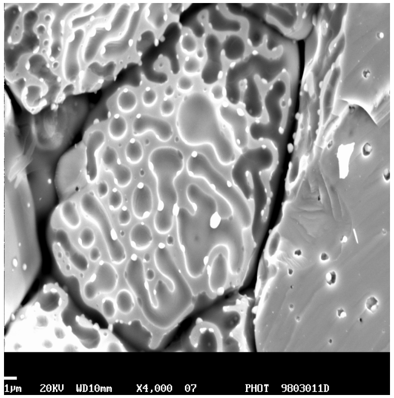
Modeling: Fission gas release

- Fission gas release (FGR) results from the limited capacity of grain boundaries to store gas. Modeled with

Fractional grain-boundary bubble coverage

$$\frac{dF_c}{dt} = \frac{d\left(N_b A_b\right)}{dt} = 0 \qquad \text{if } F_c = F_{c,sat}$$

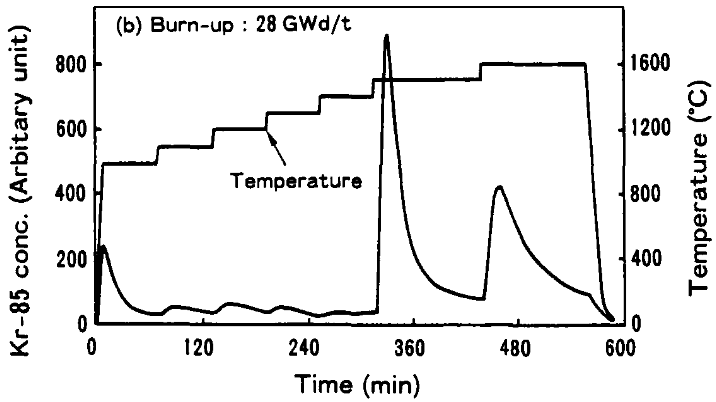




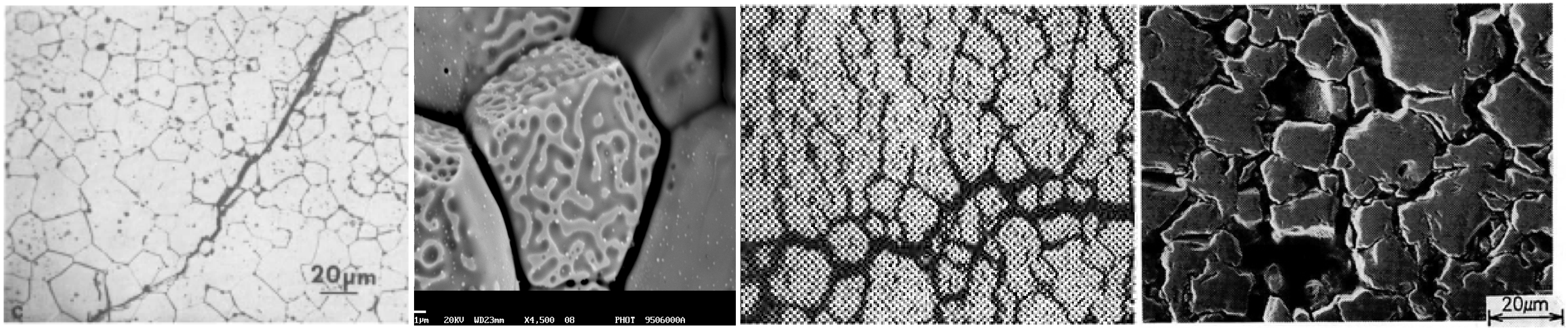
G. Pastore, L. Luzzi, V. Di Marcello, P. Van Uffelen, Physics-based modelling of fission gas swelling and release in UO_2 applied to integral fuel rod analysis, Nucl. Eng. Des. 256, 75-86, 2013

Transient fission gas release model

- Experiments show rapid FGR during transients (burst release) that cannot be explained as purely diffusion-controlled
- Theory: Grain-boundary separations due to micro-cracking causing rapid transient release as gas is vented from open grain boundaries



FGR rate during UO_2 annealing experiment
Une and Kashibe, J. Nucl. Sci. Technol. 27, 1990



Micrographs of transient-tested UO_2 showing grain boundary separations
From left to right: I.J. Hastings et al., J. Nucl. Mater. 139, 531-543, 1986; R.J. White et al., R&T/NG/EXT/REP/0206/02, 2006;
CABRI REP-Na 5 RIA test, Lemoine et al., Proc. of the 10th Int. Symp. on Thermodynamics of Nuclear Materials, Halifax, Canada, 2000;
NSRR JM-4 RIA test, T. Nakamura et al., J. Nucl. Sci. Technol. 33, 1996.

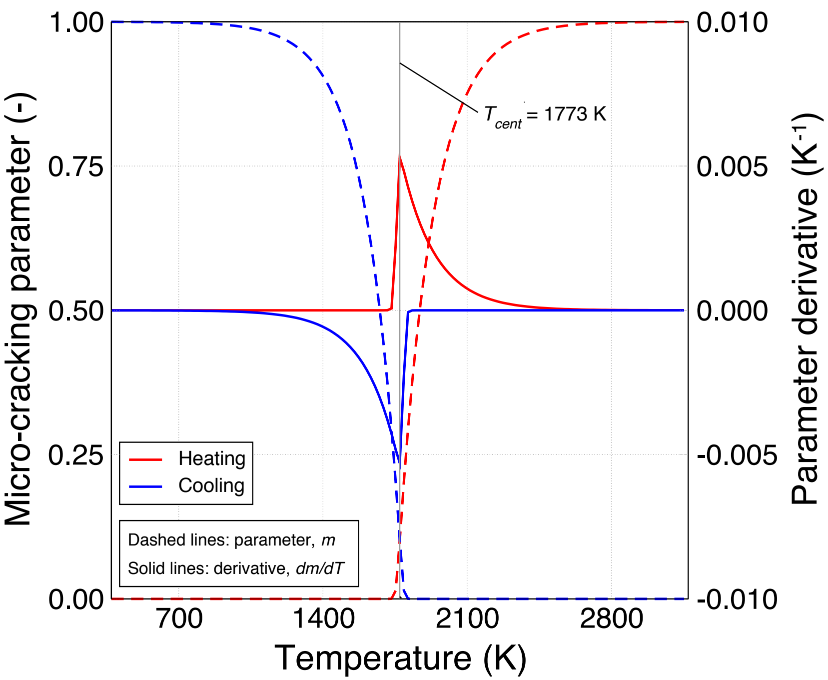
Transient fission gas release model

- Considering a contribution due to micro-cracking to the evolution of the grain-boundary bubble coverage parameters

$$\begin{cases} \dfrac{dF_c}{dt} = \left[\dfrac{dF_c}{dt}\right]_d + F_c\left[\dfrac{df}{dt}\right]_c \\ \dfrac{dF_{c,sat}}{dt} = F_{c,sat}\left(\left[\dfrac{df}{dt}\right]_c + \left[\dfrac{df}{dt}\right]_h\right) \end{cases}$$

- Modeling micro-cracking as a dependent on variations in local fuel temperature

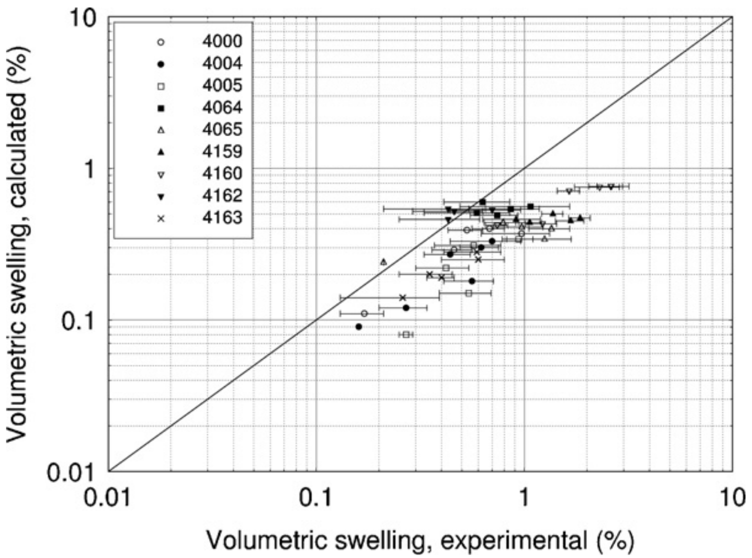
$$\left[\frac{df}{dt}\right]_c = -\frac{dm}{dt} f = -\frac{dm}{dT}\frac{dT}{dt} f$$



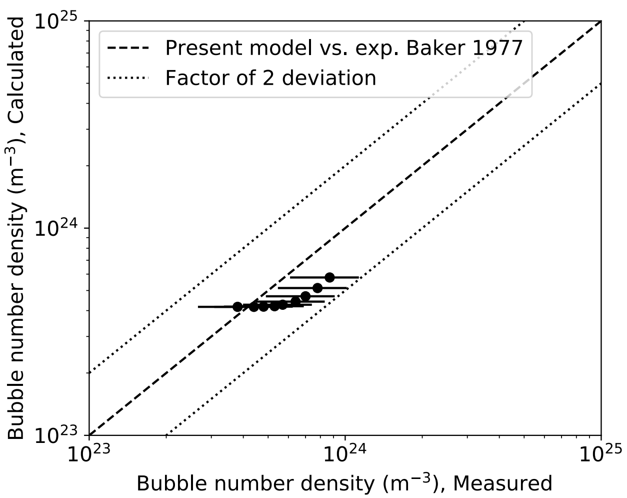
$$m(T) = 1 - \left[1 + Q\exp\left(s\frac{T - T_{cent}}{T_{span}}\right)\right]^{-\frac{1}{Q}}$$

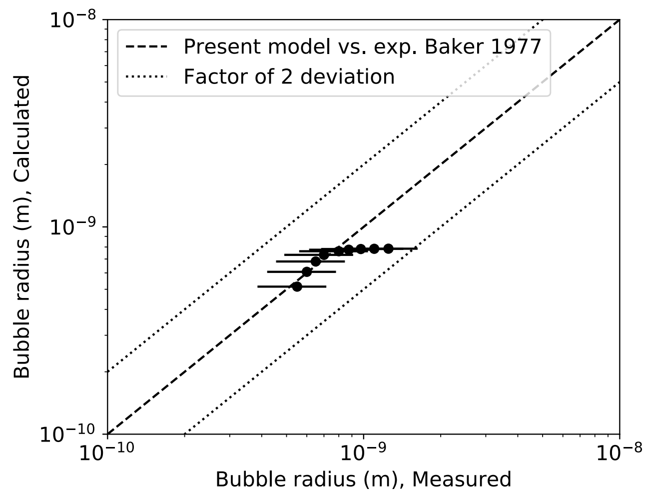
G. Pastore, D. Pizzocri, J.D. Hales, S.R. Novascone, D.M. Perez, B.W. Spencer, R.L. Williamson, P. Van Uffelen, L. Luzzi, In: Proc. of EHPG 2014, Røros, Norway, September 7-12, 2014.

Validation: Local comparisons



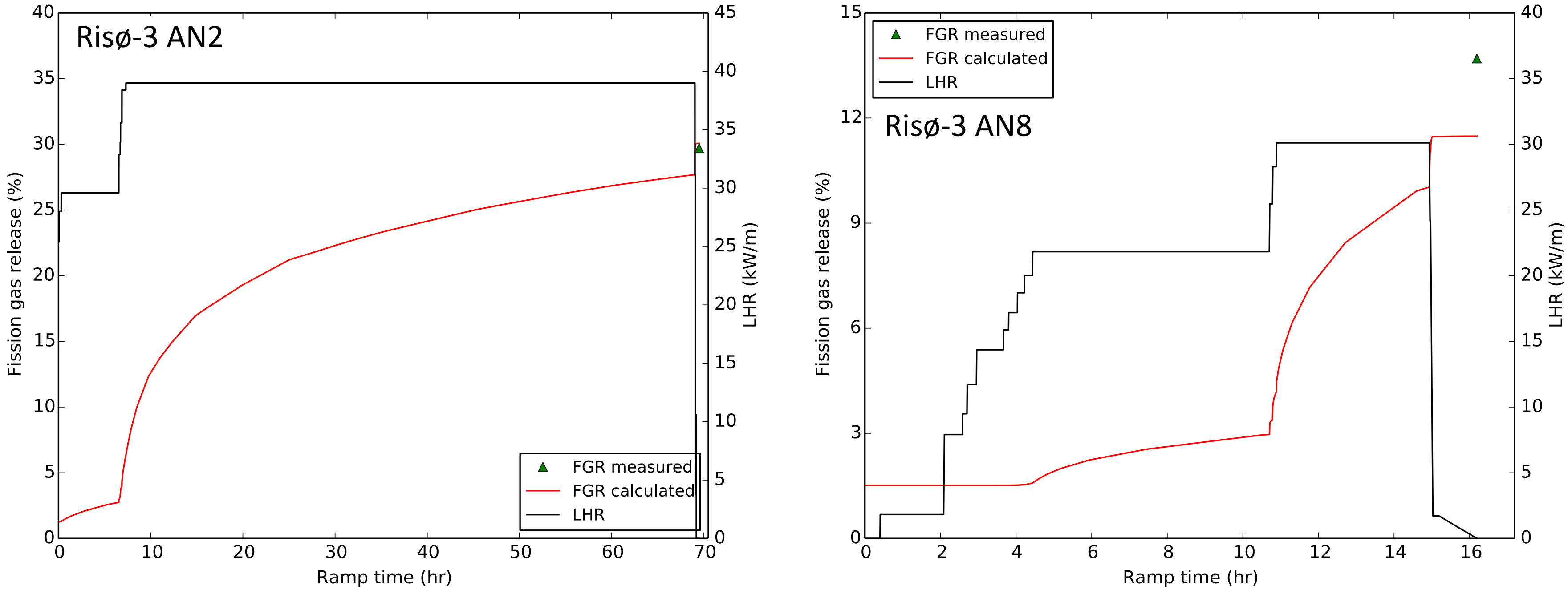
Comparisons of local grain-boundary swelling in power-ramped UO_2 samples (G. Pastore et al., NED 256, 2013). Experimental data from White et al., R&T/NG/EXT/REP/0206/02, 2006.





Comparisons of local intra-granular bubble number density and size in base-irradiated UO_2 (US DOE SciDAC project on Simulation of Fission Gas, 2018). Experimental data from Baker, JNM 66, 1977.

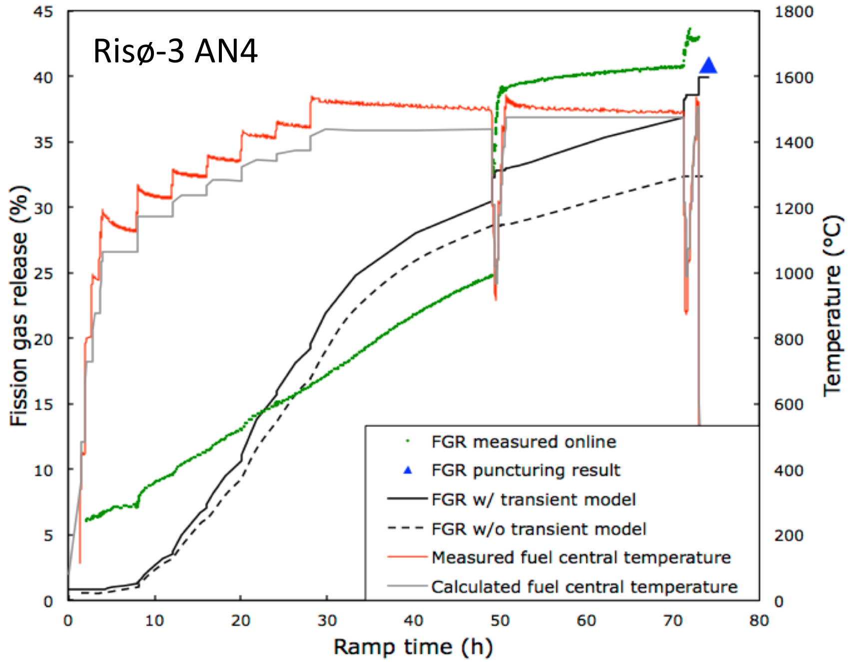
Validation: Integral fuel rod FGR



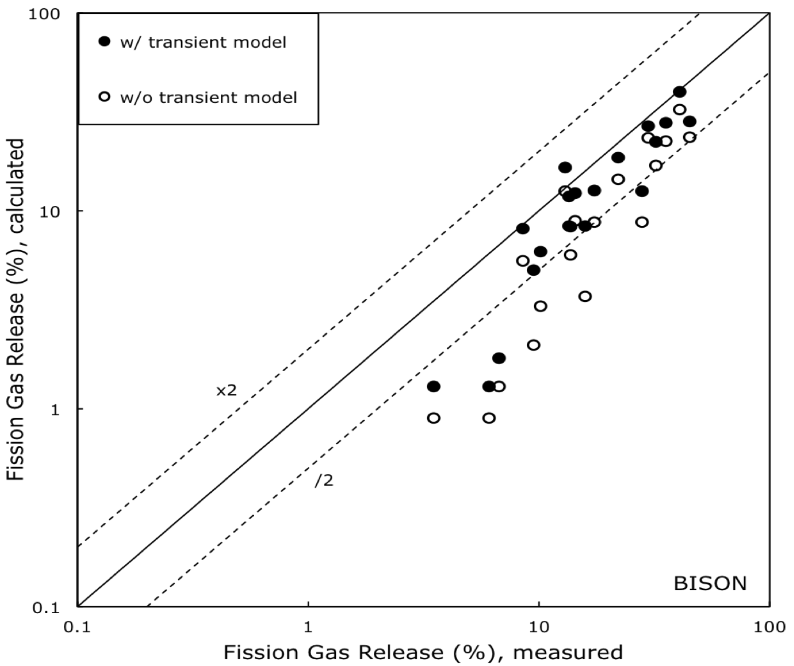
Integral FGR and rod average linear heat rate vs time LWR fuel rod power ramp experiments. FGR simulation results from the BISON code and PIE data are illustrated.

G. Pastore, T. Barani, D. Pizzocri, A. Magni, L. Luzzi, Modeling fission gas release and bubble evolution in UO_2 for engineering fuel rod analysis, in: Proc. of Top Fuel 2018, Paper A0241, Prague, Czech Republic, 30 September – 4 October 2018.

Validation: Integral fuel rod FGR



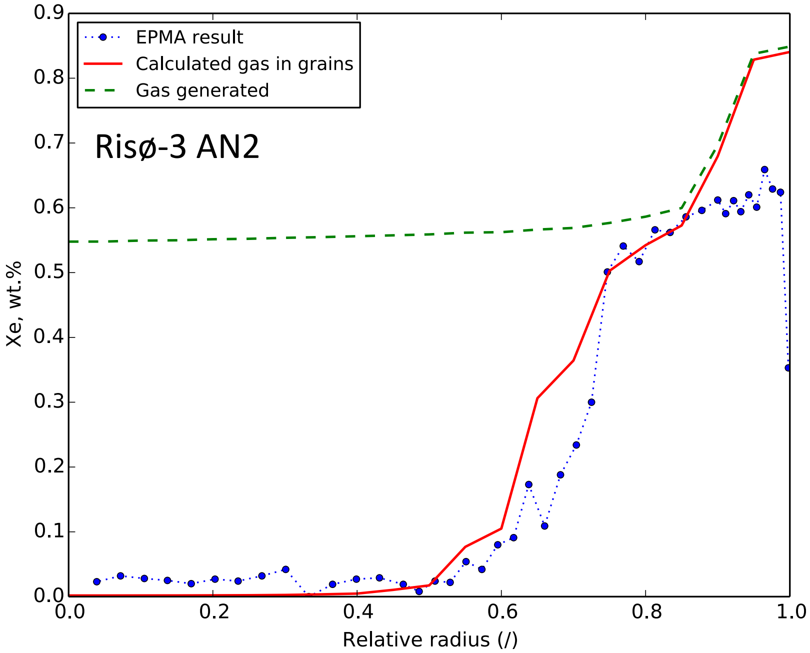
Integral FGR vs time during LWR fuel rod power ramp experiment (BISON code)

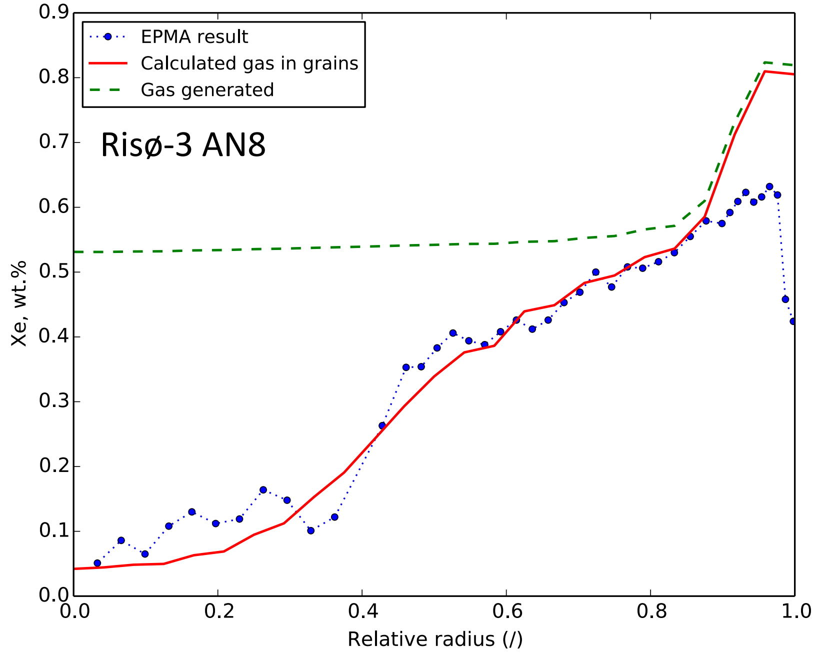


Integral FGR at EOL for 19 LWR fuel rod power ramp experiments (BISON code)

T. Barani, E. Bruschi, D. Pizzocri, G. Pastore, P. Van Uffelen, R.L. Williamson, L. Luzzi, Analysis of transient fission gas behaviour in oxide fuel using BISON and TRANSURANUS, J. Nucl. Mater. 486, 96-110, 2017.

Validation: Fission gas radial distributions

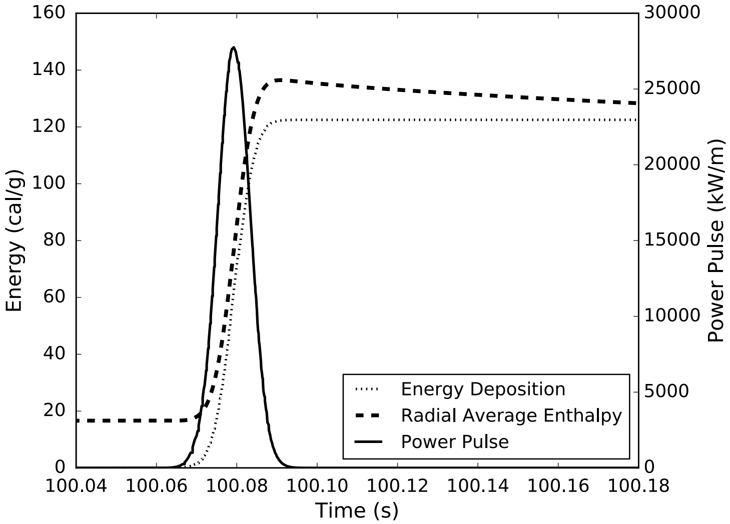


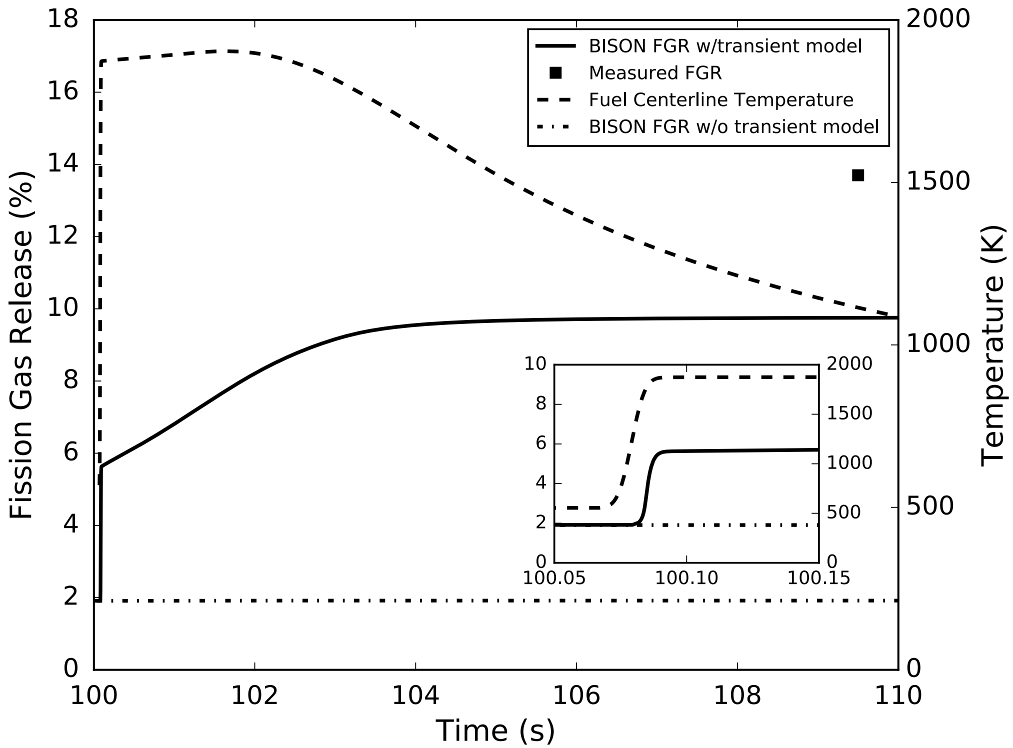


Radial profiles of Xe concentration after ramp tests calculated with BISON and PIE data

T. Barani, A. Magni, D. Pizzocri, L. Cognini, P. Van Uffelen, L. Luzzi, G. Pastore, Modeling and assessment of intra-granular bubble evolution and coarsening in uranium dioxide, In: Nuclear Materials Conference – NuMat 2018, Seattle, USA, October 15-18, 2018

RIA integral simulations

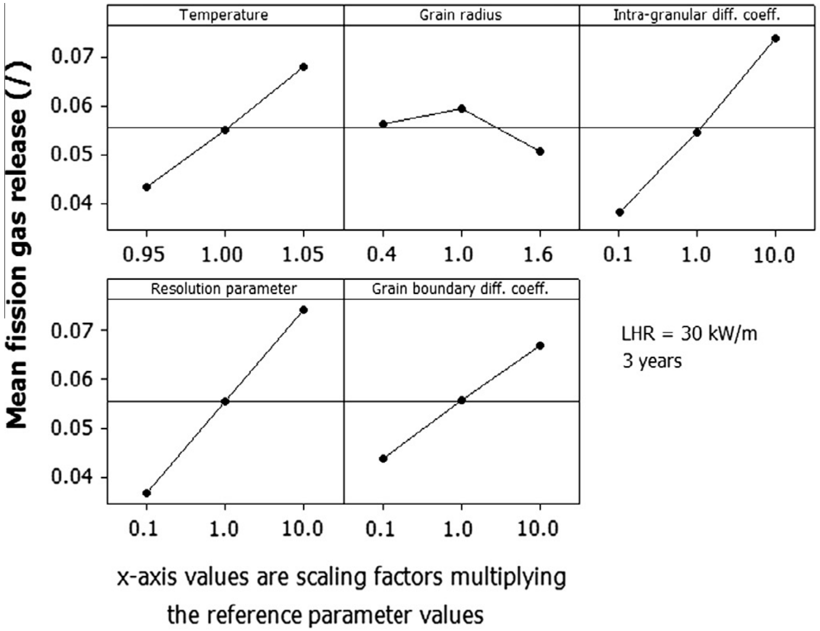


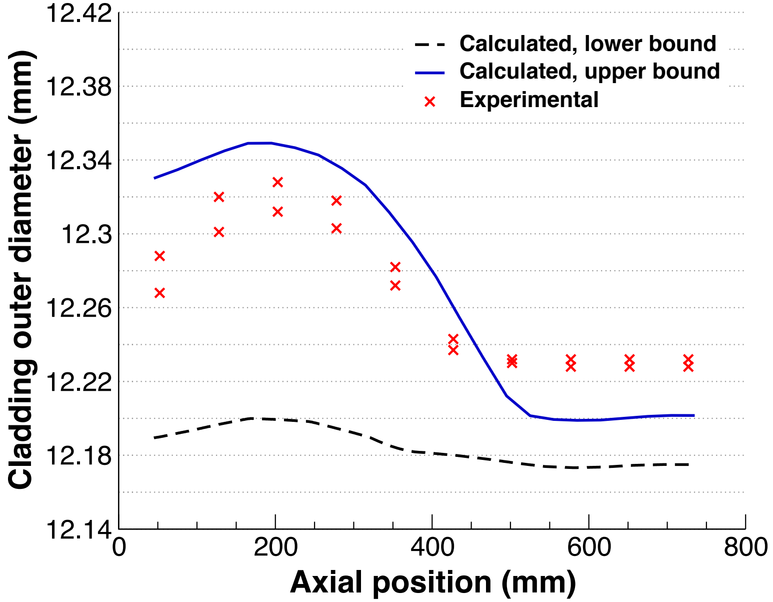


Power pulse (left) and FGR with fuel centerline temperature (right) calculated with the BISON code for the CABRI REP Na-3 RIA test. The inset shows a shorter time around the power pulse.

G. Pastore, C.P. Folsom, R.L. Williamson, J.D. Hales, L. Luzzi, D. Pizzocri, T. Barani, Modelling Fission Gas Behaviour with the BISON Fuel Performance Code, Proc. of the Enlarged Halden Programme Group Meeting – EHPG 2017, Lillehammer, Norway, September 24-29, 2017.

Uncertainty and sensitivity analysis





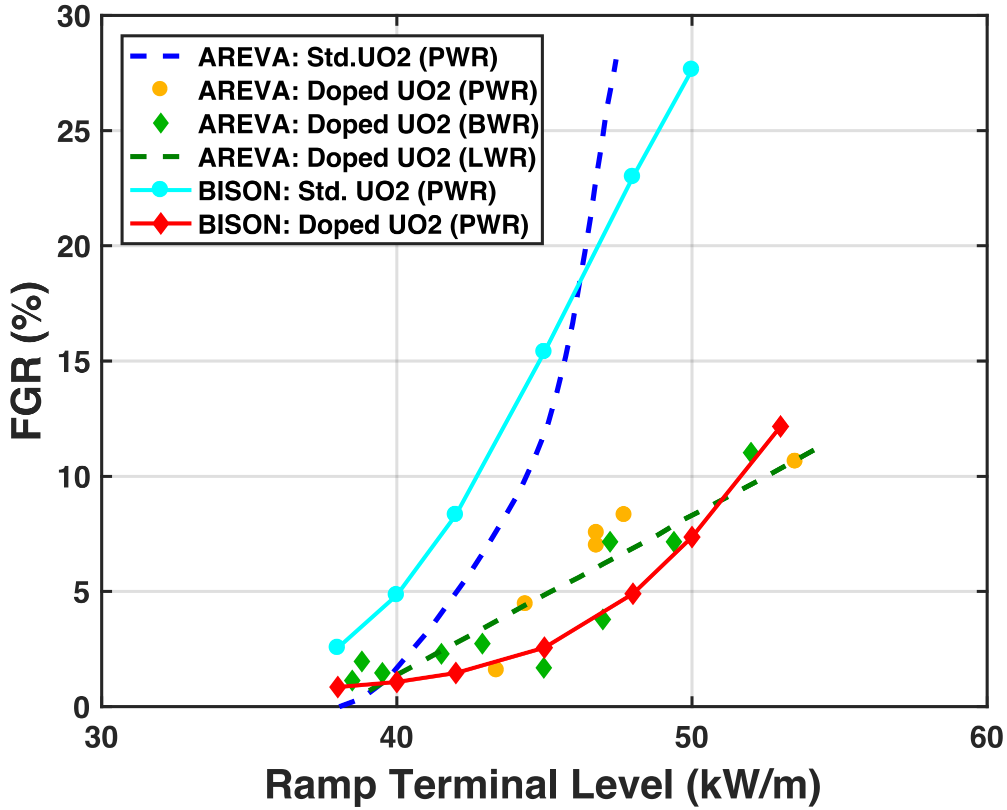
Main effects of five uncertain model parameters on calculated FGR for an irradiation time of 3 years and an LHR of 30 kW/m

Calculated cladding outer diameter profile for the Risø-3 GE7 experiment with uncertainty range from fuel gaseous swelling

G. Pastore, L.P. Swiler, J.D. Hales, S.R. Novascone, D.M. Perez, B.W. Spencer, L. Luzzi, P. Van Uffelen, R.L. Williamson, Uncertainty and sensitivity analysis of fission gas behavior in engineering-scale fuel modeling, J. Nucl. Mater. 456, 398-408, 2015.

Simulation of Cr_2O_3-doped fuel ramp tests

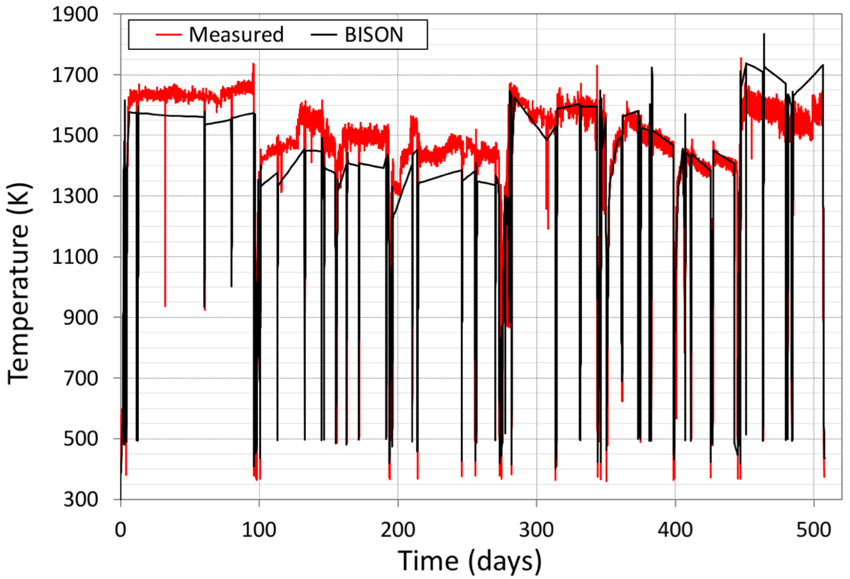
FGR for doped vs. std. UO_2

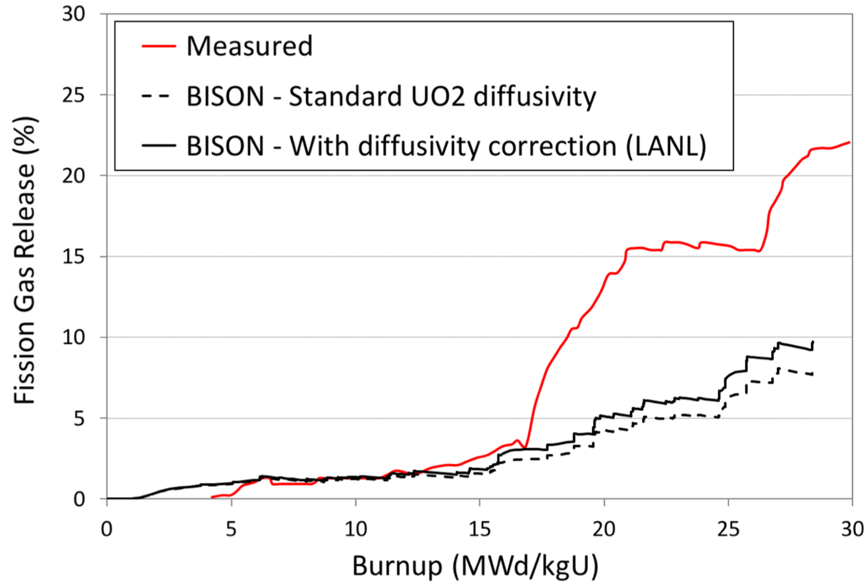


- BISON simulations of power ramp tests in the OSIRIS and Halden reactors on pre-irradiated fuel rods (various burnups) from AREVA
- Grain diameter:
  - 15.6 mm for standard UO_2
  - 56 mm for Cr-doped UO_2

Y. Che, G. Pastore, J.D. Hales, K. Shirvan, Modeling of Cr_2O_3-doped UO_2 as a near-term accident tolerant fuel for LWRs using the BISON code, Nuclear Engineering and Design 337, 271-278, 2018.

Multiscale coupling for Cr_2O_3-doped UO_2



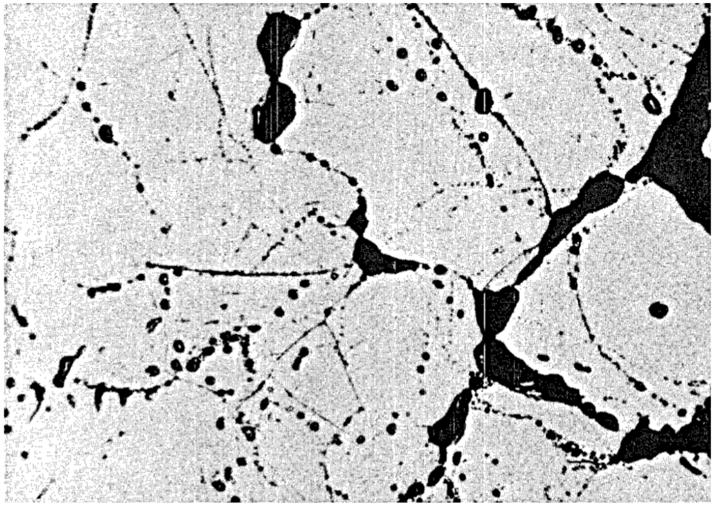


- BISON simulation of Cr_2O_3-doped UO_2 Halden test IFA-677 rod 1
- Uses fission gas diffusivity correction from point defect model developed at Los Alamos National Laboratory (*M.W.D. Cooper, D.A. Andersson, C.R. Stanek*):

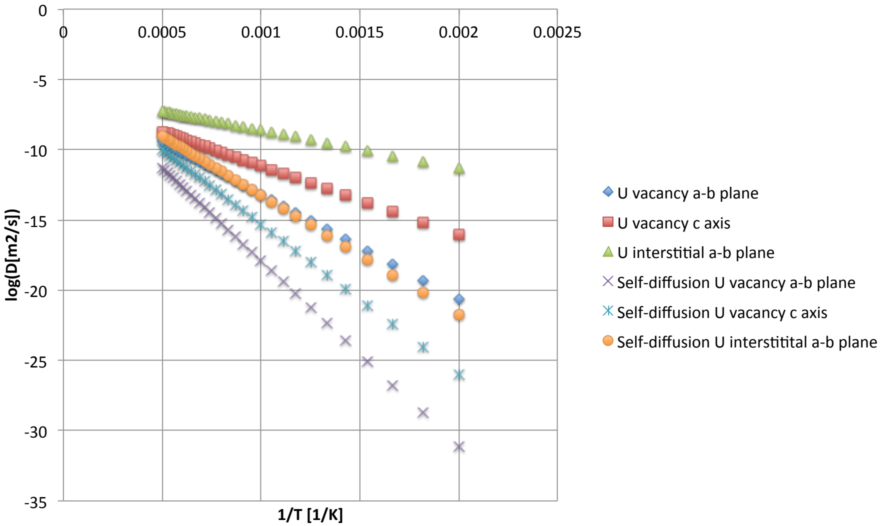
$$D^{doped} = \exp\left(-\frac{\Delta H_1}{k_B}\left[\frac{1}{T} - \frac{1}{T_1}\right]\right) D_1^{undoped} + \exp\left(-\frac{\Delta H_2}{k_B}\left[\frac{1}{T} - \frac{1}{T_2}\right]\right) D_2^{undoped} + D_3^{undoped}$$

Multiscale model for U_3Si_2

- Using a similar concept, a model has been developed for FGB in U_3Si_2
- Informed by atomistic calculations to fill the experimental data gap



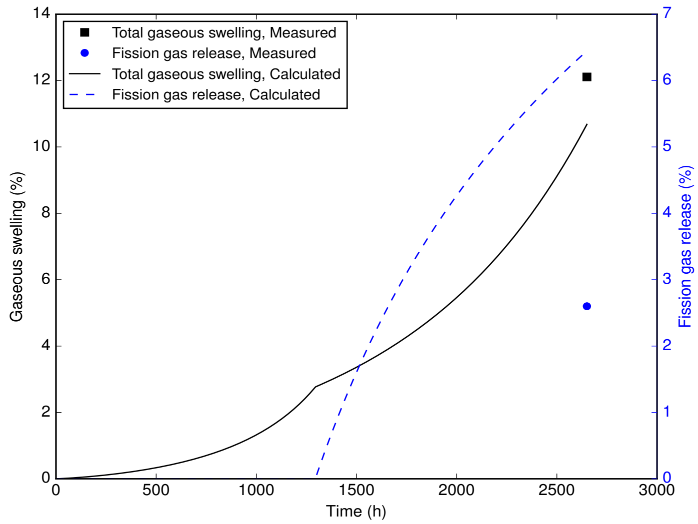
Micrograph of U_3Si_2 irradiated at ~950 K and ~6 GWd/tU (Shimizu, NAA-SR-1062, 1965). The crystalline structure as well as intra-granular and grain-boundary fission gas bubbles are evident



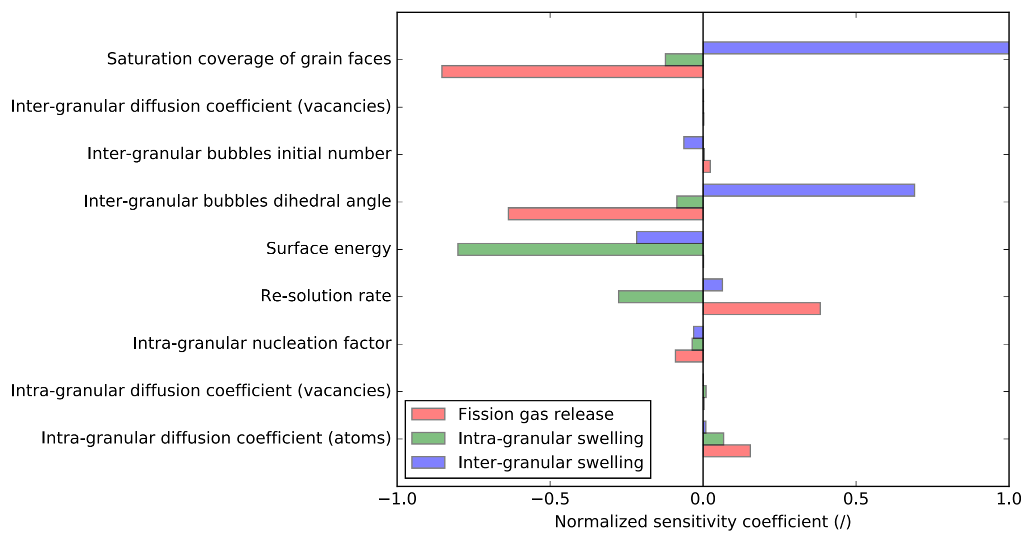
Diffusivities in U_3Si_2 from Density Functional Theory calculations (D. Andersson, Tech. Rep. Los Alamos National Laboratory, 2016)

Multiscale model for U_3Si_2

- Initial stand-alone and BISON applications of the model
- Sensitivity analysis to help addressing future research



FGR and swelling for simulation of the Shimizu experiment with stand-alone U_3Si_2 model

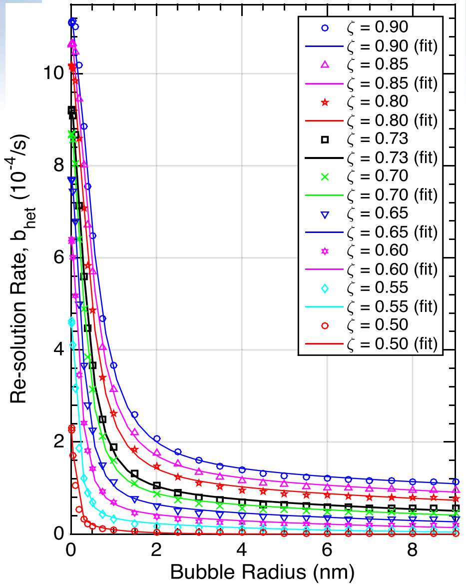


Normalized sensitivity coefficients for uncertain model parameters from SA with 10,000 Monte Carlo runs processed with RAVEN

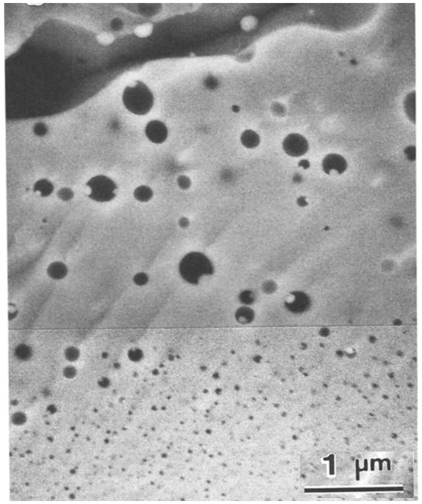
T. Barani, G. Pastore, D. Pizzocri, D. Andersson, C. Matthews, A. Alfonsi, K. Gamble, P. Van Uffelen, L. Luzzi, J. Hales, et al., J. Nucl. Mater., 2019, submitted.

Perspectives

- Further develop the multiscale approach by coupling to improved parameters (diffusion, resolution) from lower length scale models
- Extend the model to intra-granular bubble coarsening and the associated swelling during transients/high burnup
- Extend the model to gas behavior in the High Burnup Structure (HBS)
- Continue uncertainty and sensitivity analysis
- Follow usage in various fuel performance codes



Resolution rates evaluated using MD. ***Setyawan et al., J. Appl. Phys. 124, 2018***



Bubble coarsening in UO_2. ***Kashibe et al., J. Nucl. Mater. 206, 1993***

Acknowledgments

- Politecnico di Milano, Department of Energy, Milan, Italy
- European Commission, Joint Research Centre – Karlsruhe, Germany
- US DOE Office of Nuclear Energy Scientific Discovery through Advanced Computing (SciDAC) project on Fission Gas Behavior
- US DOE Nuclear Energy Advanced Modeling and Simulation (NEAMS) and Consortium for Advanced Simulation of LWRs (CASL) programs
- US/EURATOM International Nuclear Energy Research Initiative (I-NERI) project 2017-004-E on Modeling of Fission Gas Behavior in Uranium Oxide Nuclear Fuel Applied to Engineering Fuel Performance Codes
- IAEA Coordinated Research Project on Fuel Modeling in Accident Conditions (FUMAC)