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SCIANTIX: an open-source multi-scale code for fission gas behaviour modelling designed for nuclear fuel performance codes

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Software

- Review
- Repository
- Archive

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Summary

SCIANTIX is an open-source multi-scale code for modelling fission gas behaviour in oxide nuclear fuel, together with the relevant microstructural phenomena. The code behaves as a 0D meso-scale solver implementing physics-based rate-theory models, designed to be either a stand-alone tool for separate-effect calculations or a module embedded in engineering thermo-mechanical fuel performance codes (FPCs). Compared with empirical approaches used in FPCs, SCIANTIX solves evolutionary equations for stable and radioactive intra-granular gas diffusion, trapping, re-solution, grain-boundary bubble evolution, diffusional and burst release, helium behaviour and high-burnup structure (HBS) porosity. The code adopts verified numerical solvers and includes a regression suite to ensure reproducibility.

Statement of need

Engineering FPCs typically rely on empirical correlations for modelling fission gas release and gaseous swelling. The underlying physical processes are commonly described using classical rate-theory formulations (Forsberg & Massih, 1985a, 1985b), which are often simplified in engineering codes for robustness and computational speed. These implementations are usually calibrated for specific datasets or reactor conditions and are rarely available as open-source software, limiting reproducibility and research efforts for new fuel designs or irradiation scenarios.

SCIANTIX addresses these limitations by providing an open-source physics-based meso-scale module (Pizzocri et al., 2020), together with a modular C++ architecture that enables extensions and direct coupling to external multi-physics solvers (Giovanni Zullo et al., 2023). The code is supported by numerical verification through the Method of Manufactured Solutions (MMS) for all employed solvers, and by a regression testing suite covering intra- and inter-granular swelling, HBS porosity, helium behaviour and radioactive gas release. A stable API facilitates its integration into engineering-scale codes, and is already used for online coupling with TRANSURANUS, FRAPCON/FRAPTRAN and OFFBEAT (Giovanni Zullo et al., 2024).

Software description

Implementation

SCIANTIX (>2.0) adopts an object-oriented structure, in which matrices, gas, systems, models and solvers are implemented as independent classes. Separation between solvers and models supports independent MMS verification and separate-effect model validation. The spectral diffusion solver provides a meshless approach with controlled numerical error for Booth-type diffusion problems. First-order L-stable implicit time integrators ensure numerical stability. A segregated operator-splitting scheme maintains CPU-time compatibility in online coupling with engineering-scale thermo-mechanical codes.

Functionality

SCIANTIX models intra-granular diffusion, trapping and irradiation-induced re-solution; nucleation and growth of intra-granular bubbles; grain-boundary bubble growth, coalescence, saturation and fission gas release; HBS formation and porosity evolution; helium diffusion, solubility and thermal re-solution; the release of short-lived radioactive fission gases through diffusion–decay with first-precursor enhancement.

Verification and Validation

The numerical solvers are verified using the Method of Manufactured Solutions (Oberkampf et al., 2004; G. Zullo et al., 2022), with verification tests available in the repository. Separate-effect validation reproduces the published results (Pizzocri et al., 2020; Giovanni Zullo et al., 2023) without parameter tuning and using published models and parameters.

Research efforts and ongoing developments

SCIANTIX is continuously developed within international research projects (e.g., R2CA, PATRICIA, OperaHPC, TRANSPARANT). Current development covers digital-twin workflows, in which SCIANTIX provides fast calculations of helium behaviour for real-time monitoring; reduced-order models enabling accelerated surrogate evaluations of complex multi-scale phenomena; machine-learning assisted developments such as Gaussian Process regression for automatic correlation updates; and extensions towards volatile fission products including thermo-chemical evaluations.

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