# Development of the Open-Source multi-dimensional fuel performance code OFFBEAT

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The OpenFOAM Fuel Behavior Analysis Tool (OFFBEAT) is an open-source, multi-dimensional fuel performance code collaboratively developed by the École Polytechnique Fédérale de Lausanne (EPFL) and the Paul Scherrer Institut (PSI) [1]. The project started in 2017 [2], [3] motivated by the interest of the fuel modeling community [4] towards tools with multi-dimensional and multi-physics capabilities. The main objective is to allow for higher fidelity simulations, as well as to investigate poorly known aspects of fuel behavior such as an asymmetric heat exchange in the presence of non-uniform oxide or crud layers or the PCMI in the presence of pellet defects. Also, the aim is to provide the community with a flexible, readily available, general-purpose code for research and education. In this sense, a collaboration has been recently established with the JRC in Karlsruhe to develop an optimal interaction strategy between OFFBEAT and the European fuel performance code TRANSURANUS.

OFFBEAT is based on the C++ library OpenFOAM, which employs the Finite Volume Method to discretize and solve systems of partial differential equations. Its open-source nature simplifies collaborative work, thus allowing for a more sustainable development strategy. It also allows for the continuous integration of new developments from the very large and active OpenFOAM community. The code has been developed according to a modern object-oriented programming paradigm, allowing for a full encapsulation of its different features in stand-alone classes that can be easily modified without affecting the rest of the code. This paves the way for a simplified code maintenance; streamlined extension by various contributors, in terms of new models and experimental correlations; and possibility of coupling with other OpenFOAM-based solvers and routines.

Thanks to the use of OpenFOAM as base numerical library, OFFBEAT features:

* Routines for mesh generation and manipulation, with the additional possibility to readily import geometries and meshes from available tools such as Salome.
* Professional data processing and visualization with the ParaView open-source software.
* Finite volume discretization, with an intuitive formulation based on control volume balances.
* Unstructured meshes and arbitrary geometries, with the possibility of 1D, 2D or 3D analysis also for less conventional fuel configurations, such as experimental rods or plate-type fuel.
* State of the art linear algebra solvers.
* Massive parallel scalability.

OFFBEAT has been developed according to a cell-centered framework for small-strain solid mechanics. A total Lagrangian approach has been applied, with the momentum balance equations always solved in their total form. The main stress/strains solver has been coupled to a framework for thermal analysis, and the system of coupled thermo-mechanics equations solved using a segregated scheme based on fixed-source iteration.

Appropriate methodologies have been developed to simulate the heat transfer through the gap and the fuel-pellet thermo-mechanical contact. In particular, the Arbitrary Mesh Interpolation (AMI) algorithm has been employed for coupling the two surfaces of fuel and cladding in a general, flexible and consistent way. While the treatment of the gap heat transfer has been based on a thin-gap approximation and on the concept of thermal resistances (in line with the available gap conductance models used), significant efforts have been carried out for the implementation of robust contact methodologies. A first contact algorithm was based on the penalty method often used also in Finite Element codes, while a novel second contact methodology was developed specifically to improve convergence, notably when modelling multiple separated pellets. The two contact methodologies were extensively verified with well-known benchmarks. As an example, *FIG. 1* shows on the left a punch test from the NAFEMS series between a flat base and a punch with a rounded edge. The graph on the right compares the axial displacement along the bottom punch edge calculated by OFFBEAT with 3 mesh levels progressively more reined. The reference solution obtained with Code Aster [5] is included for comparison.

*FIG. 1. Punch test from the NAFEMS series between a flat base and a punch with a rounded edge. On the right, the axial displacement along the bottom punch edge calculated by OFFBEAT for 3 different mesh refinement levels is compared against the reference solution obtained with Code Aster.*

OFFBEAT has been equipped with most of the features expected from a fuel performance code, such as:

* Experimental correlations for the temperature- and burnup-dependent material properties.
* Semi-empirical models for fuel relocation, cracking, densification, and irradiation growth.
* Models for rate-independent plasticity and creep.
* Inclusion of the SCIANTIX code as a modern, mechanistic model for fission gas release and fission gas swelling.
* A simplified neutronics module derived from TUBRNP to calculate radial power profiles and isotopic evolution.
* A gap conductance model derived from the FRAPCON code but extended to a multi-dimensional framework.
* Scripts and tools that simplifies the creation of geometries and post-processing of data.

Verification of the code thermal-mechanics (including creep, plasticity and contact models) has been performed against several analytic benchmarks while a first validation base of OFFBEAT has been created including several rods from the IFPE database. In particular, the axisymmetric fuel centerline temperature was compared against thermocouple readings from the IFA-432, IFA-562.1, IFA-701 and Risoe3 experiments, while the integral fission gas release was validated against the puncture test measurements of the Super Ramp project PK-rods, and of the AN2 and AN3 segment from the Risoe3 ramp test. As an example, *FIG. 2* shows the fuel centerline temperature (FCT) predicted by OFFBEAT against the corresponding measurements provided by the fuel thermocouple for 3 rods of the IFA-432 (in a range between 0 and ~40 MWd/kg). OFFBEAT is able to predict the FCT within a ±10% error range which is for a typical range for similar validation campaigns.

*FIG. 2. Fuel centerline temperature for 3 rods of the IFA-432 assembly. The temperatures predicted by OFFBEAT are compared against the corresponding experimental values measure by the thermocouples.*

A coupling methodology between OFFBEAT and the Monte Carlo neutron transport code Serpent2 has been developed to expand the multi-physics capabilities of the code and to allow one to obtain a higher-fidelity solution for the neutron flux and for the fuel isotopic composition [6]. The methodology has been tested on simplified cases representing typical rods used in PWRs and BWRs. The objective is a high-fidelity tool for the analysis of new fuel types, unconventional configurations, and other scenarios outside the range of application of traditional models. The coupling between OFFBEAT and Serpent2 might be used to derive effective cross section for new fuel types to be later used in 1.5D codes.

As an example of a 3-D application and to showcase the current capabilities of the code, OFFBEAT has been used to analyze two fuel disc irradiation campaigns that took place in the past in the Halden Boiling Water Reactor [7]. These campaigns were characterized by large gaps and fuel stacks made of large and highly conductive molybdenum discs sandwiched between thinner and smaller UO2 discs. These characteristics, following the analysis of McNary and Bauer [8], hint at a potential significant role of eccentricity. The combination of 2-D and 3-D simulations performed with OFFBEAT revealed that the experiments might have been affected by a higher impact of eccentricity than what was originally assumed (the 3-D simulation setup is shown in *FIG. 3*). Although OFFBEAT was originally developed for the analysis of commercial LWR rods, this study has shown how this code, as well as multi-dimensional codes in general, can be valuable for the interpretation of disc irradiation experiments, with the potential to improve the investigation of separate effect tests and id in the design of new experiment.

*FIG. 3. Cross section of the 100% eccentric model used for the 3-D analysis of the fuel disc irradiation campaigns (left). Detail showing the 2-D temperature distribution on a horizontal slice at the center of the eccentric molybdenum disc (right).*

Ongoing developments of OFFBEAT are focused on: expanding the validation database; extending the code to a large-strain formulation of stress and strains; developing an optimal interaction strategy between OFFBEAT and the TRANSURANUS code for setting appropriate initial conditions to medium/high burnup multi-dimensional transients; and improving the gap conductance model to include 3-D effects.

References

[1] A. Scolaro, I. Clifford, C. Fiorina, and A. Pautz, “The OFFBEAT multi-dimensional fuel behavior solver,” *Nucl. Eng. Des.*, vol. 358, 2020, doi: 10.1016/j.nucengdes.2019.110416.

[2] I. Clifford, M. Pecchia, R. Mukin, C. Cozzo, H. Ferroukhi, and A. Gorzel, “Studies on the effects of local power peaking on heat transfer under dryout conditions in BWRs,” *Ann. Nucl. Energy*, vol. 130, pp. 440–451, Aug. 2019, doi: 10.1016/J.ANUCENE.2019.03.017.

[3] A. Scolaro, I. Clifford, C. Fiorina, and A. Pautz, “First steps towards the development of a 3D nuclear fuel behavior solver with openfoam,” in *International Conference on Nuclear Engineering, Proceedings, ICONE*, 2018, vol. 3, doi: 10.1115/ICONE26-82381.

[4] J. Y. R. Rashid, S. K. Yagnik, and R. O. Montgomery, “Overview Advanced Fuel Performance: Modeling and Simulation Light Water Reactor Fuel Performance Modeling and Multi-Dimensional Simulation.” Accessed: Dec. 12, 2018. [Online]. Available: www.tms.org/jom.html.

[5] “Code Aster.” https://www.code-aster.org/.

[6] A. Scolaro, Y. Robert, C. Fiorina, I. Clifford, and A. Pautz, “Coupling methodology for the multidimensional fuel performance code offbeat and the Monte Carlo neutron transport code SERPENT,” in *GLOBAL 2019 - International Nuclear Fuel Cycle Conference and TOP FUEL 2019 - Light Water Reactor Fuel Performance Conference*, 2020, pp. 1174–1183.

[7] A. Scolaro, P. Van Uffelen, C. Fiorina, A. Schubert, I. Clifford, and A. Pautz, “Investigation on the effect of eccentricity for fuel disc irradiation tests,” *Nucl. Eng. Technol.*, 2020, doi: 10.1016/j.net.2020.11.003.

[8] O. McNary and T. H. Bauer, “The effect of asymmetric fuel-clad gap conductance on fuel pin thermal performance,” *Nucl. Eng. Des.*, 1981, doi: 10.1016/0029-5493(81)90015-7.