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TOPIC 4

Fuel and Materials

4.2 Fuel behaviour modelling

4.2.1 Fuel performance modelling: current approach and model capabilities

extended summary

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Introduction

The ultimate goal of simulating nuclear fuel is to predict a fuel rod's behaviour and life-time in a reactor. Doing so requires taking into account the coupled effects of heat transfer, the mechanical interaction between the fuel and its surrounding protection, the isotopic evolution caused by the irradiation and the chemical interactions between fuel, fission products, cladding and coolant. The simulation of the fuel behavior requires therefore fuel performance codes, which are being used by safety authorities, research organizations and fuel vendors. The main equations implemented in the fuel performance codes will be summarized in the first part of the lecture.

Main limitations

In view of the strong interactions between the various aspects of fuel performance and the resulting mathematical problems, several assumptions are introduced for rendering the set of equations amenable to an accurate numerical solution after a reasonable computation time. The assumptions are also outlined in the first part of the lecture.

The most important assumption deals with the rod geometry. Most fuel performance codes consider a cylindrical geometry and assume axi-symmetry, i.e., they consider cylindrical UO_2 fuel pellets and metallic cladding separated by a helium filled gap. Furthermore, the radial temperature gradient is considered to be much larger in comparison with the axial temperature gradient. As a result, a majority of the codes represent the cylindrical fuel rod in a so-called one-and-a-half dimension, whereby all transport processes are solved in one (radial) dimension, and the axial segments are coupled via balance equations.

During operation the ceramic fuel pellets undergo cracking. This has a strong impact on the fuel behaviour and affects the assumptions made, as will be explained. In addition to that, the various strategies adopted in the fuel performance codes to deal with cracking will be outlined.

Advanced methods

In order to cope with large local deformations, such as those occurring in the cladding for instance during loss of coolant accidents, some codes either provide a separate tool to analyze local deformations and stresses in two dimensions by means of finite element calculations such as the FEMAXI code, or a full two dimensional mechanical computation is proposed in the FALCON code whereas a three dimensional finite element analysis is proposed in the TOUTATIS and ALCYONE codes. More recently, fuel performance codes are currently being developed either from scratch, or on the basis of commercial software for three-dimensional finite element method (FEM) simulations. Examples of such attempts are the BISON code based on ABAQUS software and the FRA-TF_global code based on COSMOSDesignSTAR/COSMOSM system or a code based on the COMSOL software. The starting point for their development is to take full advantage of the improvements in hardware and software, as well as in numerical

techniques since the conventional fuel performance codes - currently used by safety authorities – have been developed. Nevertheless, the increase in the number of dimensions goes along with a substantial increase of the computational costs and offers only an added value for the analysis of certain accident situations with large deformations. Indeed, for normal operational conditions, one dimensional codes are at least as accurate in view of the numerous uncertainties, for instance those brought about by the stochastic cracking and friction processes. The uncertainties in fuel rod powers and geometry (sphericity, pellet cracking, etc.) cannot be avoided by those multi-dimensional codes and ultimately may prevent them from replacing more simplified codes of today for licensing purposes. In any case, they will provide a deeper understanding and an excellent supporting tool for designing advanced nuclear fuels.

Apart from the main limitations caused by the geometrical assumptions, there are other limitations related to the empirical nature of material property models and some of the physical models, such as the relocation of cracked fuel segments. As a consequence of the use of empirical models, it is impossible to extrapolate the material properties and models beyond the range of operating conditions in which they have been fitted. Hence, when advanced materials are to be designed for innovative reactor types, new codes have to be developed for each combination. The required amount of experimental data is both time consuming and expensive. With the advent of advanced software and hardware many attempts have been made to introduce more physics-based models that enable extrapolation to a large range of operating conditions, and to cover a large set of potential materials. This has led to the development of meso-scopic models, micro-scopic models and even simulations tools at the scale of the electronic structure. Each simulation tool requires specific experimental data for their development and validation. There are now attempts to couple the various simulations tools in what is commonly referred to as the multi-scale approach and is considered in the second part of the fuel performance modeling by Dr. Bertolus.

Dealing with uncertainties

The parameters and models required for by the fuel performance codes are subject to uncertainties. A pragmatic manner to deal with uncertainties pertaining to power histories, fabrication data and models in the current fuel performance codes consists of applying conservative or probabilistic analysis. In order to assess the technological effect of all sources of uncertainties there are various techniques that may be considered:

- First of all, there are various so-called sensitivity methodologies, ranging from multiple runs with input data or model parameters being varied, up to a rigorous mathematical treatment based on perturbation theory.
- A second category of probabilistic approaches is the response surface technique. This is based on a careful combination of parameters called the experimental design, such as the Latin hypercube sampling or the Taguchi design.
- A third category consists of the Monte Carlo method, which is based on random sampling of all uncertain variables that are considered.
- A fourth category of methods is called semi-statistical and combines statistical as well as deterministic computations.

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