Journal of ELECTRICAL ENGINEERING, VOL. 56, NO. 1-2, 2005, 45–48

COMMUNICATIONS

TRANSURANUS VERSUS HELIOS: COMPUTATION OF SELECTED NUCLIDES IN BURNT–UP NUCLEAR FUEL

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Computer codes TRANSURANUS and HELIOS are used to compute the concentrations of nuclides in the classical UO_2 nuclear fuel and in the mixed oxide fuel (MOX) during the burn-up. The results are critically discussed.

K e y w o r d s: nuclear fuel, burn-up, uranium, plutonium, TRANSURANUS, HELIOS

1 INTRODUCTION

In 2004, as many as 444 nuclear energy reactors were operated in 31 countries worldwide. Most of them burn classical nuclear fuels, thus either uranium dioxide UO_2 containing natural uranium, uranium enriched by U-235 or, less often, the so-called MOX (Mixed Oxide) fuel, which is a mixture of UO_2 and PuO_2.

The use of nuclear fuels and introduction of their novel types requires detailed knowledge of the behaviour of the fuels in all possible states in which they occur. However, experimental studies and verifications of the behaviour of nuclear fuels often cannot be performed because of safety and instrumental reasons or because of too long times needed to conduct such studies. This is why modelling and computer simulation of the behaviour of nuclear fuels are increasingly used. Computer analyses and simulations allow obtaining the evolutions of single characteristics of the fuel at any instant in the course of its burn-up. Naturally, the knowledge of the properties of the nuclear fuel not only improves the efficiency but also the operation safety.

Numerous computer codes have been developed for nuclear fuel burn-up modelling and simulation. Nevertheless, they usually focus on different aspects and properties of the fuel. The objective of this paper is to employ the codes HELIOS and TRANSURANUS to simulate the properties of UO_2 and MOX during the burn-up and to compare the obtained results.

2 URANIUM DIOXIDE AND MOX FUEL

Uranium is the fundamental component of today's nuclear fuels. It is mined from the Earth crust in localities with content higher than 0.001 %. Natural uranium contains three isotopes of uranium: 0.0054 % of U-234, 0.7204 % of U-235 and 99.2742 % of U-238 [1]. Light water reactors (LWR) are moderated by light water, on that account fuel enrichment by U-235 is needed.

Production of the classical nuclear fuel UO_2 is based on mechanical and chemical procedures yielding the required composition of the fuel and ensuring the needed purity, enrichment, shapes and dimensions. Crystalline UO_2 has a face centred cubic (fcc) structure with a three-atomic basis. The elementary cell contains four atoms of uranium and eight atoms of oxygen. Its melting point is $2865 \pm 15\,^{\circ}\mathrm{C}$, density $10\,960\,\mathrm{kg\,m^{-3}}$, heat conductivity $3.1\,\mathrm{W\,m^{-1}K^{-1}}$ at $1000\,^{\circ}\mathrm{C}$. If non-stoichiometric, most of its thermo-mechanical properties such as the melting point, heat conductivity, and mechanical strength as well as migration of fission products and material creep vary rapidly with the content of oxygen.

During the operation of the nuclear reactor using UO_2 as a fuel, fission of U-235 and neutron capture on U-238 lead to formation of new nuclides. Hence, a nuclear reactor under operation contains, besides others, also isotopes Pu-239 to Pu-242. However, today's reactors do not reach a sufficiently high level of burn-up ensuring consumption of this accumulated plutonium. One of the remedies to this problem is reprocessing of the spent nuclear fuel, extraction of plutonium and its use in the MOX fuel, thus in the mixture of UO_2 and PuO_2. MOX fuel is a potential fuel for VVER reactors as well.

In the production of the MOX fuel, attention is paid to the homogeneity of special distribution of plutonium and to its solvability in the process of spent fuel reprocessing. While sufficient distribution uniformity can be achieved by using the classical mixing method, solvability of plutonium is a more intricate issue. Several methods have been developed allowing a very good level of solvability, as high as 99.9 %, *eg* , the Ammonium Uranyl Plutonyl Carbonate (AUPuC) method. In the case of using the MOX fuel, no changes occur in the operation mode of the reactor.

3 COMPUTER CODES

Computer technology is very efficiently used to model, simulate and analyze different states of the fuel. The mod-

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ISSN 1335-3632

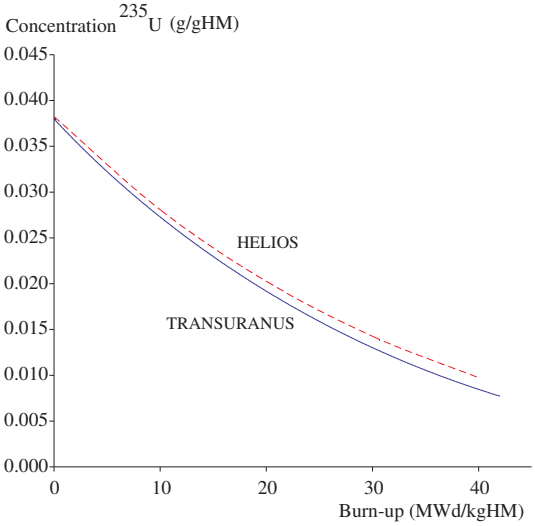

Fig. 1. The decrease of the concentration of U-235 during the burn-up of UO_2 .

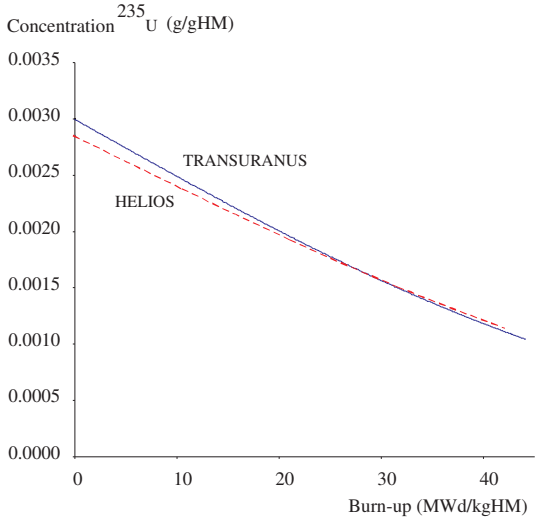

Fig. 2. The decrease of the concentration of U-235 during the burn-up of the MOX fuel.

els implemented in the computer codes may either describe the fuel element as an aggregate or analyze its local details. It is crucially important to define the maximum dimensions of the model reasonably. Usually it is enough to model just one fuel pin, to insert different defects, and to apply the obtained result to more fuel pins. In most cases, the specific computer codes are of empirical nature: they utilize the databases of existing data and empirically obtained equations describing the required parameters. Naturally, the best way of validating the results is their comparison with experimental data, which is often a very difficult task.

3.1 Helios

HELIOS [2] is a neutron gamma transport computer code. It allows modelling and simulation of the burn-up of the nuclear fuel in a lattice structure in 2D geometry. Computations of resonant shielding for nuclides are incorporated in the data of the code. The code solves various material structures of arbitrary geometry that are mutually connected by particle flows with boundary conditions. The transport method employed, Current Coupling Collision Probabilities (CCCP), is based on connecting the structures of the lattice and on the probabilities of interaction of the particles with the matter. The input data contain the geometrical representation of the fuel, definitions of sizes and distances, mutual connections and links, fuel composition, etc. The required input data may include the multiplication coefficient, atomic or mass concentrations of isotopes and pin powers. Processor AURORA reads the data, processes them and stores them in a binary file needed in subsequent computation.

One can define the desired mode of computation and of the output data. Processor ZENITH prepares the required mode of computation and the required output data of the HELIOS code. The processors are mutually interconnected by subroutine HERMES providing the flow of data between single processors, HELIOS and the database on isotopes containing, *eg* , their fission cross-sections, absorption cross-sections and other parameters.

3.2 Transuranus

TRANSURANUS [3] is a computer code intended for thermal and mechanical analyses of the fuel elements in a reactor. It allows modelling and simulation of the nuclear fuel and its operation states (or experiments) in the time period from some milliseconds to several years. Design of the program began at the University of Darmstadt, Germany in 1973. From 1978 to 1982 the works ran simultaneously at the University of Darmstadt and at the Institute for Transuranium Elements (ITU) in Karlsruhe, Germany. Since 1982, the research has been pursued solely at ITU.

TRANSURANUS is an empirically based code. It incorporates physical models of thermal and radiation densification of the fuel, models of fuel swelling, fuel cracking and relocation, a model of generation of fission gases, a model of redistribution of oxygen and plutonium, and some other physical models. The code is exploited mainly by research institutions, industries and licence bodies.

The input file of the code contains complete data needed for computation. It determines the type of reactor, cladding, coolant, fuel geometry and dimensions, surface roughness, coefficients of heat transfer, initial concentrations of uranium and plutonium isotopes, the course of power loading and the length (period) of computation. Switches 0 and 1 define the route of computing.

The output data are provided by subroutine URPLOT. It generates data files for single times, distances or locations at the fuel pin. Optionally, the output data include the pellet radius, pressure in the gap, contact pressure between the pellet and cladding, concentrations of fissionable isotopes U-235, Pu-239 to Pu-242, concentrations of

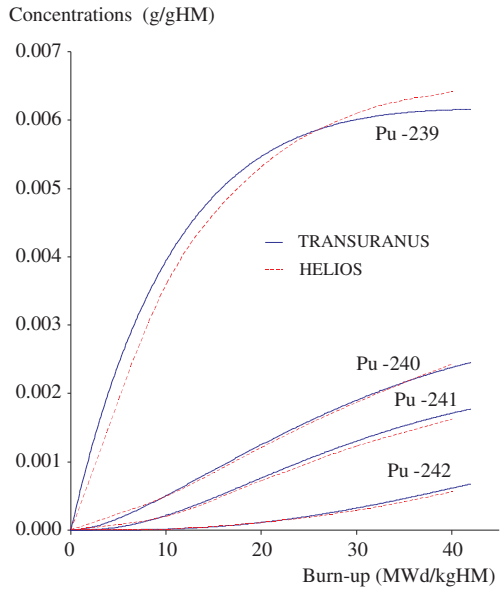

Fig. 3. The rise of the concentrations of Pu isotopes during the burn-up of UO_2.

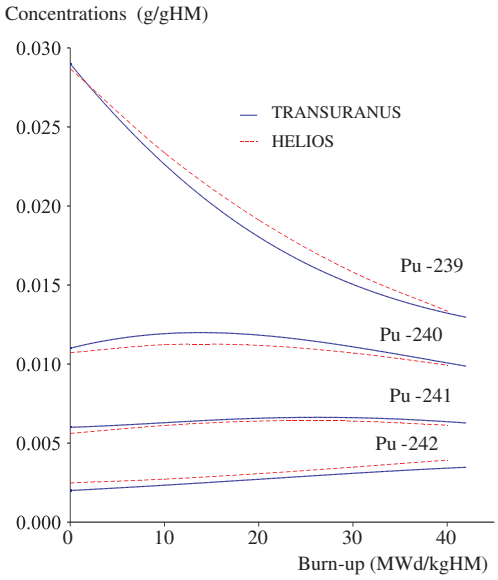

Fig. 4. The evolution of the concentrations of Pu isotopes during the burn-up of the MOX fuel.

Table 1. Dimensions of UO_2 and MOX fuels.

Inner pellet diameter	0.60000 mm
Outer pellet diameter	3.80000 mm
Inner cladding diameter	3.86000 mm
Outer cladding diameter	4.56562 mm

Table 2. U-235 and Pu isotopes concentrations.

Isotope	Concentrations (g/gHM)	
	UO_2	MOX
U-235	0.038	0.003
Pu-239	0.000	0.029
Pu-240	0.000	0.011
Pu-241	0.000	0.006
Pu-242	0.000	0.002

fission gases, temperatures of the fuel, cladding and gases in the gap and other parameters.

4 SIMULATIONS

In our study we have simulated the behaviour of fuel pins in the course of burn-up. For computing the stationary state of the classical UO_2 fuel and of MOX, thus for the case of a fault-free operation at a constant power, input files have been created defining the properties of the kinds of fuel. In these files, physical parameters have been entered starting with dimensions of the pellets and of the cladding, pellet surface roughness, stoichiometry, oxygen ratio, heat transfer coefficients, fuel grain sizes, pellet porosity, initial values of uranium enrichment and plutonium content, pin height, etc. The fuel has been divided into 10 sections, each cross-section being divided into 8 rings: 5 rings of fuel and 3 rings of cladding. At the beginning, the fuel and cladding were not in a direct contact. The chosen fuel dimensions consider the use of the distance grids in the reactor. The pins have been filled with a gas mixture composed of 98 % of helium, 1 % of nitrogen and 1 % of H_2O to a pressure of 0.6 MPa at 20 °C. The input parameters have been taken from the model of fuel pins in reactors VVER-440 provided by the Nuclear Power Plant Research Institute, Joint Stock Company, Trnava (VÚJE, a.s., Trnava).

Tables 1 and 2 summarize the fuel dimensions and initial isotopic concentrations.

The physical model employed assumes a linear power of 12.921 kW m^{-1} along the whole height of the pin. The total time of burn-up is set to 32 000 hours (3.6 years).

Figures 1 and 2 show the time evolution of the concentration of U-235 in the course of the burn-up for UO_2 and the MOX fuel, respectively. The burn-up is given in MWd/kgHM, thus in mega watt days per kilogram of heavy metal, and the concentration of nuclides in g/gHM, thus in grams per gram of heavy metal. Figures 3 and 4 show the burn-up curves for Pu isotopes.

Figures 5 and 6 present the relative deviations of the results yielded by TRANSURANUS from those obtained by HELIOS. HELIOS is generally considered to be a well-validated code for simulating the process of nuclear fuel burn-up.

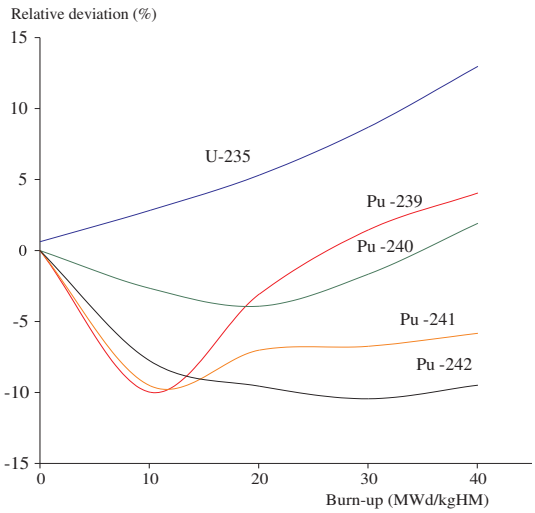

Fig. 5. Relative deviation of TRANSURANUS from HELIOS for UO_2.

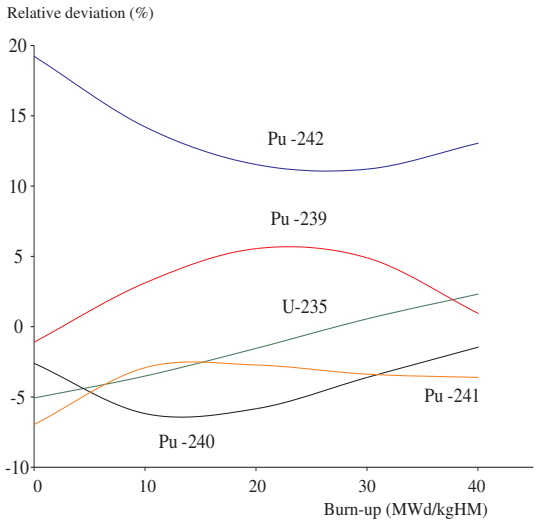

Fig. 6. Relative deviation of TRANSURANUS from HELIOS for the MOX fuel.

5 CONCLUSION

The burn-up characteristics computed by TRANSURANUS are in reasonable agreement with those yielded by HELIOS. The relative deviations range from -10 to $+10\,\%$, which is quite satisfactory for practical applications. Deviations between the simulated results are believed to be caused by different physical models employed as well as by different databases and libraries. Additionally, minor deviations may stem from different procedures and accuracies of computations. However sophisticated the computer codes for this kind of computation are, the employed databases still possess some uncertainties and they have to be further completed and updated.

From among all nuclides, TRANSURANUS allows to compute concentrations of only two elements, U and Pu. HELIOS, on the other hand, provides information on a broad range of nuclides.

TRANSURANUS allows to compute also thermomechanical properties of the fuel. Nevertheless, for these computations an advanced physical model of the fuel has to be implemented. No matter how good the agreement is between the results provided by the two codes, final verification of the data may only be achieved by experiments.

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Received 5 November 2004

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