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Specifications for a coupled neutronics thermal-hydraulics SFR test case

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Abstract. Coupling neutronics/thermal-hydraulics calculations for the design of nuclear reactors are a growing trend in the scientific community. This approach allows to properly represent the mutual feedbacks between the neutronic distribution and the thermal-hydraulics properties of the materials composing the reactor, details which are often lost when separate analysis are performed. In this work, a test case for a generation IV sodium-cooled fast reactor (SFR), based on the ASTRID concept developed by CEA, is proposed. Two sub-assemblies (SA) characterized by different fuel enrichment and layout are considered. Specifications for the test case are provided including geometrical data, material compositions, thermo-physical properties and coupling scheme details. Serpent and ANSYS-CFX are used as reference in the description of suitable inputs for the performing of the benchmark, but the use of other code combinations for the purpose of validation of the results is encouraged. The expected outcome of the test case are the axial distribution of volumetric power generation term (q'''), density and temperature for the fuel, the cladding and the coolant.

1. Introduction

Multi-physics is the field of computer-aided engineering who is interested in the simulation of multiple physical models. Although no complete multi-physics platform has yet reached the maturity for a general release, the increasing requirements of computational accuracy for design and safety analysis, especially in the nuclear industry, have caused a growing interest in the scientific community toward this approach.

Several neutronics and thermal-hydraulics codes have been coupled in the past to perform analysis of both thermal and fast reactor cores [1][2][3][4]. In particular, it has been demonstrated the possibility of employing coupled neutronics and thermal-hydraulics codes in the study of sodium cooled fast reactors (SFR), which are one of the six types of reactors actually being developed in the framework of the OECD Generation IV roadmap [5][6][7][8].

2. ASTRID core design

The Advanced Sodium Technological Reactor for Industrial Demonstration (ASTRID) is a 1500 MW_th pool-type sodium cooled fast reactor developed since 2010 by the French public government-funded research organisation CEA and its linked partners. Expected to be built after 2030, ASTRID is a industrial demonstrator for the SFR technology and can be regarded as

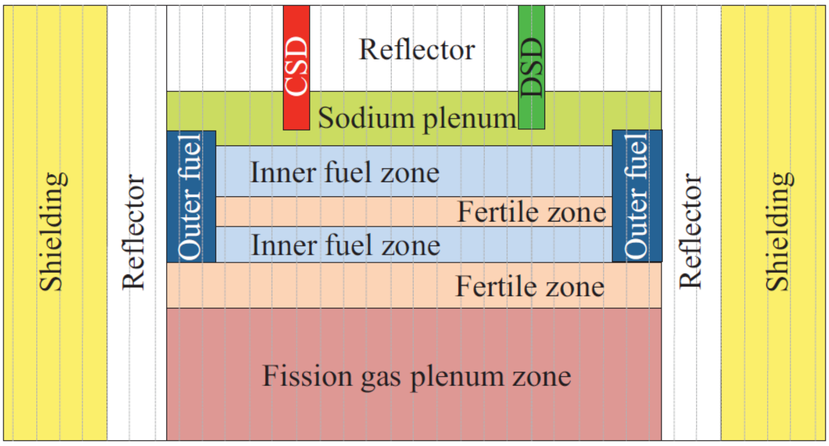

Figure 1. ASTRID core map, axial cross-section [11].

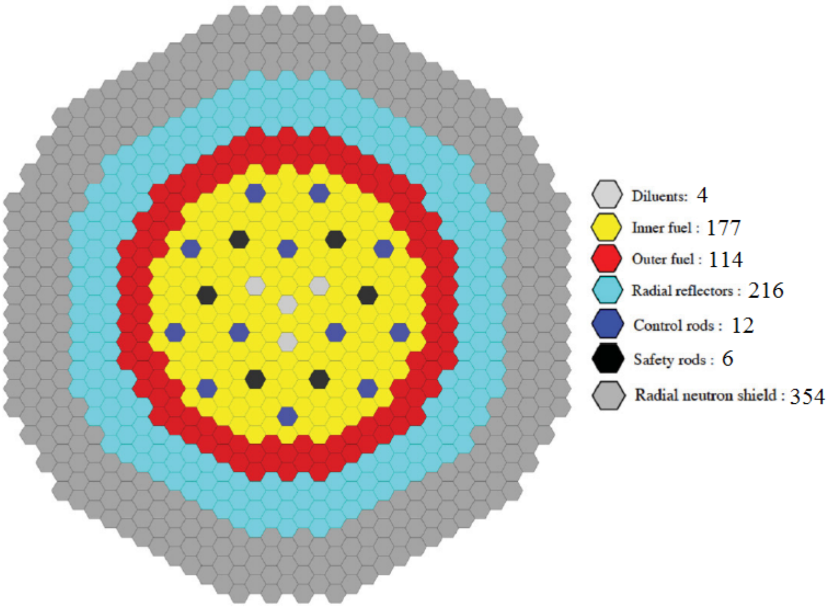

Figure 2. ASTRID core map, top view [12].

the next iteration on the French SFR reactor fleet [9][10]. To improve the safety performance of the reactor, an axially and radially heterogeneous core was designed to reduce the sodium void reactivity coefficient. ASTRID core maps are provided in Figure 1 and 2.

The reference fuel for the CFV core is a uranium-plutonium mixed oxide (MOX), with an enrichment in plutonium varying from the 20% of the outer zone to the 23.5% of the inner zone. The fuel is contained inside 291 hexagonal sub-assemblies, of which 177 are found in the inner region and 114 in the outer region. Each sub-assembly is composed of 217 fuel pins, arranged in 8 rows around the central pin, and delimited by the wrapper can. The pin are wrapped by a wire and enclosed in a cladding, a gap is present between the fuel and the cladding to house the gaseous fission products. The AIM1 austenitic stainless steel is employed as cladding, whereas the material chosen for the wrapper is the EM10 alloy.

Table 1. Pin radial dimensions and SA parameters [10][13][14].

Pin radial dimensions			SA parameters		
Pellet diameter	9.065	mm	Number of pins	217	
Gap thickness	0.075	mm	SA pin rows	8	
Clad inner diameter	9.14	mm	Inter-SAs gap	4.73	mm
Clad thickness	0.56	mm	Last pin–wrapper pitch (g)	10.44	mm
Clad outer diameter (D_p)	9.7	mm	Space between flats (e)	193.78	mm
Pin-to-Pin pitch (P)	10.8	mm	SA pitch	198.41	mm
Spacing wire diameter (D_w)	1.1	mm	q'_{max} [W cm^{-1}]	484	
Helical pitch of wire	180	mm	$\overline{q}'''$ [W cm^{-3}]	234	

Table 2. Pin axial dimensions [11].

INNER FUEL ZONE			OUTER FUEL ZONE		
Upper fissile layer	35.228	cm	Fissile fuel	90.685	cm
Middle breeder plate	20.152	cm			
Lower fissile layer	25.228	cm			
Axial blanket	30.228	cm	Axial blanket	30.228	cm
Inner zone pin height	110.836	cm	Outer zone pin height	120.913	cm

3. Benchmark specifications

Since the ASTRID design details are still under development an ASTRID-like geometry is employed. Two different test case are proposed, one for the inner and one for the outer zone sub-assembly. The radial dimensions of the fuel pin for the two cases are identical (see Table 1). The complete geometrical data for the axial direction are available in Table 2. For the purpose of the neutronics simulation the presence of the wrapping wire can be neglected, as well as the the sodium and gas plena, the structural support of the pin and of the fuel assemblies.

The fissile fuel is a mixed uranium-plutonium oxide (MOX) with an enrichment in plutonium of 23.5% for the inner zone and of 20% for the outer zone, whereas the fertile sections of the pin are composed by natural uranium oxide. The test case fuel is constituted by the isotopes U^{235}, U^{238}, Pu^{238}, Pu^{239}, Pu^{240}, Pu^{241} and Pu^{242}. The oxygen is assumed as composed completely by O^{16} and in perfect stoichiometric ratio with both the uranium and plutonium. Fresh fuel is modelled and the isotopic distribution variation it is neglected. Data about the fuel composition for both the fissile and fertile sections are available in Table 3.

The pin-cladding gap is filled by gaseous helium at 4 MPa, which it is composed exclusively by He^4. Moreover, the coolant is considered as natural and perfectly pure sodium. The composition of the AIM1 cladding and the EM10 wrapper is assumed to be equal to the average data in the reference [16]. Thermo-physical properties about the fuel, the coolant, the cladding and helium can be found in the references [17], [18] and [19].

4. Coupling scheme

The approaches that can be followed to couple a neutronics code and a thermal-hydraulics one are divided in two categories: a loose coupling, where the calculations are performed separately and informations between the models is exchanged only at specified points, and an internal coupling, where to models are integrated in the same platform and communicate continuosly.

The loose coupling can considered equivalent to the solving of a set of differential equations through the operator splitting method. The main advantage of this approach is that it is possible

Table 3. Fissile and fertile fuel mass and atomic fractions [15].

	MOX outer zone		MOX inner zone		UO_2	
Isotope	WF	AF	WF	AF	WF	AF
U-235	0.507%	0.194 %	0.485%	0.186%	0.220%	0.084 %
U-238	69.910%	26.440 %	66.837%	25.283%	87.929%	33.241 %
Pu-238	0.496%	0.188 %	0.579%	0.219%		
Pu-239	9.132%	3.439 %	10.696%	4.029%		
Pu-240	4.770%	1.789 %	5.610%	2.105%		
Pu-241	1.880%	0.702 %	2.220%	0.829%		
Pu-242	1.454%	0.541 %	1.724%	0.642%		
O-16	11.851%	66.707 %	11.849%	66.707%	11.850%	66.674 %

to employ verified and validate code for the solution of each model, without the necessity to modify the source code. It is the state-of-the-art for coupled calculations and it is implemented for this test case [7].

The codes used as reference for this test case are Serpent, for the neutronics part, and ANSYS-CFX, for the thermal-hydraulics part.

Serpent is a three-dimensional continuous-energy Monte Carlo reactor physics burnup calculation code developed by the VTT Technical Research Center of Finland since 2004 and first distributed in 2009. Serpent allows the description of any two- or three-dimensional fuel or reactor configuration. Integrated in the code are cross section libraries based on JEF-2.2, JEFF-3.1, JEFF-3.1.1, ENDF/B-VI.8 and ENDFB/B-VII for 432 nuclides at 6 temperatures between 300 and 1800 K. [20]

ANSYS-CFX is a general purpose Computational Fluid Dynamics three-dimensional code. The program is able to simulate a wide range of physical phenomena and flows. A tailored programming language (CEL) is available to extend the capability of the code, i.e. adding new materials to the software libraries and modifying the solver equations. [21].

The Serpent output supplies the distribution of the volumetric power generation (q''') inside the fuel, which is employed in the writing of the CFX input file. In turn, the CFX results provide the distribution of the temperature and the density of the fuel, the cladding and the coolant which are integrated as input for the next iteration of Serpent. Local power, k_{eff} and the temperature distribution are proposed as convergence parameters. At the end of each coupling cycle, the parameters chosen are checked against the following convergence criteria

(i) $k_{eff} = 1.0 \pm 0.001$ in two successive iterations
(ii) $Q < 0.1\%$
(iii) $T_f, T_c, T_{Na} < 0.1\%$

for the local power and temperature distribution, the criterion should be intended for the residual of the parameter discussed. In particular, for the criterion (iii) representative temperatures must be selected, i.e. central point for pin and cladding, outlet for the sodium. When all the criteria are satisfied, the calculation is considered complete. In Tables 4 and 5, data necessary for the setup of the coupled simulations are provided.

5. Expected results

In this work, specifications for a coupled neutronics/thermal-hydraulics test case based on a generation IV sodium-cooled fast reactor were presented. The design chosen to serve as a model

Table 4. Neutronics simulation initial conditions.

	T[K]	ρ [kg m^{-}3]
MOX fuel	1500	10120.04
UO_2 fuel	900	10219.43
Cladding	750	7746.00
Helium	750	1.87
Sodium coolant	750	837.95

Table 5. Thermal-hydraulics simulation initial conditions [13][14].

Γ_{core}	7900	kg s^{-}1	Na inlet properties		
I/Outer FA power	6/3.84	MW	ρ	855	kg m^{-}3
Na inlet T	673	K	c_p	1289	J kg K^{-}1
Na outlet T	823	K	λ_t	73.11	W m^{-}1 K^{-}1
Re	$5\,10^4$		μ	2.76 10−4	Pa s

for the test case was the ASTRID, a technological demonstrator actually in development by the CEA. Two test cases were proposed: in the first one the inner zone fuel assembly conditions is studied, whereas in the second the outer zone assembly is considered. A loose coupling scheme was analysed with Serpent for the neutronic part and ANSYS-CFX for the thermal-hydraulic one. Since the computational resources needed to model the whole assembly might be too high, it is possible to restrict the thermal-hydraulics analysis to the single central fuel pin of the sub-assembly through the setup of appropriate boundary conditions. However, whenever possible, the authors advise to model the complete assembly.

The expected results for this benchmark can be summarized as the following

- The coupled neutronics/thermal-hydraulics steady-state simulation of the test cases proposed should be performed until the convergence of the parameters of interest.
- Axial distribution of volumetric power generation and fission rates in the fuel
- k_{eff}
- Axial distribution of temperature and density for the fuel, the cladding and the coolant
- Pressure drop across the channel for the sodium

The validation is conducted through code-by-code comparisons. However, results for similar configurations can be found in the literature, i.e. [7] and [14].

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