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## An extended version of the SERPENT-2 code to investigate fuel burn-up and core material evolution of the Molten Salt Fast Reactor

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### ABSTRACT

In this work, the Monte Carlo burn-up code SERPENT-2 has been extended and employed to study the material isotopic evolution of the Molten Salt Fast Reactor (MSFR).

This promising GEN-IV nuclear reactor concept features peculiar characteristics such as the on-line fuel reprocessing, which prevents the use of commonly available burn-up codes. Besides, the presence of circulating nuclear fuel and radioactive streams from the core to the reprocessing plant requires a precise knowledge of the fuel isotopic composition during the plant operation.

The developed extension of SERPENT-2 directly takes into account the effects of on-line fuel reprocessing on burn-up calculations and features a reactivity control algorithm. It is here assessed against a dedicated version of the deterministic ERANOS-based EQL3D procedure (PSI-Switzerland) and adopted to analyze the MSFR fuel salt isotopic evolution.

Particular attention is devoted to study the effects of reprocessing time constants and efficiencies on the conversion ratio and the molar concentration of elements relevant for solubility issues (e.g., trivalent actinides and lanthanides). Quantities of interest for fuel handling and safety issues are investigated, including decay heat and activities of hazardous isotopes (neutron and high energy gamma emitters) in the core and in the reprocessing stream. The radiotoxicity generation is also analyzed for the MSFR nominal conditions.

The production of helium and the depletion in tungsten content due to nuclear reactions are calculated for the nickel-based alloy selected as reactor structural material of the MSFR. These preliminary evaluations can be helpful in studying the radiation damage of both the primary salt container and the axial reflectors.

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### 1. Introduction

Recent studies have highlighted the promising features of the Molten Salt Fast Reactor (MSFR) [1], developed in the 7th EURATOM Framework Programme. This system offers the possibility to fully benefit from the adoption of a thorium-based closed fuel cycle [2]. Moreover, the fast neutron spectrum adopted, unlike previous experiences with moderated Molten Salt Reactors (MSR),<sup>1</sup> allows more effective incineration of transuranic (TRU) isotopes [3]. Nonetheless, several open issues still exist on different aspects of this innovative system. The adoption of an on-line (continuous) reprocessing scheme offers several advantages but may lead to some problems due to the necessity of handling highly radioactive streams. Moreover, the structural materials have to withstand severe conditions in terms of temperature, chemical environment and neutron flux [4].

The presence of a continuous fuel reprocessing prevents the adoption of commonly available fuel burn-up codes. Few codes were developed specially for this purpose in the past (e.g., [9,5,2,6]). In Table 1, a list of recent works concerning burn-up calculations in MSRs is presented, along with the main features of the employed codes. Some of these codes adopt approximations that may lead to inaccurate fuel evolution predictions or are not fully available. For this reason, a purpose-made extension of the continuous-energy Monte Carlo reactor physics and burn-up code SERPENT-2 [10] is proposed in the present work.<sup>2</sup> The developed extension of SERPENT-2 code directly takes into account the effects of on-line fuel reprocessing on burn-up calculations and features a reactivity control algorithm. It is here assessed against a dedicated version of the deterministic ERANOS-based EQL3D procedure [11,2] and adopted to accurately study the isotopic evolution of

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<sup>1</sup> See, e.g., documents related to liquid-halide (fluoride and chloride) reactor research and development, available at <http://www.energyfromthorium.com/pdf/>.

<sup>2</sup> The extended SERPENT-2 version has been preliminarily presented at the 2nd International SERPENT User Group Meeting. The methods for MSR burn-up calculations presented in this work will be implemented in the official distribution version of SERPENT-2. [http://montecarlo.vtt.fi/mtg/2012\\_Madrid/index.htm](http://montecarlo.vtt.fi/mtg/2012_Madrid/index.htm).

## Nomenclature

### Latin symbols

$b_{j \rightarrow i}$	branching ration from nuclide $j$ to nuclide $i$
$C_i$	atomic fraction of the isotope $i$ in the feed vector
$FY_{k \rightarrow l}$	fission yield for the production of the fission product $l$ from a fission of the heavy metal $k$
$k_{eff}$	effective multiplication factor
$k_{eff,tgt}$	target effective multiplication factor for the reactivity control algorithm
$k_{inf}$	infinite multiplication factor
$N_i$	atomic density of the generic isotope, $i$ ( $\text{cm}^{-3}$ )
$r$	radial coordinate (m)
$r_{abs}$	absorption rate ( $\text{s}^{-1}$ )
$r_{capt}$	capture rate ( $\text{s}^{-1}$ )
$z$	axial coordinate (m)

### Greek symbols

$\varepsilon$	user-defined tolerance for the reactivity control algorithm
$\lambda_i$	decay constant of the generic nuclide $i$
$\lambda_{i,repr}$	effective removal constant for the reprocessing of the fission product $l$
$\rho$	reactivity

$\sigma_{j \rightarrow i}$	one-group transmutation cross-section from nuclide $j$ to nuclide $i$
$\sigma_{kf}$	one-group fission cross-section of the heavy metal nuclide $k$
$\phi$	neutron flux ( $\text{cm}^{-2} \text{s}^{-1}$ )

### Acronyms

ARR	Advanced Recycling Reactor
CR	Conversion Ratio
CRAM	Chebyshev Rational Approximation Method
EPFY	Effective Full Power Years
EVOL	Evaluation and Viability of Liquid Fuel Fast Reactor Systems
FP	Fission Product
HM	Heavy Metal
LWR	Light-Water Reactor
MSFR	Molten Salt Fast Reactor
MSR	Molten Salt Reactor
pcm	per cent mille
ppm	parts per million
PSI	Paul Scherrer Institut
RHS	Right-Hand Side
TRU	transuranic isotopes

**Table 1**

Comparison of different works dealing with burn-up calculations in MSRs available in recent open literature.

	Nuttin et al. [5] <sup>a</sup>	Fiorina et al. [2] <sup>b</sup>	Sheu et al. [6]	Present work
Neutron transport code	MCNP	ERANOS	KENO-VI	SERPENT-2
Neutron transport method	Monte Carlo continuous energy	Deterministic $S_n$ -16	Monte Carlo multi-group (238)	Monte Carlo continuous energy
Burn-up code	REM (in-house code)	ERANOS	ORIGEN-S	SERPENT-2
Solution of the Bateman equations	Fourth order Runge–Kutta method	Power series approximation of the matrix exponential	Power series approximation of the matrix exponential	Chebyshev rational approximation of the matrix exponential
Number of isotopes considered	All the isotopes available in the nuclear data library Short lived isotopes are treated separately	167 Short-cut and simplified decay chains	388 Short lived isotopes are treated separately	All the isotopes available in the nuclear data library All the isotopes are included in the burn-up matrix
Non-soluble FP removal	Continuous (non-soluble FP are treated separately)	Continuous	Batch	Continuous
Soluble FP removal	Continuous	Continuous	Batch	Continuous
Feed material injection	Continuous	Batch	Batch	Continuous
Reactivity control	Yes Continuous adjustment of fissile material injection/extraction rate	Only guarantees criticality at equilibrium –	Yes Batch injection of fissile material	Yes Continuous adjustment of fissile material injection/extraction rate

<sup>a</sup> For the work of [5], the information not available in the paper has been taken from the PhD thesis of Nuttin [7].

<sup>b</sup> For the work of [2], the information not available in the paper has been taken from the PhD thesis of Fiorina [8].

MSFR core materials. The work is focused on the study of the breeding performance of the reactor and the analysis of some parameters that are thought to be critical for the deployment of this technology.

The paper is organized as follows. In Section 2, a brief introduction to the MSFR concept is given, along with a description of the fuel cycle scenarios considered in the present work. In Section 3, a detailed description of the methodology adopted and of the extension of the SERPENT-2 code is presented. A comparison with the ERANOS-based EQL3D procedure is also reported for a selected case. In Section 4, the newly implemented reactivity control algorithm is presented. Finally, the main results related to isotopic evolution of the fuel salt (Section 5) and of the nickel-based alloy

selected as structural material for the primary salt container and the axial reflectors (Section 6) are discussed. The main conclusion are drawn in Section 7.

## 2. Investigated reactor concept

### 2.1. The Molten Salt Fast Reactor

Details about the MSFR configuration can be found in Refs. [3,1,12]. In the following, a brief description of the reactor is given. Fig. 1 shows a schematic view of the MSFR. The molten salt mixture of the primary circuit acts as fuel and coolant at the same

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