

MODELLING THE CORROSION PRODUCT TRANSFER IN FUSION SYSTEMS: THE OSCAR-FUSION CODE

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1. INTRODUCTION

Predicting the radioactive contamination of nuclear reactor circuits is a significant challenge for plant designers and operators. To simulate the transfer of contamination in the primary system of PWRs, the CEA, in cooperation with EDF and Framatome, has been developing a simulation code called OSCAR (tOol for Simulating ContAmination in Reactors) since the 1970s. OSCAR is the merging of two previous codes in 2008 [1]: PACTOLE for activated corrosion products (ACPs) and PROFIP for actinides and fission products [2].

Despite differences in design and operating conditions between the PWR primary system and the primary heat transport systems (PHTSs) of the tokamak water cooling system (TCWS) of fusion reactors like ITER and DEMO, the OSCAR code has been applied to fusion reactors, resulting in OSCAR-Fusion (formerly known as PACTITER, which was an adaptation of PACTOLE to ITER [3, 4]). This adaptation was made possible due the physical modelling and modularity of the OSCAR code [5].

This paper describes the modelling of ACPs transfer applicable to different types of nuclear reactors, with specific details provided for fusion reactors. Finally, further improvements and needs are discussed.

2. OSCAR CODE MODELLING

2.1. Modelling of nuclear systems

The OSCAR code modelling is based on the arrangement of control volumes (also called regions). A system is discretized into as many regions as necessary defined according to their geometric, thermal-hydraulic, neutronic, material and operational characteristics (see an example of the OSCAR discretization of an ITER PHTS in Fig. 1).

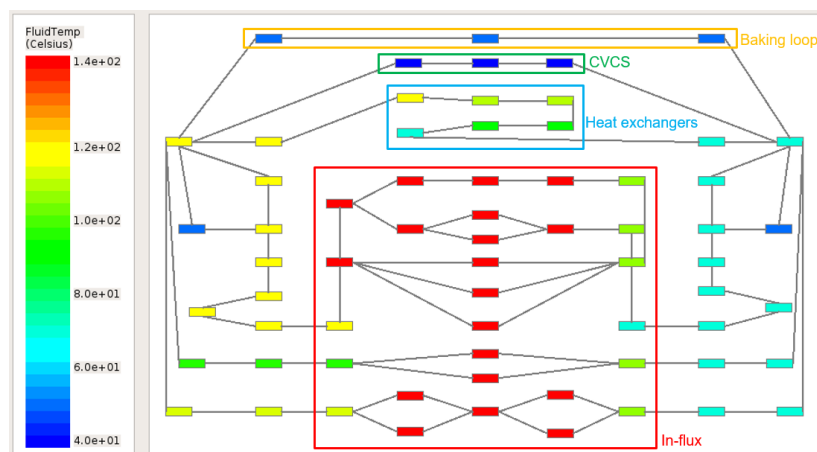


FIG. 1. OSCAR-Fusion v1.4.a - Discretization of the ITER IBED PHTS (coolant temperatures for burn phase) [6].

Several media can be defined in each control volume (see Fig. 2):

- Immobile media:
 - Base metal: material composing the system components (stainless steels, Ni-base alloys, RAFM (reduced activation ferritic-martensitic) steels and Cu-base alloys for fusion reactors...);
 - Inner oxide layer: a non-porous rough Cr-rich layer, which completely coats the base metal;
 - Deposit / Outer oxide layer: a porous rough Fe-Ni-rich layer with Cu for fusion reactors, which coats the inner oxide layer.
- Moving media due to the coolant advection:
 - Particles: assumed to be spherical with a grain size distribution following a log-normal law;
 - Ions: dissolved species.
- Trapping media for the coolant purification in the CVCS:
 - Filter for Particles;
 - Ion-exchange resins (IER) for Ions.

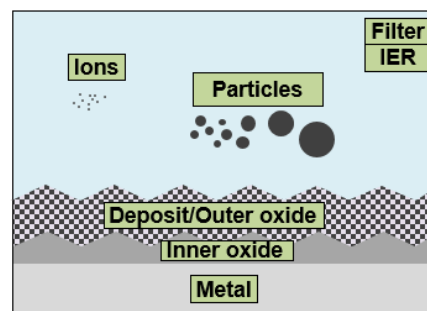


FIG. 2. OSCAR v1.4.a - Media taken into account in the modelling.

2.2. Chemical elements and isotopes

The main chemical elements and their isotopes taken into account in the OSCAR v1.4.a code are those composing the materials of the reactor nuclear systems that generate the main ACPs: Co, Cu (for fusion reactors), Cr, Fe, Mn, Ni, Ag, Sb, Zn and Zr. The radioactive half-lives of the radioisotopes taken into account in the OSCAR code range from seconds up to millions of years [7].

2.3. Mass balance and transfer mechanisms

The OSCAR code calculation kernel solves a system of mass balance equations for all isotopes (stable and radioactive) in all media in all regions at each adaptive time step (from some seconds to some days) using Eq. (1) below:

$$\frac{\partial m^i}{\partial t} + (\dot{m}_{out}^i - \dot{m}_{in}^i) = \sum_{sources} J_{transfer}^i - \sum_{sinks} J_{transfer}^i \quad (1)$$

where m^i is the mass of isotope i in a given medium [kg], t the time [s], $(\dot{m}_{out}^i - \dot{m}_{in}^i)$ the advection term of isotope i [$\text{kg}\cdot\text{s}^{-1}$] and $J_{transfer}^i$ a transfer mass rate of isotope i between 2 media or 2 isotopes [$\text{kg}\cdot\text{s}^{-1}$].

Thus, the OSCAR code calculates the masses of corrosion products and the activities of ACPs in the solid and liquid phases of nuclear systems as a function of time during normal operation over several decades and during transients down to a few seconds.

The transfer mechanisms taken into account in OSCAR v1.4.a are indicated in the yellow boxes in Fig. 3.

The models of the main mechanisms, i.e. corrosion-release, dissolution/precipitation, erosion, and deposition, are briefly presented below.

The OSCAR chemistry module, PHREEQCEA (a version of the PHREEQC code [11] extended to the PWR temperature range) and a CEA thermodynamic database gathering experimental, extrapolated and literature data [12] are used to calculate the thermodynamic equilibrium concentration of each element in the coolant C_{eq}^{elt} , the molar fraction of each solid phase (solid speciation), the pH at temperature, and the dihydrogen or dioxygen partial pressure p_{H_2} or p_{O_2} . For fusion reactors, Cu data were integrated into the PHREEQCEA thermodynamic database, especially based on an experimental campaign conducted by the CEA to acquire Cu solubility data for ITER divertor PHTS conditions [3].

2.3.3. Erosion

Erosion of a deposit results from the coolant friction forces. The erosion mass rate of isotope i , $J_{erosion}^i$ [kg.s⁻¹], is given by:

$$J_{erosion}^i = f_{dep}^i m_{eros} E_{eros} / \Psi_{eros} \quad (5)$$

where f_{dep}^i is the mass fraction of isotope i in the deposit / outer oxide layer, m_{eros} the mass of the deposit that can be eroded [kg], E_{eros} is the erosion coefficient [s⁻¹] based on the Cleaver and Yates model [13] depending on the shear stress at the wall and the dynamic viscosity of the coolant, and Ψ_{eros} the erosion resistance coefficient.

2.3.4. Deposition

The deposition mass rate of particles takes into account:

- Laminar [14] and turbulent [15] diffusion (mass transfer coefficient h [m.s⁻¹]),
- Sedimentation for horizontal components [16],
- Thermophoresis for temperature gradients between the coolant and the walls [17],
- Nucleate boiling deposition [18, 19],
- Flow disturbances caused by valves, elbows, etc., through relaxation lengths.

The deposition mass rate of isotope i , $J_{deposition}^i$ [kg.s⁻¹], is given by:

$$J_{deposition}^i = f_{part}^i S_w v_{depos} C_{part} \quad (6)$$

where f_{part}^i is the mass fraction of isotope i in the particles, v_{depos} the deposition velocity of particles [m.s⁻¹], and C_{part} the particle concentration [kg.m⁻³].

2.4. Input and output data

To use OSCAR, it is first necessary to provide a set of input data by using an input graphical user interface (GUI):

- Geometric and thermal-hydraulic data of each control volume: hydraulic diameter, wet surface, fluid velocity, flow rate, bulk and wall coolant temperatures, horizontal/vertical position;
- Material characteristics: initial composition, initial thickness, density, roughness, porosity and tortuosity. Any possible surface treatment is taken into account via the experimental corrosion and release rates;
- Neutronic data: nuclear power fraction in each in-flux region, associated with the NUCLEO database defining neutron reactions and activation rates for OSCAR. For fusion reactors, NUCLEO comprises all pertinent neutron reactions on all elements, including Cu, like $^{63}\text{Cu}(n, \gamma)^{64}\text{Cu}$ or $^{63}\text{Cu}(n, \alpha)^{60}\text{Co}$, along with the associated activation rates arising from the fast neutron flux.

- Operating data: nominal power, boron, lithium, dihydrogen and dioxygen concentrations as a function of time. A Zn injection rate can also be defined;
- Reloading of components when necessary (e.g., PWR fuel assemblies, steam generator replacement);
- Purification: efficiency of the filter and ion exchange resins for the CVCS.

It is possible to simulate transients such as the cold shutdown procedure or plasma pulses for fusion reactors by adjusting operating parameters like the nominal power, pressure, temperature, flow rate, boron, lithium and concentrations of dihydrogen and dioxygen.

The OSCAR results are plotted using an output GUI. These results include masses, activities, dose rates, transfer mass rates, chemistry parameters (equilibrium concentrations, solid speciation, pH_T , partial pressures, dissolution surface reaction rates, dissolution velocities, etc.) and thermal hydraulic parameters (density, viscosity, Reynolds number, Schmidt number, mass transfer coefficient, etc.).

2.5. Calibration-Validation

The transfer mechanisms need to be calibrated because some parameters of the physical models presented above (dissolution surface kinetic constants, proton reaction orders, erosion coefficient, and deposition velocity) are scarcely known in primary system conditions. These parameters are determined by simulating experiments in test loops [10, 20] and operation of a typical PWR [21].

Global validation of the OSCAR code was ensured by comparing the simulation of the power operation for several cycles and cold shutdowns of 6 PWR units with contamination measurements in these 6 PWRs (see one of the units in [7]). The calibration and the validation of OSCAR was possible thanks to the wealth of operating experience (OPEX) collected from the EMECC contamination expertise assessments. To date, about 430 EMECC campaigns have been performed by the CEA in 76 different French and foreign PWRs since 1971 [22, 23]. In addition to the γ surface activities of ACPs (^{58}Co , ^{60}Co , ^{54}Mn , ^{59}Fe , ^{51}Cr ...) measured using the EMECC device [24], the OSCAR results were compared to other on-site measurements: volume activities and chemical element concentrations.

3. DISCUSSION

Thanks to the world-unique feedback from the EMECC campaigns, the OSCAR code's validation domain encompasses both power operation and cold shutdowns of PWRs under primary and auxiliary circuit conditions. This includes a temperature range from 20 to 350 °C, covering both reducing and oxidizing environments, basic and acidic conditions, and laminar or turbulent flow regimes. Considering the similarities between the PHTS conditions in fusion reactors and PWRs¹, the OSCAR-Fusion code can benefit from the validation of OSCAR.

However, because of the distinct characteristics of fusion reactors compared to PWRs, such as pulsed operation, the use of Cu-base alloys and RAFM steels, the presence of a magnetic field, higher thermal flux and neutron flux, and distinct thermal-hydraulic conditions, it is essential to carry out studies and experiments in test loops to obtain data on these factors for the development and validation of the OSCAR-Fusion code.

¹ The conditions in the water-cooled lithium-lead breeder blanket (WCLL-BB) PHTS of DEMO are similar to those in the reactor coolant system of PWRs [25]. For the divertor PHTS of DEMO, the water temperature can reach 250 °C or even higher [26].

The materials in the water cooling systems of European DEMO (Eurofer-97 for the WCLL-BB and CuCrZr for the divertor plasma-facing components (PFC)) will be exposed to similar or even one order of magnitude higher heat fluxes (up to 10-20 MW/m² for the divertor [27]) compared to the fuel cladding in PWRs. It is well-known that high-duty core PWRs experience subcooled nucleate boiling, which intensifies the formation of corrosion product deposits on the fuel rods (commonly referred to as crud) [28]. This phenomenon can potentially result in crud-induced localized corrosion (CILC) events that may lead to cladding failure. It is highly probable that subcooled nucleate boiling will occur in the WCLL-BB and divertor PHTSs of DEMO [25], resulting in the formation of thicker corrosion product deposits, consequently ACPs, increasing material temperatures, and thus exacerbating corrosion. Therefore, experiments to determine the corrosion rates of RAFM steels should be conducted up to a temperature of 350 °C ($T_{\text{sat}@15,5\text{MPa}} = 345 \text{ °C}$), which has not been the case so far, possibly even higher due to the likely presence of a significant deposit thickness caused by subcooled nucleate boiling. It should be noted that the OSCAR code takes into account the effect of subcooled nucleate boiling on deposition (see section 2.3.4).

Similarly to PWRs [29], colloidal transport, which can be significant in fusion reactors, will require measuring the zeta potential of Cu-rich particles and RAFM steel oxide particles under various thermal and chemical conditions. These data will contribute to the new deposition model implemented in the version of the OSCAR code under development [29, 30]. Regarding this matter, particle size distributions in various PHTSs need to be determined since the particle deposition rate depends on their size.

The effect of chemistry on the deposition of colloids under subcooled nucleate boiling conditions should also be studied in DEMO conditions, as this effect could be significant, as suggested by a test conducted under PWR conditions [31].

Due to fast neutron reactions, reaction products have high recoil energy, which can eject nuclides from oxide particles. This process tends to introduce radioactive nuclides into the fluid from materials exposed to the high neutron flux of fusion reactors. The consideration of recoil nuclei was part of the PACTITER modelling, and this model will also be incorporated into a future version of OSCAR-Fusion.

The high flow velocity of 13-15 m.s⁻¹ in CuCrZr PFCs is likely to result in flow-assisted corrosion (FAC), especially considering the environment may periodically become slightly oxidizing (cyclic variation from reducing to oxidizing due to the plasma pulsed mode) [26, 32]. Indeed, despite the addition of hydrogen into the PHTs water, due to the high neutron flux in the PFCs, it is possible that the oxidizing species formed by radiolysis may not be completely recombined, thus making the environment slightly oxidizing [26]. The effects of erosion corrosion can be simulated using the corrosion model of the OSCAR code (see section 2.3).

The intense magnetic field in fusion reactors can have effects on material corrosion and the deposition of corrosion products [33], especially ferrite particles. A study is currently underway as part of M. Molinari's thesis (Sapienza University of Rome) to develop models for the OSCAR-Fusion code that consider the effect of the magnetic field.

The injection of zinc into PWRs can, under certain conditions, have a beneficial effect on primary circuit contamination (especially reducing the incorporation of Co-60 into chromites and corrosion) [34]. Particularly due to their low Cr content, it is uncertain whether zinc can have a beneficial effect on RAFM steels and copper alloys. Experimental tests with zinc injection should be conducted on these materials under fusion reactor PHTS conditions. Zinc injection can be simulated using the OSCAR code [10, 35].

Finally, it should be noted that there is a plan to develop a version of OSCAR for the lithium-lead circuit of DEMO, known as OSCAR-LiPb, following the development of OSCAR-Na for sodium-cooled fast reactors (SFRs) [5].

4. CONCLUSION

The OSCAR code is a tool for simulating the transfer of ACPs in nuclear reactor circuits. It is based on a modular approach that allows it to be applied to different types of reactors, including fusion reactors (e.g., [6, 36-38]). While OSCAR-Fusion benefits from the validation of OSCAR for PWRs in a wide range of conditions, distinct features require additional validation for fusion reactors. Challenges related to the interactions between coolants and materials, especially RAFM steels and Cu-base alloys, in fusion reactors include subcooled nucleate boiling, high neutron flux, high coolant velocity, plasma pulsed operation, the magnetic field, and colloidal transport.

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