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First Numerical Simulations of Contamination of the PWR Primary Circuit by Activated Corrosion Products with the PACTOLE V3.0 Code

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Abstract --- Operating nuclear reactors are faced to occupational dose rate caused by activated corrosion products. In order to reduce this radiation field, the CEA, EDF and Framatome-ANP have developed the PACTOLE code aiming at the prediction of corrosion product behaviour in the Pressurized Water Reactor (PWR) primary circuit. The latest version of the code has been released in 2003. This version has been completely rewritten in an Oriented Object Language (in C++) in order to be able to include new physical modeling.

The goal of this paper is to present the latest version of the PACTOLE code, namely V3.0. One first describes the code modelling, and the resolution of the resulting instationary equations of mass balance. One highlights the new empirical approach for corrosion and release modelling which allows to take into account the impact of surface treatment. The PACTOLE V3 numerical method is detailed.

A comparison of the PACTOLE V3 code results with on-site measurements, deposited and volume activities of French PWR primary circuits (900 MWe PWR with alloy 600 and 1300 MWe PWR with alloy 690), is given. One finds a reasonable agreement between on-site measurement and numerical simulation for the deposited activities.

I. INTRODUCTION

The PACTOLE code, developed by the CEA, in co-operation with EDF and Framatome-ANP, aims at predicting the Pressurized Water Reactor (PWR) primary circuit contamination.

In a challenging industrial environment, the development of the PACTOLE code is still of major concern for CEA, EDF and Framatome-ANP.

Taking into account recent development relevant to corrosion product behavior, the latest PACTOLE code version, namely V3.0.f, has been released in 2003. The V3 version of the PACTOLE code has been completely reengineering and is intended to evolve as soon as new developments are available. Written in a fully object-oriented design, the PACTOLE V3 code is modular and easily evolving.

The aim of this paper is to present the PACTOLE V3.0 code and a comparison of numerical simulations with measurement of deposited and volume activities in two types of nuclear power plants (900 MWe and 1300 MWe PWRs).

In the first part of this paper, the modeling of the corrosion product behavior is described. It focuses on

improvements that take into account surface treatment impact on corrosion/release processes^a.

Typical applications of the PACTOLE code are reactor fuel cycle simulations (one fuel cycle corresponds approximately to one year). The consequence on the PACTOLE V3 development was the implementation of a numerical resolution for the instationary corrosion product transport equations. So, the second part of this paper presents the implicit time scheme used for the discretization of the equations and the numerical methods used for the resolution of the discretized equations. The comparison of the numerical simulations with experimental measurements is discussed in the next section. The last part of the paper gives an overview of the foreseen PACTOLE developments.

II. PACTOLE V3 GENERAL OUTLINES

The aim of the PACTOLE code is to predict the primary circuit contamination caused by activated corrosion products (volume and deposited activities), in nuclear reactors. PACTOLE has been used in the past either to help in reducing the contamination of operating PWR¹ or to help at designing new reactor concept such as tokamak, cooling loops of ITER for instance².

The former PACTOLE code version, named V2, showed some lacks of modeling³. Therefore, a new code version, namely PACTOLE V3.0, has been designed to account for recent developments relevant to the behavior of corrosion products and to help in understanding and modeling the physico-chemical processes.

II.A. Primary Circuit Representation

Based on a control volume approach, the primary circuit is represented by an arrangement of several volumes in which mass balance equations are solved. As shown in Fig. 1, displaying a typical modelization of a primary circuit, the loops are gathered into one because a homogeneous contamination is assumed for the loops. Nevertheless, the loops can be individually computed in order to study, for instance, the effect of Steam Generator (SG) composition or surface treatment on contamination repartition between loops.

The primary circuit is composed of one mainstream line to which derived circuits (like the CVCS) are connected. The reactor core can be multifold (e.g. threefold or fourfold), depending on the fuel management^b.

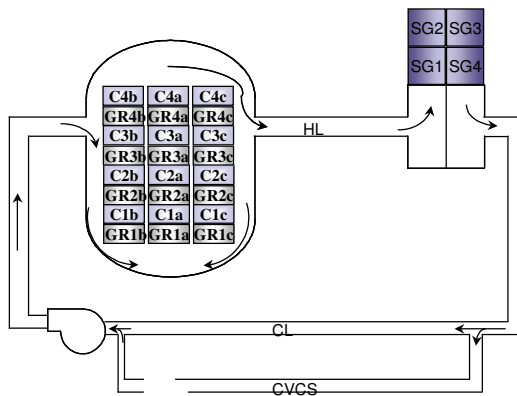


Fig. 1: Typical representation of a PWR primary circuit

II.B. General Input

For each control volume, representing a part of the primary circuit, input parameters are relevant to geometrical aspects, thermohydraulics considerations and material properties.

Since the PACTOLE code is based on control volume approach, the only requested geometrical parameters are hydraulics diameter and wet surface. The

^b 1/3 or 1/4 core assemblies are removed at every fuel cycle.

later is defined as the surface that can be oxidized and on which corrosion products can be deposited.

Concerning thermohydraulics data, classical parameters such as fluid velocity, flow rate and fluid temperature have to be provided. Furthermore, wall temperature is of major concern, since corrosion product equilibrium concentrations depend on the wall temperature gradient along the primary circuit.

Concerning material properties, the metal composition of each part of the primary circuit has to be given. In addition, surface roughness and surface treatments that appear to have a large influence^{4, 5} are provided in term of release and corrosion rates.

Obviously, corrosion product activation in reactor core is directly proportional to the neutron flux. Thus the power fraction, relative to the nominal power, has to be specified with care in every part of the core.

Reactor operating conditions, which may impact primary circuit contamination, are also provided in the PACTOLE input data. These data can be summarized as follows: power history, water chemistry (Li, B(pH), dissolved hydrogen) and reactor shutdown.

II.C. Form of Corrosion Products in a Control Volume

Although the PACTOLE code is based on a control volume approach, different physical states can be found in one control volume, also called region. These states, called media in what follows, have different behaviors, different corrosion products concentrations and can interact. Fig. 2 displays the different media that can exist in a control volume.

Directly produced by metal oxidation^c, the inner oxide is an enriched chromium layer. Dense and relatively thin, it is a low soluble oxide and acts as a protective barrier against metal oxidation.

The outer oxide, more soluble in reactor operating conditions than the inner oxide, is mainly composed of nickel ferrite. As a result of metal oxidation combined with ion precipitation, the outer oxide becomes contaminated by incorporating activated corrosion products.

Released from base metal, ions are carried by the fluid in the different part of the primary circuit where they can precipitate in the bulk, producing particles, which form another medium. Both particles and ions, which can be activated when crossing a core region, can respectively

^c Corrosion of zirconium base metal is not accounted for in the PACTOLE code.

deposit on the piping walls and precipitate either on the deposit or on the outer oxide.

At last, a peculiar medium, which aims at clearing the primary circuit, can be represented: the filter and ion exchanger resin devices.

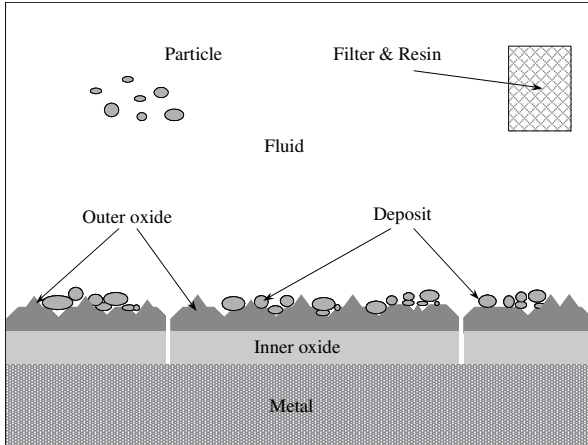


Fig. 2 : Media in a Control Volume for a PACTOLE representation (Fluid means ions)

II.D. Isotopes and Nuclear Reactions

The chemical elements and derived isotopes are declared by the user. In addition, the nuclear characteristics such as reaction rates or half-life and the filiations between active and stable isotopes can be specified by the input data.

II.E. General Mass Balance Equation

In every control volume, constituting the primary circuit, corrosion product behavior is described by mass balance equations, which are formulated as follows:

$$\frac{\partial m_i}{\partial t} + (\dot{m}_s - \dot{m}_e) = \sum_{\text{Source}} J_m - \sum_{\text{Sink}} J_m$$

Where m_i is the mass of the i^{th} isotope in a considered medium (see Fig. 2), t is the time, $\dot{m}_s - \dot{m}_e$ is the convective term (balance between input and output). Except for nuclear reactions, which are mass production/loss within the considered medium, J_m is an exchange mass rate between two different media.

II.F. Computer Aspects

Combined with a fully object programming language (C++), the PACTOLE V3 code has been written and designed using the Unified Method Language (UML).

Thanks to its code architecture, and confirmed by the development of a mock-up, the latest PACTOLE version is an easy evolving computer tool in which new media can be added and in which new models can be tested. Moreover, the class management process, introduced in the PACTOLE code, allows a non-limited number of control volumes, isotopes, fuel cycles... The only restriction comes from the memory of the computer on which the code runs.

The PACTOLE V3 code version is available on UNIX workstation and on personal computers using Windows operating system.

III. PACTOLE V3 MAIN MODELS

Major phenomena, which are involved in corrosion product transport, are accounted for in the PACTOLE code. The transfer mechanisms between all considered media are summarized in Fig. 3.

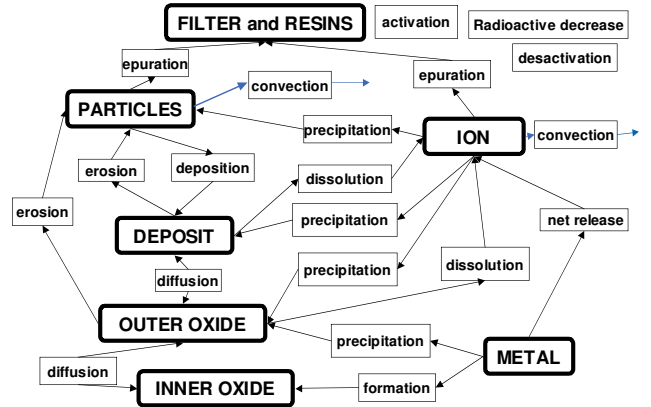


Fig. 3 : main mass transfers in the PACTOLE code

III.A. Corrosion, Ion Release and Ion Incorporation in Oxides

Experimental investigations and on-site deposited activity measurements have demonstrated the impact of surface treatment on corrosion and ion release in the fluid⁴. Even though the experimental evidences are nowadays clearly identified, their mathematical expressions are up to now still under questions⁵. In a first step, an empirical approach for corrosion and ion release processes has been chosen for the PACTOLE code modeling.

In the proposed modeling, corrosion is the process by which the base metal becomes oxidized. This oxidation leads to several mass transfers, which are: generation of an inner oxide, generation of an outer oxide and release of metallic ions directly in the fluid. These transfers are shown in Fig. 4. In the PACTOLE V3 code, corrosion and

release mass transfers are, respectively, directly dependent of a corrosion and of a release velocity, which are defined by the user. The experimental background results from a common work between EDF, Framatome-ANP and CEA^{6,7}.

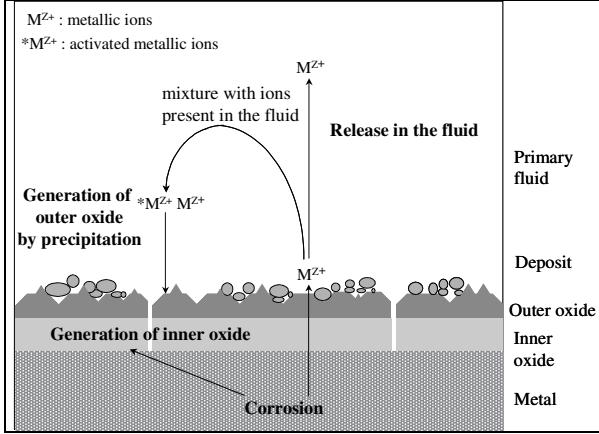


Fig. 4 : PACTOLE local modeling for inner and outer oxide generations and ion release

III.B. Ions Incorporation in the Oxide Layers

Various authors^{8,9} have highlighted that activated ions, which are present in the fluid, are incorporated either to the inner oxide or to the outer oxide while growing.

For the outer oxide, the ions incorporation mechanism is described as a function of the release velocity. This modeling allows to take into account the impact of the material surface treatment on the oxide contamination.

III.C. Ion and Particle Transport

After being released from base metal, metallic ions are transported in the primary circuit. Since solubility law depends on temperature and on water chemistry¹⁰, metallic ions can reach regions where their concentration exceed the saturation and therefore precipitate on wall surfaces or in the bulk, forming particles. When the ion concentration is below the saturation, the dissolution of the oxide and deposit occurs.

Transported by the fluid under particulate form, the corrosion products deposit on wall surfaces when submitted to the Brownian and turbulent diffusions and to thermophoresis effect. This last effect is important in steam generator tubes in which the thermal gradient between the fluid and the wall is high and positive¹¹. Moreover, the particles assume to follow a lognormal probability function in the PACTOLE modeling.

Both deposited particles and oxides can be eroded when hydrodynamics forces become higher than those from adhesion. Erosion produces new particles in the bulk fluid, which can be transported by convection in the other regions of the primary circuit. Concerning erosion process, the PACTOLE modeling assumes that above a threshold deposit thickness limit, deposit and oxide may be eroded.

The key point of these interactions, between the wall surfaces and the fluid, occurs when the deposit/oxides are submitted to a neutron flux (in-core regions). Indeed, deposited corrosion products become activated and therefore can be again transported in out-of flux regions of the primary circuit where they participated to the dose rate.

III.D. Reactor outages

During refueling shutdown of French PWR equipped with nickel based steam generator alloys (Inconel 600 or 690), due to controlled oxygenation of the primary circuit which increases the solubility by a factor of 100 to 1000, most of the ⁵⁸Co, along with other isotopes, deposited on the zircaloy rods, is released in the primary water¹². Even though the present PACTOLE modeling is simple for these operating conditions, it accounts for the global behavior of the corrosion products during reactor shutdown. Nevertheless when data concerning corrosion product solubility in oxidizing condition are available, the PACTOLE V3 version will be easily improved thanks to its new architecture.

IV. PACTOLE V3 NUMERICAL RESOLUTION

In order to obtain the isotope mass values, the global equations system must be solved with appropriated numerical methods¹³.

First, the equation system has been discretized in time. Two different time schemes have been used. In order to obtain large time-step, an implicit time scheme has been chosen for the equations of ions, particles, deposit, outer and inner oxides as follows:

Discretized equations for ions and particles:

$$\frac{m_i^{n+1} - m_i^n}{\Delta t} + d_m \left[\frac{C_i^{n+1}}{\frac{1}{2}(\rho_{f_{i+1}} + \rho_{f_i})} - \frac{C_{i-1}^{n+1}}{\frac{1}{2}(\rho_{f_i} + \rho_{f_{i-1}})} \right] = q_i^{n+1}$$

where Δt is the time-step defined as follows $t^{n+1} = t^n + \Delta t$, m_i^{n+1} (respectively m_i^n) is the i^{th} isotope mass at t^{n+1} (respectively t^n) in the considered media. Sink and source

terms are gathered in q_i . C is the concentration of the isotope and p is volume mass of water in a defined control volume.

Discretized equations for inner and outer oxide and deposit:

$$\frac{m_i^{n+1} - m_i^n}{\Delta t} = q_i^{n+1}$$

Since the metal and filter mass balance equations are not coupled with the others and no convective terms appear in these equations, an explicit time scheme has been chosen as follows:

Discretized equations for metal and filter:

$$\frac{m_i^{n+1} - m_i^n}{\Delta t} = q_i^n$$

The resolution of the discretized system is performed in three steps. In a first step, the metal masses are determined directly thanks to the explicit time scheme. In a second step, equations of ions, particles, outer oxide, inner oxide and deposit are linearized with a Newton method and then solved with a preconditioned GMRES method. In a third step, isotope masses in the filter and resin are determined thanks to the explicit time scheme.

In addition, a time-step auto-adaptive management has been implemented based on the Newton method iterations. This code feature allows the time-step to be larger when equilibrium states are reached. On the other side, when the code deals with transient behavior of corrosion products, such as reactor shutdown and initial cycle, the time-step is automatically reduced.

V. PARAMETRIC STUDY WITH PACTOLE V3.0

Considering the large number of interactions between the different media, lots of physical models had to be implemented in the code, meaning that a great deal of parameters have to be given. Some of these parameters could be found in the literature, some could be determined experimentally on analytical experiments and others have to be provided by the user. It is thus very important to determine the parameter that produces the greatest effects on the final results in order to know where to put the emphasis on physical modeling and experimental measurements. A parametric study has then been achieved on the parameters of the physical models: 35 parameters have been chosen and the simulation results considered are the surface activity of the deposit, the total surface activity and the volume activity of nuclides ^{58}Co , ^{60}Co , and ^{59}Fe in six regions (spacer grid made of Inconel 718,

core, hot leg, SG hot side, SG cold side, crossover leg and cold leg). The four most important parameters are finally the following (in decreasing order): enthalpy, activation reaction rate, release velocities for spacer grids and SG tubing, fraction of elements governing the release of spacer grid and SG regions.

VI. SIMULATIONS WITH THE PACTOLE V3 CODE

The objective of this section is to present the PACTOLE capabilities by comparing simulation results with experimental data. Two simulations are presented below: simulations of the contamination of running 900 MWe PWR (reactor A with alloy 600) and 1300 MWe PWR (reactor B with alloy 690). These simulations are compared to experimental data of volume and deposited activities¹⁴. Comparing PACTOLE simulations to on-site measurements is an important step for the code validation.

Reactor A (respectively B) is a PWR with a nominal power of 900 MWe (resp. 1300 MWe) that contains three (resp. four) individual loops. The following table gives an overview of the main characteristics, which may have an influence on corrosion products behavior, of the reactor A.

Table 1 : Main characteristics of reactor A

| | | |
|------------------|-----------------|--|
| In core surfaces | Fuel cladding | Zry-4 - 5020 m ² |
| | Spacer grids | In 718 / Zry-4 - 513 m ² |
| | Other | Stainless Steel - 182 m ² |
| | Steam Generator | Inconel 600 - 13413 m ² |
| | CVCS flow rate | 2.7 10 ⁻² % |
| | Chemistry | pH _{300°C} = 7.0 / 7.2 |
| | Remarks | Fluid chemistry was changed at fuel cycle #4 |
| | | Grid assembly composition changed at fuel cycle #6 |

Made of Inconel 600, the steam generator tube bundles are the largest source of nickel. Indeed, their total wet surface is more than 13000 m² (representing approximately 60 % of the total surface) and nickel represents 70 % of the metal alloy.

The second largest surface in contact with water, is the fuel assemblies made of zircaloy. As previously mentioned, the zirconium base metal does not participate to the corrosion product inventory but this surface is directly submitted to neutron flux and is therefore responsible to the activation of the corrosion products transported and deposited on fuel rods.

It is also important to mention that in the reactor A, the assembly spacer grids were made of Inconel 718^d for the 5 first fuel cycles, and that even though their surface is small, the spacer grids are nonetheless submitted to the neutron flux.

Concerning operating conditions, reactors A and B were operating under load follow as almost all French nuclear power plants. Fig. 5 shows the evolution of the power fraction, as used by the PACTOLE code, for the first seven fuel cycles of reactor A and five first cycles of reactor B.

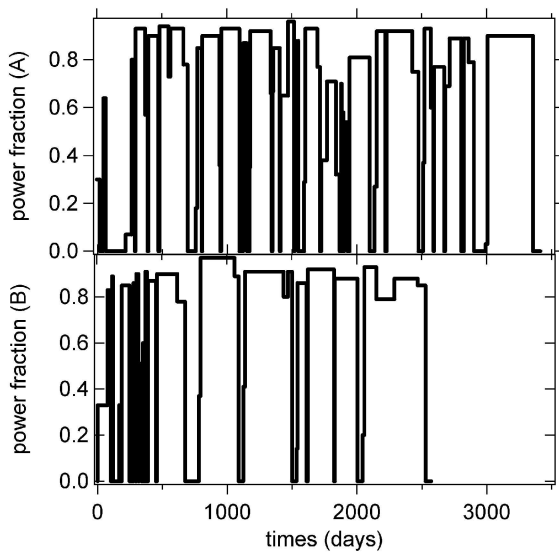


Fig. 5 : Nominal reactor power fraction of the reactor A first seven fuel cycles and first five fuel cycles of reactor B.

Nowadays, all French units are running with a so-called coordinated water chemistry¹⁵ at $\text{pH}_{300^\circ\text{C}}$ 7.2. When the reactor A started operating, its water chemistry was set to former specifications: the water $\text{pH}_{300^\circ\text{C}}$ was 7.0 for the first part of the fuel cycle and increased up to 7.4 at the end of the fuel cycle. Fig. 6 shows the pH evolution of the reactors A and B fuel as used by the PACTOLE code. Up to fuel cycle 3, the reactors A and B were running with the coordinated water chemistry at $\text{pH}_{300^\circ\text{C}}$ 7.0, from cycle 4, they have been operated with the coordinated chemistry at $\text{pH}_{300^\circ\text{C}}$ 7.2.

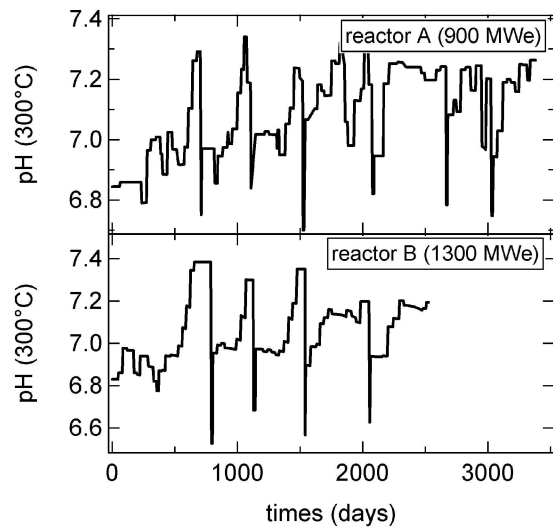


Fig. 6 Reactors A and B water pH (PACTOLE representation)

Fig. 7 and Fig. 8 respectively show the ^{58}Co and ^{60}Co deposited activities calculated by the PACTOLE code and the experimental gamma-spectrometry data on the Steam Generator (SG) tubing. The experimental uncertainties, which are about 20 %, are represented on the figures.

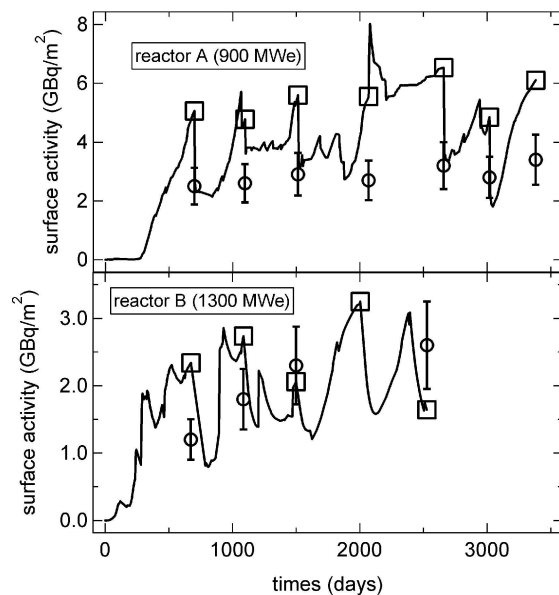


Fig. 7 : ^{58}Co deposited activity on SG tubing from PACTOLE results (continuous line with the squares for the times of measurements) and on-site measurements (circles with error bars)

^d Inconel 718 is approximately made of 52 % nickel.

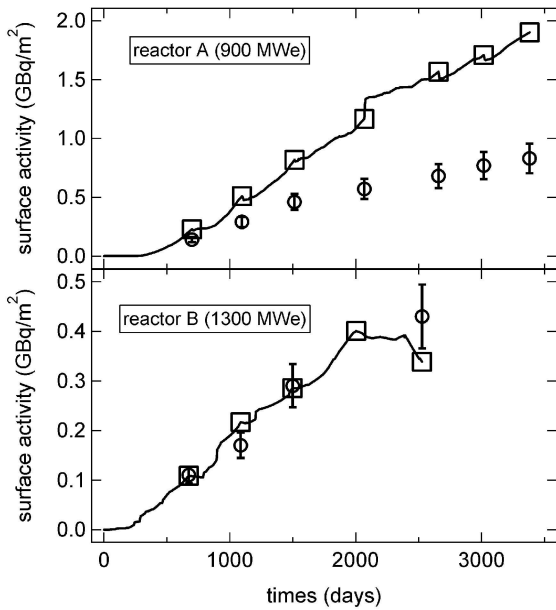


Fig. 8 : ^{60}Co deposited activity on SG tubing from PACTOLE results (continuous line with the squares for the times of measurements) and on-site measurements (circles with error bars))

It can be seen from these figures, that the PACTOLE code provides a reasonable estimation of the ^{58}Co and ^{60}Co deposited activity for the reactor B (1300 MWe PWR with alloy 690). On the other hand, the ^{58}Co and ^{60}Co deposited activity calculated by the PACTOLE code is over estimated for reactor A (900 MWe PWR with alloy 600).

Fig. 9 and Fig. 10 respectively represent the ^{58}Co and ^{60}Co deposited activities on the cold legs. Both computed results and on-site measurements are represented in these figures. Slightly different conclusions can be drawn from these two figures: the PACTOLE code also gives reasonable estimation prediction for ^{58}Co and ^{60}Co deposited activities but with a tendency to underestimation compared to on-site measurements. One should note however that the simulation presents a much better matching with experimental results at the end of the simulation (fifth shutdown for reactor A and seventh shutdown for reactor B).

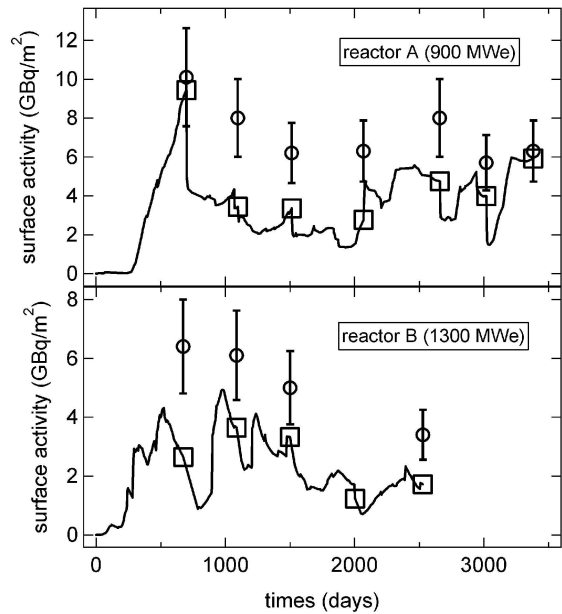


Fig. 9 : ^{58}Co deposited activity on the cold legs results from numerical simulations (continuous line with the squares for the times of measurements) and on-site measurements (circles with error bars)

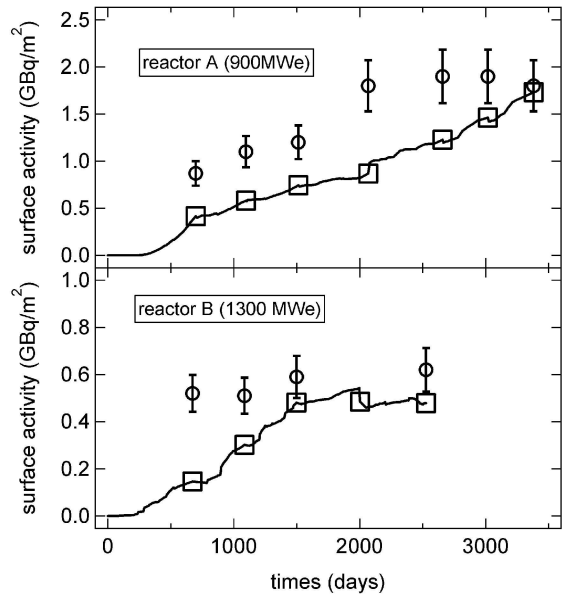


Fig. 10 : ^{60}Co deposited activity on the cold legs results from numerical simulations (continuous line with the squares for the times of measurements) and on-site measurements (circles with error bars)

Fig. 11 represents the ^{58}Co and ^{60}Co fluid activities (both ions and particles are accounted for) calculated with the PACTOLE code for reactor A. The correct tendency, i.e. a large increase, is reproduced for the first cycle for

^{58}Co and ^{60}Co . On the contrary, the following decrease and stabilization of the volume activities are not reproduced. One should note that the numerical simulations done with the previous version of the PACTOLE code (V2) suffered from the same drawback.

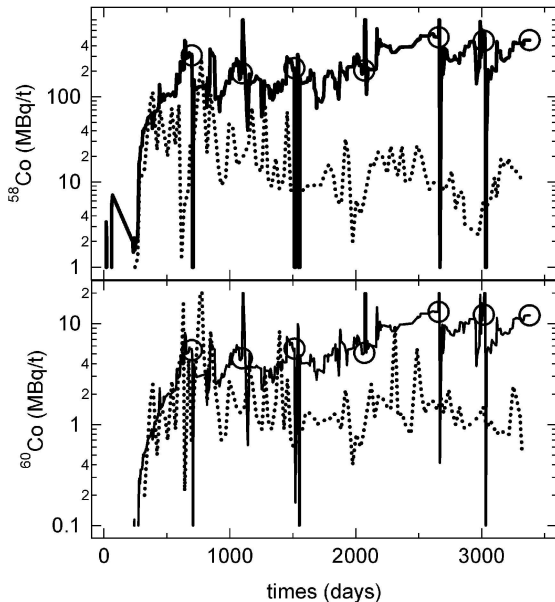


Fig. 11 : ^{58}Co and ^{60}Co volume activities simulated for reactor A (900 MWe) (continuous lines with the circles for the times of shutdown) and on-site measurements (dotted lines).

The new PACTOLE code is able to compute the global deposited activities in the different regions of the primary circuit even though some discrepancies can be found. On the other hand, the problem of computing in an accurate way the ion and particle concentration in the fluid remains: this problem is intended to be alleviated in a near future with a new solubility modeling as it will be seen in the last section of this paper.

Considering that some physical models are different in the V3 version of the PACTOLE code (in particular for the corrosion and release velocities) compared to the previous one (V2), a strict comparison of numerical results between the two code versions is then difficult in the sense that the input data could not be strictly identical.

One should note that the numerical simulations presented above are the first achieved with the new version of the PACTOLE code, meaning that the input data have not been ultimately adjusted so that the matching between calculations and on-site measurements would be even better. Considering the number of interactions between the different media, and thus of physical models, the number of physical parameters is

also quite large: this explains the interest of the parametric study presented in section V. This parametric study has considered physical parameters, excluding operation parameters (power fraction, activation rate, water, chemistry, fluid velocities, wall and fluid temperatures, geometrical parameters, etc.) that are supposed to be known. Of course, the physical parameters are identical for the two simulations when they have to be, meaning that only parameters related to different alloys (Inconel 600 or 690) are different. As already mentioned, the parametric study will allow to put more emphasis on the most influent parameters: a workprogram including modeling and experiments on analytical loops is being defined. In addition, a multicriteria calibration, using optimisation methods with or without constraints, is also foreseen afterwards to determine relevantly the remaining unknown parameters: it will require the simulation of a large number of different PWRs to take into account the great variability in the contamination of different PWRs.

VII. PACTOLE V3 FURTHER DEVELOPMENTS

Major improvements have been achieved in the V3.0 PACTOLE code version for the data processing architecture (design using UML combined with a fully object programming language, C++) and numerical analysis for solving stationary equations. This new architecture will allow the PACTOLE code of being an integration tool for the complex physics involved in contamination transfer studies. Some physical models have been already modified (among them corrosion and release velocities), but there are still both existing models to improve and new models to implement. In consequence, the three partners (CEA, EDF, Framatome-ANP) have decided to make a large effort to improve the physical modeling and every future version of the PACTOLE will present a significant appreciation of the physics. A particular attention will again be devoted to the validation process that includes verification of elementary models, of model couplings, comparison between simulations and experiments on system loops and finally comparison between simulations and measurements in reactors. One will undertake for every new version of the code this rigorous validation process that ends by a series of calculations of a list of validation cases (that remains identical for all versions of the code): this allows to identify the physical models that should be developed and completed for the next version. As mentioned in the previous section, the making of a wilful workprogram for improving the physical models and the data is thus under way and performed by CEA, EDF and Framatome-ANP. One could already identify some of the future important steps in the PACTOLE code development:

- Improvement of the corrosion/release mechanism.

Based on the present empirical mathematical expression,

the impact of macroscopic parameters such as solubility or temperature will be accounted for. This work will be performed on the basis of EDF and CEA experimental results obtained recently.

- Improvement of the oxide composition determination. A new approach for oxide determination and solubility calculation has been developed in the CEA. This model based on a survey of oxides thermodynamic behavior is aimed to predict in a more accurate way solubility values. It is designed, for instance, at predicting with a better confidence the corrosion product ion concentration that can be measured in operating PWRs.

- Addition of a specific module for shutdown. In the present code modeling, only reducing conditions can be treated: a real simulation of oxygenation phase is therefore impossible. Due, for a large part, to the lack of available data, an important effort is devoting to the data collection of oxide characteristics in oxidizing conditions.

VIII. CONCLUSIONS

Modeling the behavior of corrosion products in the PWR primary circuit is still of major concern as regards to present and future industrial challenges.

The latest code version, PACTOLE V3.0, is a major step forward for the prediction of reactor contamination by activated corrosion products. The main improvements are related to surface treatment impact on corrosion and release mechanisms and to a numerical scheme for solving transient behaviors. In addition, the code has been developed using oriented object methods (programming language, architecture design method) in order to get a flexible, and easily evolving computer tool.

The comparison of the simulations made with the PACTOLE code with on-site measurements of deposited activities demonstrates a reasonable agreement between numerical simulations and experimental data. Nevertheless, further calculations have to be performed with other reactors and with experimental loop results to get a good picture of the code capabilities.

Further code developments are already planned. Along with the improvements of existing models, new code capabilities will be available in a close future.

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