OVERVIEW OF ACP SIMULATION CODES SUITABLE FOR THE FUSION FIELD

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Abstract

Water corrosion codes in the nuclear industry are primarily developed to predict Activated Corrosion Products (ACP) generation and transport in cooling systems of nuclear fission power reactors. Adaptations of similar fission codes have been used to estimate this essential source term in the fusion field. Examples of codes built specifically for fusion cooling water systems include the TRACT and CATE series. OSCAR-Fusion is the most promising code in the field of fusion energy cooling systems, leveraging 30 years of expertise and on-field and experimental validation. However, the code is not fully validated due to unique features in fusion, such as pulsed operation, neutron fluxes, water chemistry, and magnetic field presence. The ACP inventory assessment for EU-DEMO water cooling systems will benefit from ITER modelling, and the breeding blanket WCLL Primary Heat Transport System (PHTS) will benefit from long-term simulation experience in the nuclear fission field. Gas corrosion codes are briefly discussed, as the only source of radioactive contamination is due to sputtering products. The theory of liquid metal corrosion is summarized, along with several mathematical models to represent the physical-chemical process.

1. INTRODUCTION

An overview of the water corrosion codes used in the nuclear industry, namely for fission and fusion reactors, is presented in this paper as the first topic. Some water corrosion codes have been identified, most of which were created to forecast the development and movement of ACPs in the cooling loop of nuclear fission power reactors.

The PWR-analogous PACTITER and OSCAR-Fusion codes were developed for fusion applications but starting from the fission versions, while the code TRACT was created particularly for the cooling water system of fusion reactors.

In the paper, the problem of gas corrosion codes is briefly discussed, in which the only source of radioactive contamination of the cooling loop is sputtering products.

The fundamentals of the theory governing liquid metal corrosion have been reviewed, along with a number of mathematical models that must be applied under specific circumstances to represent the physical-chemical process that includes species dissolution and transport, chemical reactions, and new phase formation. There are three key phases in this process:

Transport in the solid (metal or alloy), dissolving of the components of steel into the liquid, or mass exchange at the solid/liquid interface, and transport of corrosion products and impurities in the liquid are the first two.

2. WATER CORROSION CODES IN NUCLEAR INDUSTRY

Uniform corrosion in nuclear plant coolant primary circuits is crucial for the production of activated corrosion products (ACP) and water purification. Light Water Reactors (LWRs) experience undesirable effects such as corrosion, erosion, and deposition of corrosion products on heat transfer surfaces. Removal of corrosion products can be challenging due to their amount and activity. Rules and specifications are provided for LWRs to control water chemistry, ensure acceptable radioactive contamination, and minimize deposition within pressurized components.

To evaluate the risks associated with ACPs in fission nuclear plants due to water corrosion, codes and models have been developed. These codes provide basic information on the ACP inventory of cooling loops, corrosion rate of structural materials, radioactive inventory in the water purification system, and dose rates required to evaluate occupational radiation exposure.

In nuclear fission, ACPs are primarily from the fuel's cladding, structural materials of the cooling system, and radiolysis of water. Combining information from codes on water chemistry and radiolysis with those on ACP inventory is essential for a complete picture of operating conditions in nuclear plant cooling systems.

ACP codes are made by combining chemical and physical parameters to get the desired output, such as ACP inventory, water chemistry, and dose rate. Validation of codes is necessary due to the unique characteristics of each nuclear plant, and experimental testing is necessary for validation. Examples include the CORELE apparatus used for ITER plant to validate the release model of the PACTITER code.

2.1 Main water corrosion codes for fission and fusion cooling systems

In the following Table 1 main features of some fission and fusion corrosion codes are summarized. For the sake of the brevity of the paper further details and explanations are given in separate paragraphs for the codes that have been used

for ACP prediction in fusion power plants. They are PACTITER and OSCAR Fusion derived from analogous for the FPPs, and TRACT and CATE specifically developed for fusion water system.

2.2 PACTOLE code

The PACTOLE computer code, developed by CEA [1], predicts the time-dependent behavior of Activated Corrosion Products (ACPs) in PWR primary systems. It is considered the most updated activity transport code. PACTOLE v3.0 was developed to explain ACP behavior in PWRs and model physical-chemical processes, following PACTOLE v2.0 [2]. PACTOLE v3.0 received upgrades with two new releases, enhancing its main characteristics [3]. PACTOLE v3.1 improves the chemistry module and provides empirical expressions for corrosion and release rates. PACTOLE v3.2 treats oxidizing conditions and validates the transfer of corrosion products in ionic form, ensuring similar surface and volume activities to on-site measurements.

2.3 PACTITER code

The PACTITER code, derived from the PACTOLE code, simulates Activated Corrosion Products (ACPs) behavior in fusion reactor primary cooling systems [4]. The latest version, v3.3, is based on a control volume approach, with the primary circuit represented by multiple volumes. The code solves transient mass balance equations, as shown below:

$$\frac{\partial m_i}{\partial t} + (\dot{m}_s - \dot{m}_e) = \frac{\partial m_i}{\partial t} = \sum_{source} J_m - \sum_{sink} J_m$$

where mi is the mass of the ith isotope in a considered medium defined as a form for the corrosion products, t is the time, $(\dot{m}_s - \dot{m}_e)$ is the convective term (balance between input and output) and except for nuclear reactions, which are mass production/loss within the considered medium, Jm is the exchange mass rate between two different media.

Improvements in version 3.3 include: improved corrosion and release processes, treatment of oxidizing conditions, improved chemistry module (PHREEQC-CEA), corrosion and release kinetics, no solubility correction, an instationary mass balance equation, a non-limited number of control volumes, elements, and isotopes, a new approach for oxide determination and equilibrium concentration calculation, and a model based on a survey of oxides thermodynamic behavior.

Seven different media are taken into account in a control volume as depicted in FIG. 1.
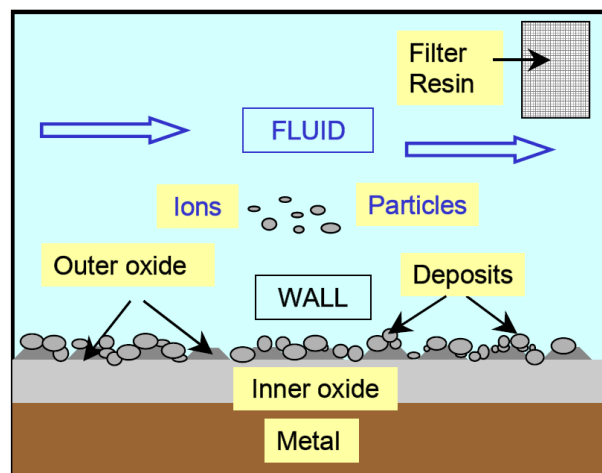.

FIG. 1- Media in a Control Volume for a PACTOLE/PACTITER v3.x representation

The mass balance equations determine corrosion and release processes based on time production rates, affecting material surface treatments and circuit contamination.

2.4 OSCAR code

OSCAR merges two previous codes [5]: PACTOLE for corrosion product transfer in PWR primary systems [2] and PROFIP for fission product transfer [6]. Validated against data from in-situ gamma spectrometry measurements, primary

coolant sampling, and experimental reactors, OSCAR offers a comprehensive solution for predicting contamination in reactors. The OSCAR code, developed through R&D cooperation between CEA, EdF, and Framatome, simulates contamination transfer in nuclear reactor systems during power operation and cold shutdown (20 °C - 350 °C - reducing/oxidizing - acid/alkaline) . It serves as a numerical tool for simulations, predictions, and knowledge-sharing on contamination. The code analyses corrosion product behavior and assesses ACP volume and surface activities of primary and auxiliary systems.

OSCAR has made several improvements compared to PACTOLE, including reviewing transfer mechanism models, making bug corrections, and updating the CEA thermodynamic database of the PHREEQC code. Numerical instabilities have been suppressed, and a user-friendly interface has been developed for generating input files and exploiting output files. OSCAR modelling is based on subdividing PWR circuits into elementary regions, solving mass balance equations for isotopes using the previous equation (1) described for PACTITER. Corrosion product transfer phenomena are simulated, and the dissemination rate for fuel damage is specified by the user in the input file. The isotopic distribution of disseminated fissile material is the same as at the fuel pellet surface, calculated by a specific module integrated in the code.

The fusion version of OSCAR-Fusion was developed in 2016 for ITER PHTS ACPs assessment purposes, adding copper as a ninth element. Additional information on OSCAR-Fusion latest version (v1.4) can be found in the paper presented in this TM [] and in the IAEA TECDOC-1912 (2020) [7] reporting contributions for IAEA events on "Challenges for Coolants in Fast Neutron Spectrum Systems: Chemistry and Materials (2017 and 2018).

2.5 TRACT code

The TRansport and ACTivation code, developed by UKAEA [8], simulates the flow and mass transport of isotopes in 1-D channels, handling liquid or gaseous coolants in fusion devices. The code calculates pressure drops, flow velocities, pumping power, and mass transfer of corrosion and dissolution rates of the bulk solid cooling channel material. It also predicts precipitation and/or crud formation and deposition, and radioactive decay (activation) of isotopes in irradiation conditions. The code is written in the IDL language with a graphical user interface and has been widely used in water cooling loops for ITER and power plant studies, with success in corrosion and activation of products. The code follows automatically unstable network isotopes' radioactive decay without user input, allowing arbitrary transmutations through a neutron irradiation field. It has two types of filters at nodes, retaining dissolved or crud isotope flow. The TRACT model was widely used for analyses of water cooling loops for ITER and power plant studies, predicting corrosion and activation of products. It has been successful in predicting hydraulic parameters of piping and loop components of austenitic stainless steel. The model was used to predict corrosion, transport behavior, and activity in the central column cooling loop of the Spherical Tokamak power plant.

2.6 CATE 2.0 code

The CATE code, developed by North China Electric Power University [9], aims to simulate the production and transport of ACPs in fusion reactor cooling loops. The first version of CATE has a two-phase homogeneous model covering main ACP behavior, including corrosion, release, dissolution, deposition, purification, activation, and decay. The Runge-Kutta method is used for numerical solutions, and special treatments on short-life nuclides and adaptive time step algorithms are implemented for high calculation efficiency. CATE v2.0 includes the production mechanism, three-node transport, and solution models. The code provides the composition and activity of ACPs in coolant and pipe wall, and version 2.1 [10] implements the water chemistry module and handling method for pulsed operation in fusion reactors.

TABLE 1 - Summary table with features of water corrosion codes

Code/model	Developed for	Features / Validation	Corrosion products	Fluids	Models
Error! Reference source not found.	CANDU PWR	Constant coolant chemistry	Appear both as particles and as solute in the coolant	Water + Boron Water+ LiOH	
Error! Reference source not found.	Specific PWR plant Oconee Unit 1, USA	Transport of both radioactive and non radioactive cruds relies on particulate removal mechanism from structural materials	They come from SS and from Inconel	Water	
Error! Reference source not found. Developed by Nuclear Development Corporation with Mitsubishi Heavy Industries Ltd.	Prediction of radioactivity level and evaluation of the effect of countermeasures in the primary circuit of Japanese PWRs.	The qualification of the ACE code was done by means of comparison of ACE simulated results with actual Japanese plant data.	Co58, Co60	Water	Corrosion rate, Deposition, Erosion, Dissolution, Precipitation, Incorporation in oxide film
Error! Reference source not found. Developed **by** KAERI	Prediction of the corrosion products and radioactivity transport in the primary coolant system of PWR	Validation done by comparison with results of in-pile PWR-simulating loop tests in the research reactor (MITR) with different water chemistry conditions.	The CPs formed on the SG Inconel and SS tubing surfaces under nominal PWR coolant chemistry are mainly nickel-ferrite or nickel-cobalt-ferrite	Water	PWR circuit comprises core, coolant, and SG, influenced by water chemistry. Main models are: • Soluble Transport • Particulate transport • Solubility of Iron
Error! Reference source not found. Developed by Dept of Nuclear Energy Reactor and System Chemistry Group, (Bulgaria)	For the calculation of time-accumulated activity of the main corrosion products radionuclides 60Co and 58Co on different parts of the primary system of WWER and NPPs.	The qualification of the MIGA-RT code was tested in NPPs EBO-1, LOVIISA-1, LOVIISA-2 and in French Beznau PWR NPP	MIGA-RT considers only Co58 and Co60 radionuclides.	Water with specific KNH2. KOH is introduced as a pH control agent	Corrosion product particle transport Activation Ionic transport Mass transfer of particles Release rate of corrosion products
Error! Reference source not found. Developed by Kang and Sejvar at Westinghouse	Predicting corrosion-product transport and radiation field buildup in PWRs using scientific understanding.	The semi-empirical model used is based on a theoretical understanding of the physical processes involved in radiation field build-up, it also uses experimental data from plants.		Water	Nodal transport diagram and the crud transport mechanism are modelled semi-empirically between nodes. Solubility directly impacts corrosion product release rate. Particles are transported in various regions of the loop in both particulate and soluble forms.
Error! Reference source not found. Developed by Nuclear Research Institute Rez plc, Czech Republic	Prediction of corrosion products behaviour and radioactivity build-up on the WWER and PWR primary system surfaces	VALIDATION FIELD: DISER code qualification involved comparing simulated results with actual WWER plant data from NPP Dukovany, LOVIISA, and Bohunice. Reactor	Co58, Co60, Mn54, Cr51, Fe59	Water	Thermodynamic models of solubility are used. The code considers a double oxide layer, with corrosion products being soluble ions, colloids, and particles. Ion transport is described as diffusion, while colloidal transport is governed by

		primary circuit is divided into 15 nodes with different conditions.			interaction with charged surfaces and potential barriers.
Error! Reference source not found. **Developed** by the Electric Power Research Institute	Prediction of corrosion products in PWR primary coolant circuits.	Good comparison with measured plant histories can be obtained using parametrically selected transport characterization data.	Co58, Co60	Water	The crud and activity transport is predicted only on the basis of a solubility difference as a driving force Coolant transients on corrosion product activity build-up are overlooked
Error! Reference source not found. **Developed** at the Kurchatov Institute in Moscow	The evaluation of radiation conditions in the vicinity of primary equipment in WWER-1000	The Russian Scientific-Technical Centre of Radiation Safety validated a code using operational data from NPP Zaporizhzhia, containing modeling algorithms for generating, transporting, and accumulating corrosion product species on primary circuit internal surfaces.	Co58, Co60, Mn54, and Fe59	Water	Loop segments are described by surface hydraulic diameter, wall temperature, fluid flow, and velocity. Mass transport between fluid and wall, and adjacent segments. considered with the following processes: •Corrosion and release from the base metal •Precipitation and particle dissolution in the coolant •Surface layer formed by crystallisation and deposition •Dissolution and erosion of the surface layer •Transport of soluble and particulate forms •Neutron activation and radioactive decay •Incorporation of activated products into both inner and outer oxide.
Error! Reference source not found. Developed by Mirza et al. in 1997.	Simulation of corrosion product build-up in reactor core, inner piping, and primary coolant loop, considering flow rate and power transients.	CPAIR code initially simulated corrosion product activity under flow rate transients, later modified for power perturbations.	Na24, Mn56, Fe59, Co58, Co60 and Mo99	Water	The model is based on the following physical processes: 1. production of ACPs through neutron flux core, 2. removal through water purification, 3. removal of activated isotopes from primary coolant loop structures, Simulation of coolant leakage and ACP decay.
Error! Reference source not found. Developed by Panos J. Karditsas (UKAEA Fusion)	To simulate the flow and mass transport of isotopes inside a network of 1-D channel for fusion reactors.	TRACT is written in the IDL language with a graphical user interface. TRACT simulates corrosion, erosion, dissolution, precipitation, and deposition	Basically, all the major radioisotopes present in the base metal under irradiation and in contact with water.	Water	This is how the physical model is organized: a. Fluid flow simulation calculates pressure drops, velocities, pumping

		processes in fixed channels with multiple layers.	Example: V52, Al28, V53, Mn56, W187, Cr51, Mn54, Ta182, Fe55, Long-lived isotopes		power using loop components from library. b. Mass transfer of corrosion and dissolution rates in bulk solid channel material; solubility influences precipitation, formation, and deposition.. c. Isotopes radioactive decay and convection downstream
Error! Reference source not found. Develop by CEA Cadarache The first version of PACTOLE was released in 1973. Subsequent versions have followed since then. Information provided in this Table refer to v3.2	For the prediction of contamination in the primary circuit of PWRs. The goal is to analyze the behaviour of corrosion products, activated or not, in order to determine the activity in the fluid and the deposited activity of out-of flux surfaces.	The PACTOLE code's qualification process began over 30 years ago, comparing simulated results with in-situ measurements. PACTOLE V3 code was reengineered to implement a numerical solution for corrosion product transport equations, tested using 900 MWe PWRs, and CIRENE loop test.	Fe59, Mn54, Co58, Ni59, Ni63, Co60, Cr51, Mn56, Zr93, Zr95	Water with LiOH, Boron and H2	Based on a control volume approach, the primary circuit is represented by an arrangement of several volumes in which mass balance equations are solved. Main models are: Corrosion, ion release and ion incorporation in oxides Ion and particle transport Activation
Error! Reference source not found. Develop by CEA Cadarache The first version of PACTITER was released in 1996, the latest v3.3 was released in 2008	To predict contamination in ITER's Primary Heat Transfer System (PHTS), analyze corrosion product behavior to determine fluid activity and out-of-flux surface deposited activity.It is the fusion version of PACTOLE v3.2	PACTITER v3.3 replaces Zr with Cu Validation not specifically in fusion environment, but exploits the experience gained in the validation in French PWR field	Fe55, Fe59, Mn54, Mn56, Co58, Co59, Co60, Cr51, Ni57, Co57, Cu64, Cu63, Cu65	Water with LiOH, and H2	Based on a control volume approach, the primary circuit is represented by an arrangement of several volumes in which mass balance equations are solved. Main models are: • Corrosion, ion release and ion incorporation in oxides • Ion and particle transport • Activation
Error! Reference source not found. Developed by CEA Cadarache The 1st version was released in 2008. The last version is v1.4 (2017). **OSCAR-Fusion** is the fusion version of OSCAR developed in 2016.	For the prediction of contamination in the primary circuit of PWRs, due to fission products and ACPs.	OSCAR combines PACTOLE and PROFIP codes for corrosion and fission product transfer in PWR primary systems, validated using 40+ years of in-situ gamma spectrometry data for accurate primary coolant control..	Elements/Radioisotopes: 8 elements (Ni, Co, Fe, Mn, Cr, Zn, Ag, Zr) 36 isotopes including 17 radioisotopes): Activated water products: N16, Ar41 radioisotope $t_{1/2}$: 7 s - 1,5 Ma	Water with LiOH, Boron and H2	Cooling loops divided in control volumes by material, geometry, thermal-hydraulics, neutronics, and operation Transfer mechanisms of CPs Corrosion-Release Dissolution/Precipitation Erosion/Deposition
Error! Reference source not found.	Simulation of the production and transport process of ACPs	The cooling loop is divided into three zones, which are the	V49, V52, V53, Cr51, Cr55, Mn56, Fe55, Fe59,	Water	Code includes production mechanism, three-node transport, and solution

Developed by the North China Electric Power University	in the cooling loops of fusion reactor, especially for CFETR of China in the future.	coolant, the in-flux pipe and the out-flux pipe.	Co-57, Co58m, Co58, Co60m, Co60, Ni57, Ni63	models. Phenomena modelled are corrosion, release, dissolution, deposition, purification, activation and decay

3. GAS CORROSION CODES

Simulation codes for the generation and transport of ACPs in nuclear fusion reactor gas cooling loops are unavailable due to the practical absence of corrosion products. Helium cooling gas is chemically inert and does not activate by irradiation. For fusion gas-cooled reactors, radioactive contamination is primarily due to sputtering products. The two gases considered as refrigerant for nuclear power plants (including also fusion are helium and CO2, with CO2 and He) is have different chemical stability and corrosion properties.

TABLE 2 below compares, amongst other properties, the chemical stability and corrosion [11] of CO_2 and He.

TABLE 2 - Chemical stability and corrosion properties of CO2 and He

	CO_2	Helium
Thermodynamic properties	Good heat capacity (for a gas). Good energy conversion capacity (low Cp/Cv ratio).	Good thermal conductivity (for a gas).
Chemical stability, corrosion	CO2 exhibits high chemical reactivity above 650°C, causing metal carburization and graphite oxidation. Exposure to radiation increases this reactivity, producing oxidizing and corrosive agents due to radiolytic decomposition.	Chemically inert, regardless of temperature. No usage limitation under high temperatures.
Availability, resources	Abundant and very inexpensive	Available and inexpensive

4. LIQUID METAL CORROSION MODELS

4.1 Introduction

Liquid metal corrosion is a crucial factor in heat transfer, particularly in fusion nuclear reactors. It involves species dissolution, transport, chemical reactions, and new phase formation. The process involves three steps: transport in solid metal or alloy, dissolution of steel constituents into liquid, and transport of corrosion products and impurities.

The first step is regulated by mass mobility in the solid, the second by dissolution/chemical processes at the liquid/solid interface, and the third by both mass convection and diffusion in the liquid. Through mass exchange, the transport processes in liquid and solid are associated with each other at the solid/liquid interface. Transport in liquid and solid can also result in impurity redistribution and the creation of new phases at the solid-liquid metal interface. The movement of corrosion products in liquids and their interactions with contaminants are significant in the corrosion of liquid metals.

Dissimilar metal mass transfer and temperature gradient mass transfer are the two types of mass transfer in liquid metal corrosion. Because of the thermodynamic necessity for equal element chemical potentials in all phases, dissimilar metal mass transfer happens in isothermal closed loops, whereas thermal gradient mass transfer occurs in non-isothermal systems. Depending on the transportation of CPs in the solid and liquid phases, as well as the dissolution reaction at the interface, liquid metal corrosion may result in surface recession of structural materials. The mass transfer rate governs mass transfer-controlled corrosion, whereas the diffusion rate in the solid phase governs activation controlled or dissolution controlled corrosion. Liquid metal corrosion is caused by a number of physical and chemical processes, including mass diffusion, convection, oxidation, and impurity formation.

4.2 Liquid metal corrosion theory

4.2.1 Basic equations

The mass transfer equation and mass flux for diverse species in solid or liquid mediums are the fundamental equations. The first can be written as follows:

$$\frac{\partial c}{\partial t} = \nabla J + q \quad [\text{g·m}^{-3}\text{·s}^{-1}] \qquad (2)$$

where q is a homogeneous reaction term in the material bulk and J is the flux.

The flux J can be expressed for liquid as it follows:

$$J_1' = -D_i' \cdot \nabla c_i' + \vec{u} c_i' \quad [\text{g·m}^{-2}\text{·s}^{-1}] \qquad (3) \qquad \text{for the liquid}$$

$\vec{u}$ is the velocity vector and D'i [m2·s-1] is the diffusion coefficient in the liquid.

For the species i in the solid with a corrosion rate R(t) as a function of the time and with the original point fixed on the surface of the solid material as shown in the next FIG. 2, the mass flux can be expressed as follows:

$$J_1 = -D_i \cdot \nabla c_i + R(t)c_i \qquad (4)$$

where Di is the diffusion coefficient of species i in the solid.
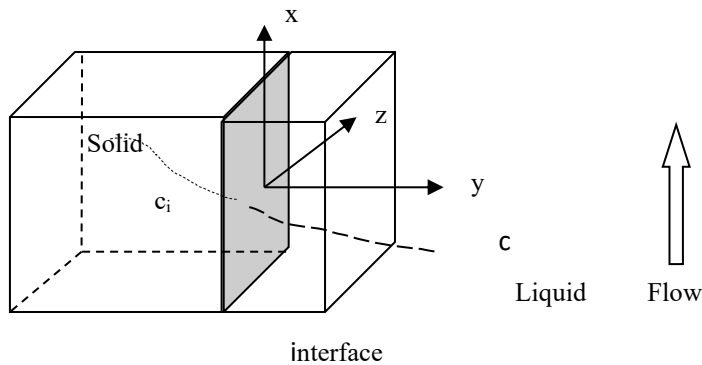

FIG. 2 - Coordinate of the corrosion by liquid metal

4.2.2   Mass Exchange at solid/liquid interface

At the interface along the normal direction, as shown in there is (a) mass flux in the liquid, Ji,1; (b) mass flux in the solid, Ji,2 and (c) mass flux through the interface due to absorption and desorption, Ji,3.

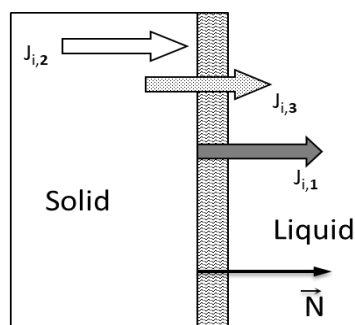FIG. 3 - Mass fluxes at solid/liquid interface

Considering a steady state or a quasi-steady state at the surface, we get:
$J_{i,1} = J_{i,2} = J_{i,3}$

Therefore, the transports in liquid and solid are coupled to each other through mass balance at the interface.

4.2.3   Corrosion rate for general cases

The dissolution reaction is the first step in liquid metal corrosion control, followed by mass transfer control. Net corrosion is controlled by either dissolution at the surface (activation control) or mass transfer in the liquid (mass transfer control). If the diffusion flux is less than the mass transfer rate, the surface will dissolve, resulting in a finite surface recession rate. In high flow velocity cases, the corrosion rate becomes independent of flow velocity, and the process becomes activation controlled. If the diffusion rate in the solid is greater than the dissolution rate, there is no surface recession. However, diffusion in solid can result in a selective corrosion layer at the surface, which can lead to material failure. In low diffusion rates, the diffusion layer or selective corrosion layer can be avoided, allowing all corrosion products entering the liquid from the dissolution of the surface or surface recession.

4.3 Corrosion product transport in liquid phase (non-isothermal cases)

The primary coolant loop of a liquid metal-cooled fast reactor experiences non-isothermal corrosion product transfer. The liquid metal flows through the reactor core, reaching its peak temperature at the core outflow, before passing via a

heat exchanger and reducing to its lowest value. The corrosion/precipitation process is sustained by the temperature gradient. Because of the solubility of the steel components, thermal gradient mass transfer is the primary corrosion process. The core outlet has the highest corrosion rate, whereas the heat exchanger exit has the highest precipitation rate.

The most relevant models to simulate this phenomena are

- Esptein Model [12]
- Sannier and Santarini's model [13]
- Kinetic corrosion model [14]
- Particulate model [15, 16, 17]

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4.4 Corrosion product transport in solid phase

Liquid metal corrosion can be classified into three types:

- stoichiometric corrosion,
- selective corrosion, and
- surface corrosion (with or without recession).

Stoichiometric corrosion involves all solid material constituents dissolved into the liquid, causing weight loss as a function of time. Selective corrosion occurs due to different diffusion rates of steel constituents, with the initial corrosion rate for noble elements being less than the rate dictated by their bulk fraction.

4.5 Oxygen effects on liquid metal corrosion

Oxygen is the primary contaminant affecting liquid metal corrosion. Iron-based steels experience increased corrosion in light liquid metals like sodium and sodium-potassium alloys, while heavy liquid metals like lead and lead-bismuth alloys may have protective oxide layers. Oxygen redistribution occurs between the liquid metal and structural components until the chemical potentials of oxygen in solid and liquid phases are equal.44

4.6 Discussion on liquid metal corrosion models

Corrosion by liquid metal does not involve electron transport in the liquid and is a physical-chemical process as opposed to corrosion by aqueous solution, which is an electro-chemical process. Some models of liquid metal corrosion were developed based on solid-phase mass transport, while others were developed based on liquid-phase mass transfer. In the survey presented the two types of models were coupled through mass exchange at the solid/liquid interface to determine the bulk corrosion rate or the solid surface recession rate.

Different corrosion models have been proposed for different situations and assumptions, but their applicability ranges have not been specified. These models were used for studying corrosion in nuclear reactors' major coolant loops and were compared to experimental data. Most studies agree, while others provide contradicting results. When flow velocity is high, activation controlled corrosion develops, which should be avoided in nuclear reactor design owing to probable mechanical erosion. The three models, Epstein's, Sannier and Santarini's, and the kinetic model, all agree that mass transport in the liquid phase controls corrosion.

Epstein's model predicts constant corrosion rate in a non-isothermal loop, assuming bulk concentration equilibrates to surface equilibrium concentration at the lowest temperature section. This results in a high corrosion rate, as the bulk concentration is higher than the average surface concentration throughout the loop. The other two corrosion models predict downstream effects and corrosion/precipitation zones, with the kinetic model being more complex and Sannier and Santarini's model requiring more assumptions. Most of the models for solid phase transport involve sodium corrosion. The two-region model predicts ferritic layer thickness within experimental errors, while the transient model shows a short transient process time compared to reactor operational periods. It is realistic to consider corrosion in the steady state in the liquid phase. In mass transfer control range, concentrations are the boundary conditions, while fluxes are the solid phase transport conditions. In activation control range, concentrations and fluxes are constant at the interface. The transport in the solid may be utilized for predicting the constituent distribution shift caused by corrosion in the solid phase, and the transport in the liquid can predict the surface recession rate by merging the models at the interface. In cases where model constants are unavailable, they can be estimated by fitting experimental data using simplified solutions. For instance, the bulk corrosion rate and parabolic oxidation constant in the oxidation-corrosion interaction model can be obtained by fitting the measured oxide layer thickness. This allows for long-term predictions of corrosion and oxidation interactions in Lead-Bismuth Eutectic (LBE) systems. Liquid corrosion models do not include pitting, stress, embrittlement, or penetration corrosion due to scarcity of studies. However, these corrosion types must be mitigated to prevent structural material degradation in fusion reactors. Further experimental studies and realistic models are recommended. Table 3 summarizes the main features of liquid metal corrosion models in Chapter 4, defining their relevance for estimating corrosion in fusion power reactors, even with non-fundamental changes.

Table 3 highlights the major aspects of liquid metal corrosion models discussed in this section 4, establishing their applicability for predicting corrosion in fusion power facilities even with non-fundamental changes.

TABLE 3 - Summary table with features oc liquid metal corrosion models

Model/Phenomenon	Relevance	Note
Mass Exchange at solid/liquid interface	YES	To be included in the simulation code
Corrosion product transport in liquid phase (isothermal cases)	NO	Because isothermal conditions do not exist for cooling system / some relevance might exist for liquid metal breeder systems
Corrosion product transport in liquid phase (non-isothermal case)		
Epstein's models)	YES For an ideal case of a loop with a hot and a cool isothermal zone, a heat exchanger and a heater.	Verify the relevance of various assumptions made, it cannot predict the downstream effects which have been reported experimentally, it can be applied to a loop with small ΔT It might be also applied to liquid metal breeder systems
Sannier and Santarini's model	YES	The model can predict both corrosion and deposition in a closed loop system. Four different cases to be chosen for simulating actual conditions
Kinetic corrosion model	YES	Verify the relevance of assumptions made to derive the solving equations giving • the concentration distribution in the mass transfer boundary layer, • the corrosion flux through the boundary layer, • the concentration of corrosion products in the bulk flow
Particulate model	YES	This model simulates the transport deposition and re-dissolution of small particles of corrosion products. For applying this model, the particle concentration, particle size and distribution must be known
Transport in solid	YES	Being one of the main steps involved in the corrosion by liquid metal must be complemented for an integral assessment of corrosion products by the other major phenomena involved: 1. mass transfer in the liquid phase 2. mass exchange at the solid/liquid interface
Transport in solid (Two region problem with): Model 1. surface with zero recession rate) Model 2. Surface with constant recession rate	YES	1. Model 1 is for the particular condition when the constituents of initially austenitic steel are depleted by corrosion process beyond a specific minimum threshold level, with the depleted layer becoming ferritic as in liquid Na 2. This model provides the thickness of the ferritic layer at the steady state, the concentration at the austenite/ferrite interface and the corrosion rate in term of weight loss
Surface recession rate determination	YES	Assuming, in the case of steels in contact with the liquid metal, the corrosion of iron that determines surface recession rate or the bulk corrosion rate
Oxygen effects on liquid metal corrosion	YES	Each integral assessment tool shall consider the oxygen effect, through the calculation of O2 solubility in the liquid metal and its distribution between the liquid metal and the structural materials in contact with. Effects have been calculated for liquid lead and Lead-Bismuth Eutectic (LBE)
Models of corrosion–oxidation interactions in liquid lead and LBE with oxygen control	NO	They might be of some interests in the case that liquid metal were lead or LBE

4.7 OSCAR-Na code

CEA developed the OSCAR-Na code to calculate the mass transfer of corrosion products and contamination in sodium fast reactors (SFR) [18]. The code includes a solution/precipitation model, focusing on diffusion in steel, diffusion through the sodium laminar boundary layer, equilibrium concentration of elements, and interface velocity due to bulk corrosion and deposition. The interfacial velocity due to corrosion or deposition is calculated using a numerical method and mass balance. The model's parameters, including iron equilibrium concentration and oxygen enhanced dissolution rate, have been assessed from literature reviews. The simulation of the French SFR reactor PHENIX with the first version V1.3 of OSCAR-Na was able to assess the correct amount of contamination and contamination profiles on heat exchanger surfaces for Mn54, Co58, and Co60 radionuclides. The analysis of the solution/precipitation model enables prediction of the impact of key parameters on contamination in a PHENIX-like reactor.

5. DISCUSSION AND CONCLUSIONS

This paper reviews water corrosion codes in nuclear reactors, focusing on fission and fusion reactors. Most codes were developed for predicting ACP formation and transport in cooling loops, with PACTITER and OSCAR Fusion codes being derived from PWRs. OSCAR-Fusion is the most promising code, utilizing 30-year experience in PACTOLE/OSCAR codes. However, validation experience is lacking, and its application to ITER and DEMO water cooling systems needs the support of the experimental validation. The paper also discusses gas corrosion codes, where only radioactive contamination is due to sputtering products.

The paper analyses liquid metal corrosion models and calculation tools, focusing on the physical-chemical process of species dissolution and transport, chemical reactions, and new phase formation. The OSCAR-Na code is aimed at calculating mass transfer of corrosion products and contamination in primary circuits of sodium fast reactors.

Given the complexity of the phenomena to be simulated with different models, it appears from analysis of the various codes listed in Table 1 for the simulation of corrosion phenomena in the cooling systems of nuclear plants and, more specifically, for the determination of the ACPs inventory, that the development of these was most often referred to specific situations of which a large number of physical parameters were well known, such as the single typology of nuclear reactor type or even the single plant or unit .

The models developed are based on semi-empirical parameters or on data that requires carrying out field measurements, while nevertheless accurately characterizing the physical phenomenon in accordance with computation capabilities. Therefore, the definition of a model or the development of a code should involve an exhaustive set of modeling experiments. It is important to consider both the role of experiments and the predictions made by computer codes. In combination with the selection of relevant materials, the ability to employ proven computer codes to simulate various water chemistries and operating circumstances for cooling primary systems offers the advantage of quickly scanning through possibilities while saving time and money.

On the other hand, experiments play a crucial role in the integral validation of computer code models, which are primarily concerned with metal release and corrosion mechanisms, oxide and particle dissolution, but also with oxide and deposit formation, oxide and deposit erosion, particle dissolution and deposition, and ion and particle convection. Obtaining determinant input data, such as metal corrosion and release rates over time, oxide morphology (such as inner porosity) and composition for the pertinent material composition and roughness, and water chemistry parameters, is another significant contribution anticipated from the research.

Fission-derived experience teaches us that some variations in less important input conditions of the problem, such as the variation of the composition of a given material in contact with the coolant or the state of surface finish of a material in contact, may lead to discrepancies between predictions of the model and experimental data, not previously recorded in the varied conditions. Additionally, the construction of codes for the estimation of the ACPs in the case of fusion must deal with other sources of uncertainty, such as the different refrigerant's temperature range in some cases (e.g.: 100-150°C and 240°C for ITER), which is different from that existing in a PWR, instead considered for DEMO WCLL cooling water system. Other notable variations include a lack of boron-required water chemistry and the presence of a strong magnetic field, to mention a few.

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