Overview of ACP Simulation Codes Suitable for the Fission and the Fusion Fields

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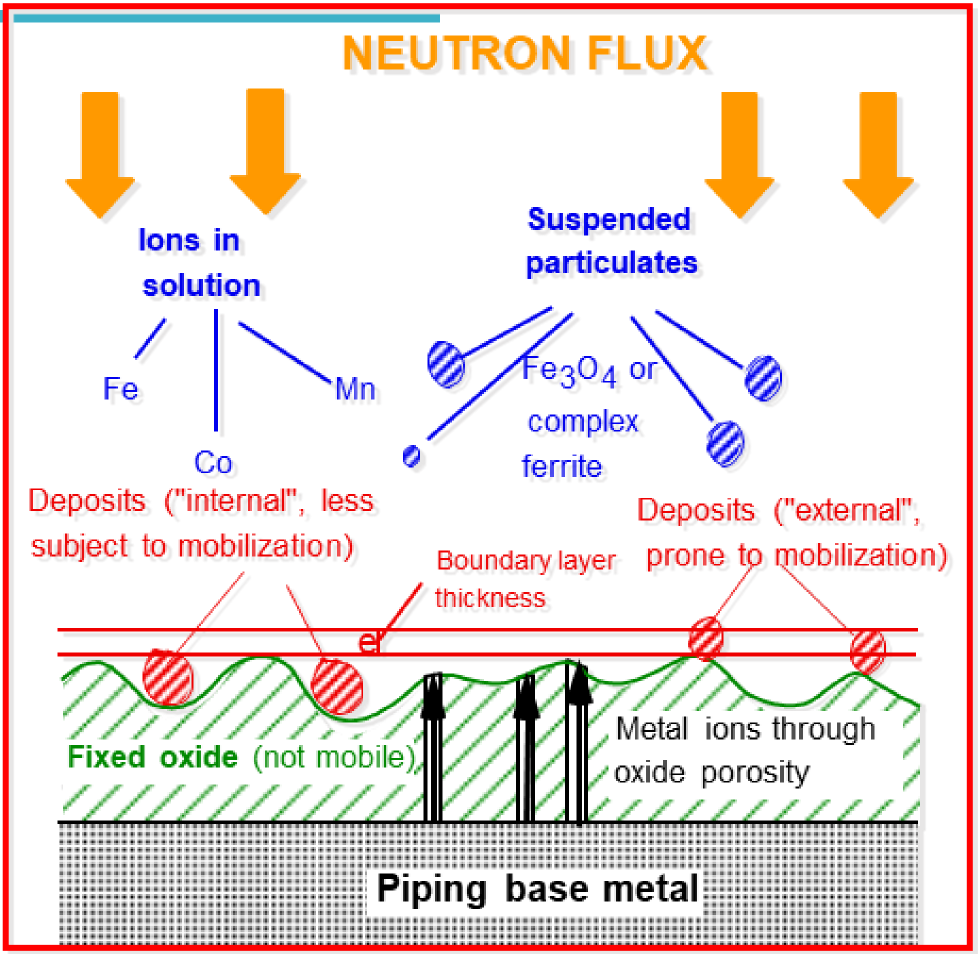
Technical Meeting (CM) on Preparing the Technical Meeting on Compatibility Between
Coolants and Materials for Fusion Facilities and Advanced Fission Reactors
IAEA Headquarters, Vienna 30 October-3 November 2023

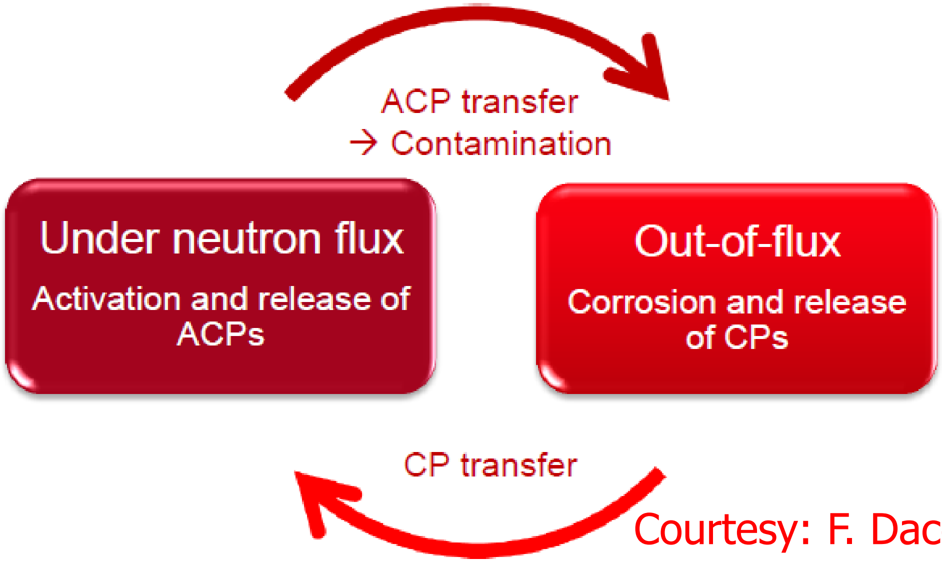
Summary

- ACPs generation and transport
- ACPs issues
- Water Chemistry Control
- Fusion phenomena not modelled in ACP codes
- Computer Codes for ACPs assessment in water
- Gas Corrosion Codes
- Liquid Metal Corrosion Models
- Experimental loops
- Conclusions

ACPs generation and transport



Principle of contamination transfer in a nuclear cooling system



ACP transfer → Contamination

Under neutron flux
Activation and release of ACPs

Out-of-flux
Corrosion and release of CPs

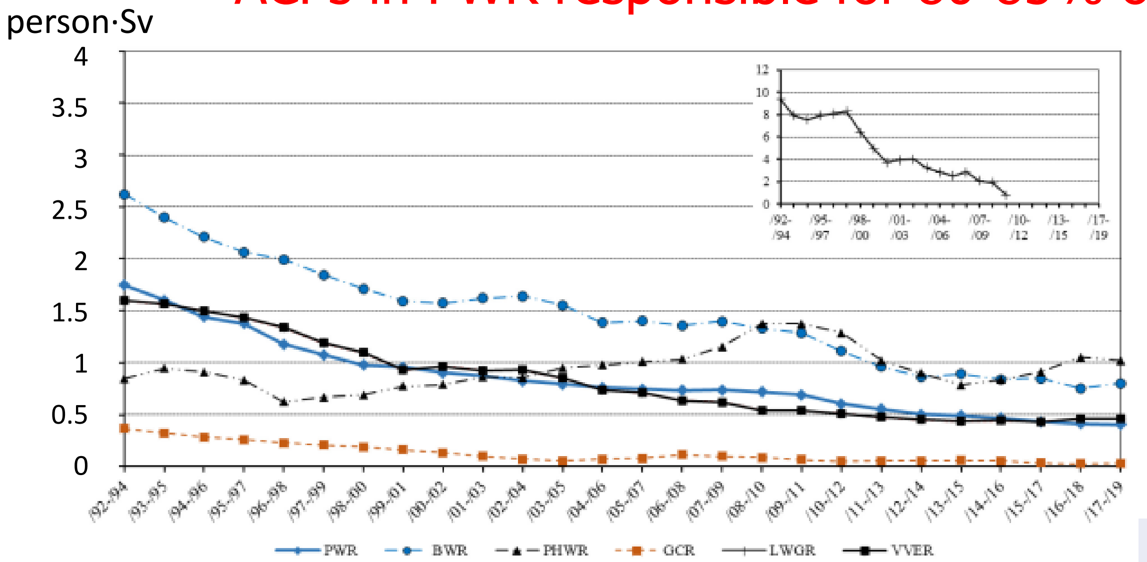
CP transfer

Courtesy: F. Dacquait, CEA

- **Radioprotection**: Reduction of ORE;
- **Environment**: Minimization of release/waste – Optimization of dismantling process – Source term in case of accident/incident
- **Availability**: Optimization of reactor operation

ACPs: an issue for worker collective doses

- ACPs in PWR responsible for 80-85% of ORE

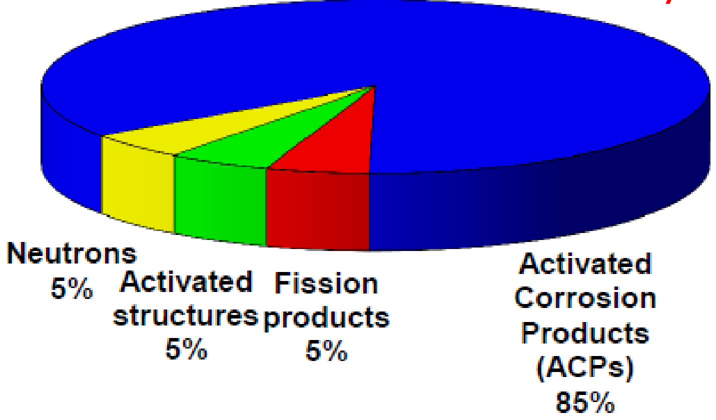


Three-year rolling average collective dose per reactor for all operating reactors
included in ISOE by reactor type, 1992-2019
(person·Sv/reactor) **Ref. [1]**

[1] Occupational Exposures at Nuclear Power Plants
Twenty-Ninth Annual Report of the ISOE Programme, 2019

Collective dose for operation and maintenance of PWRs

Courtesy: F. Dacquait, CEA



Ref. [1]	2019 average annual collective dose (person·Sv/reactor)	3-year rolling aver. 2017-2019 (person·Sv/reactor)
Pressurised water reactors (PWR)	0.41	0.41
Pressurised water reactors (VVER)	0.45	0.47
Boiling water reactors (BWR)	0.89	0.82
Pressurised heavy water reactors (PHWR)	0.82	1.01
Gas Cooled Reactor	0.03	0.033

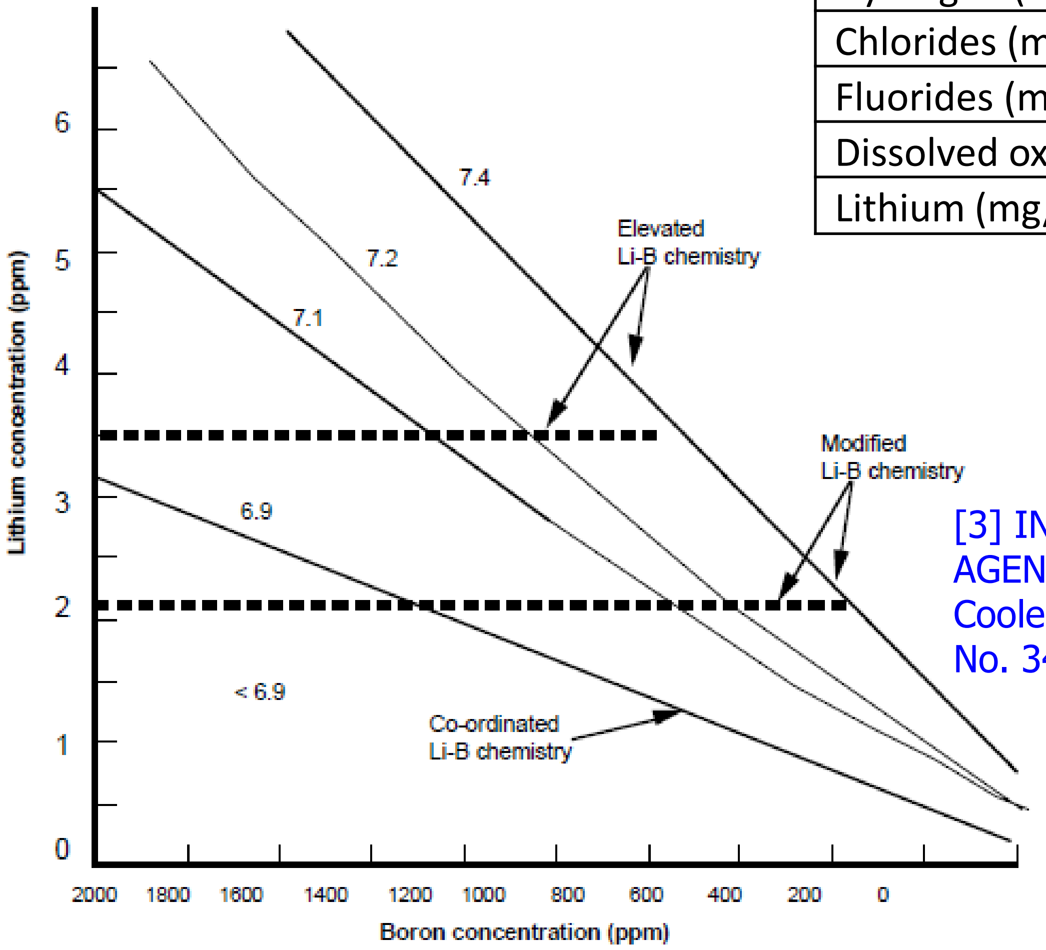
ACPs: issue for structural integrity and operation

1. Control of Corrosion is a MUST in reactor coolant
   - System integrity jeopardized
   - Activity transport
   - Build-up of corrosion → barriers to heat transfer (SG tube plugging)
2. How? By control of coolant chemical parameters (*pH, Eh,* H_2*, B, LiOH, KOH*)

- Activity transport in PWRs controlled by high pH
- Oxidising conditions promoting SSC in BWRs counteracted by H_2 addition
- Hydriding of Zr alloys in CANDU cores minimised by adjusting dissolved [H_2]

Water Chemistry Control in PWRs [3] with LiOH as pH control agent

Hydrogen (cm^3($_{STP}$)/kg H_2O)	25-50
Chlorides (mg/kg)	< 0.15
Fluorides (mg/kg)	< 0.15
Dissolved oxygen (mg/kg)	< 0.01
Lithium (mg/kg)	Consistent with station lithium programme



[3] INTERNATIONAL ATOMIC ENERGY AGENCY, Coolant Technology of Water Cooled Reactors, Technical Reports Series, No. 347 1993

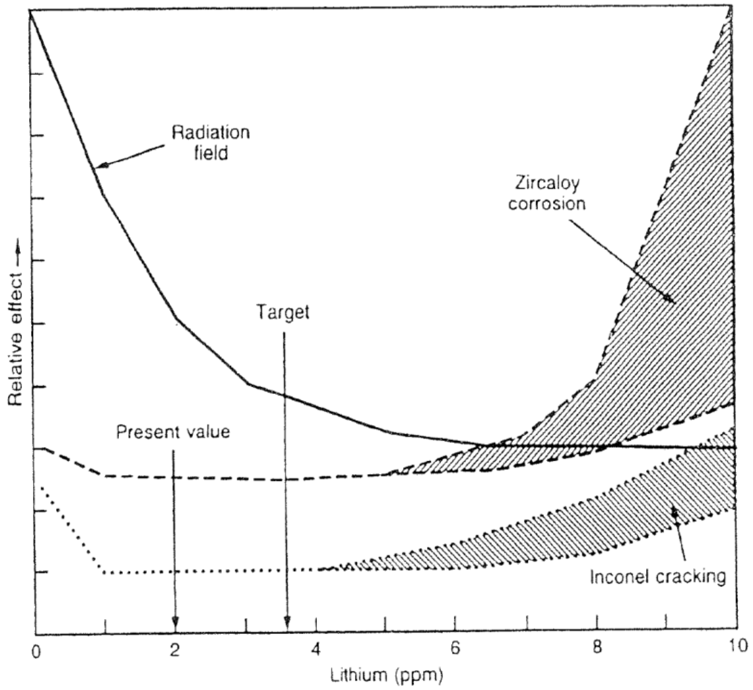


FIG. 13. Schematic diagram of PWR primary coolant chemistry; effect of lithium concentration (1200 ppm boron).

Water Chemistry Control
in PWRs [3] with KOH or ammonia as pH control agent

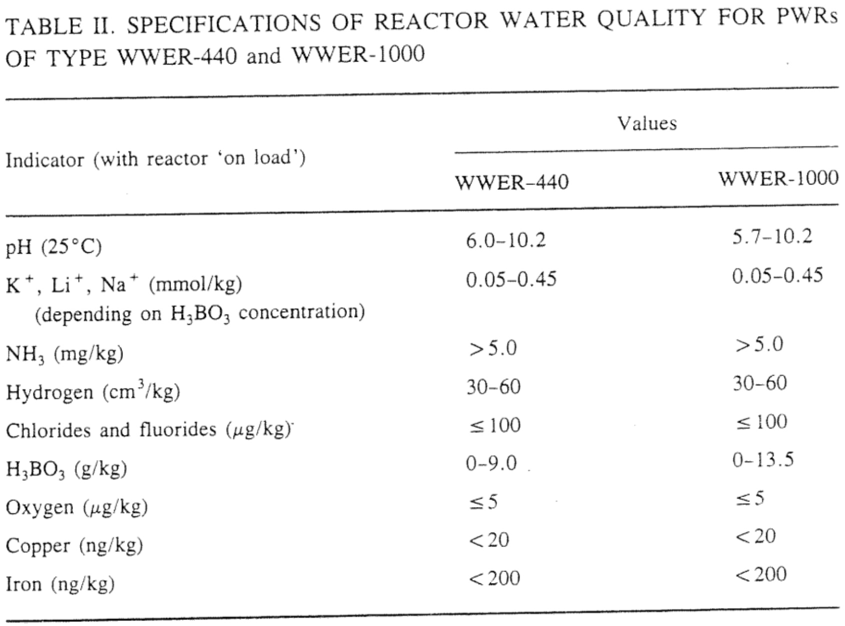
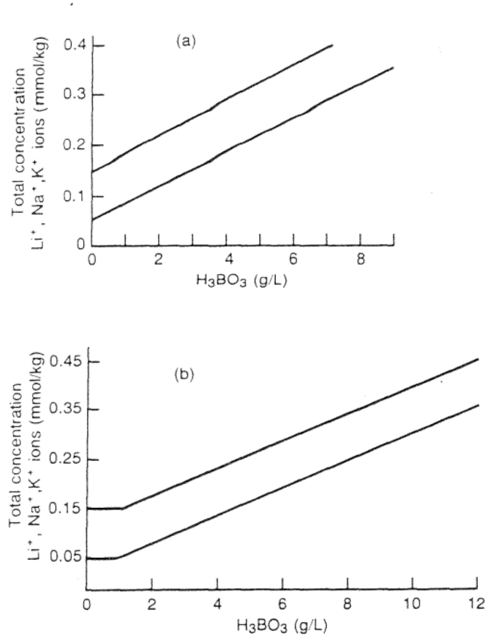


TABLE II. SPECIFICATIONS OF REACTOR WATER QUALITY FOR PWRs OF TYPE WWER-440 and WWER-1000

Indicator (with reactor 'on load')	Values	
	WWER-440	WWER-1000
pH (25°C)	6.0–10.2	5.7–10.2
K^+, Li^+, Na^+ (mmol/kg) (depending on H_3BO_3 concentration)	0.05–0.45	0.05–0.45
NH_3 (mg/kg)	>5.0	>5.0
Hydrogen (cm^3/kg)	30–60	30–60
Chlorides and fluorides (μg/kg)	≤100	≤100
H_3BO_3 (g/kg)	0–9.0	0–13.5
Oxygen (μg/kg)	≤5	≤5
Copper (ng/kg)	<20	<20
Iron (ng/kg)	<200	<200



Maximum and minimum values of total alkali ion concentrations plotted against Boric acid concentrations for (a) WWER-440 and (b) WWER-1000 reactors.

Addition of NH_4OH (hydrazine)

- Generates H2 under radiolysis
- Works better to control pH at lower temperatures

KOH qualification process launched by EPRI includes also materials qualification

[3] INTERNATIONAL ATOMIC ENERGY AGENCY, Coolant Technology of Water Cooled Reactors, Technical Reports Series, No. 347 1993

Water Chemistry Control in Fusion Facilities

ITER, EU-DEMO, JT-60SA & DTT, 4 facilities → 3 different water chemistries

ITER IBED PHTS water chemistry [4]

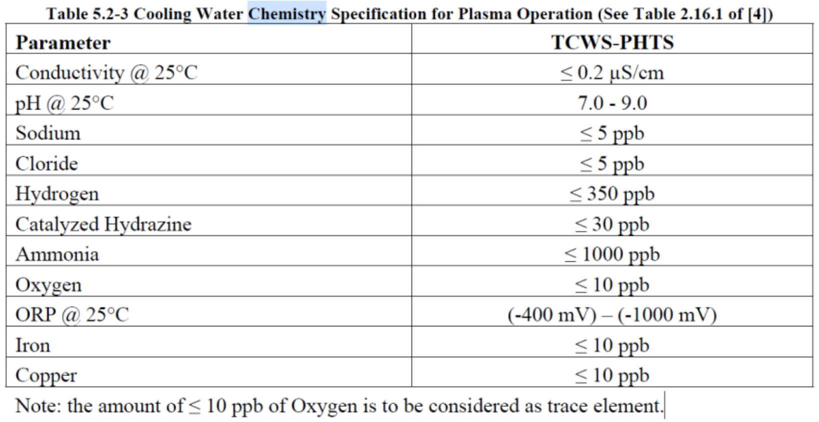


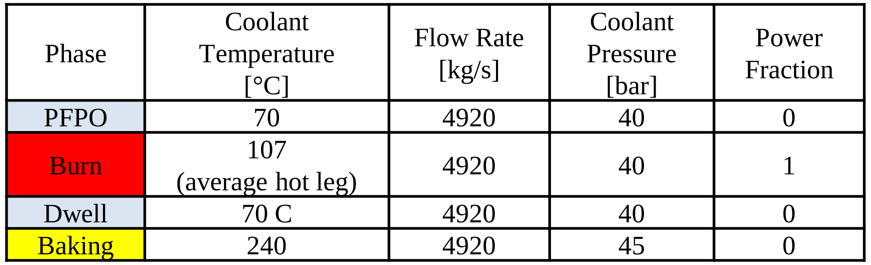
Table 5.2-3 Cooling Water Chemistry Specification for Plasma Operation (See Table 2.16.1 of [4])

Parameter	TCWS-PHTS
Conductivity @ 25°C	≤ 0.2 µS/cm
pH @ 25°C	7.0 - 9.0
Sodium	≤ 5 ppb
Cloride	≤ 5 ppb
Hydrogen	≤ 350 ppb
Catalyzed Hydrazine	≤ 30 ppb
Ammonia	≤ 1000 ppb
Oxygen	≤ 10 ppb
ORP @ 25°C	(-400 mV) – (-1000 mV)
Iron	≤ 10 ppb
Copper	≤ 10 ppb

Note: the amount of ≤ 10 ppb of Oxygen is to be considered as trace element.

[4] SRD-26-PH, -CV, -DR, -DY, -SA (TCWS) from DOORS (2823A2 v6.4/E) (current)

Slightly different for VVPHTS and NBI PHTS



Phase	Coolant Temperature [°C]	Flow Rate [kg/s]	Coolant Pressure [bar]	Power Fraction
PFPO	70	4920	40	0
Burn	107 (average hot leg)	4920	40	1
Dwell	70 C	4920	40	0
Baking	240	4920	45	0

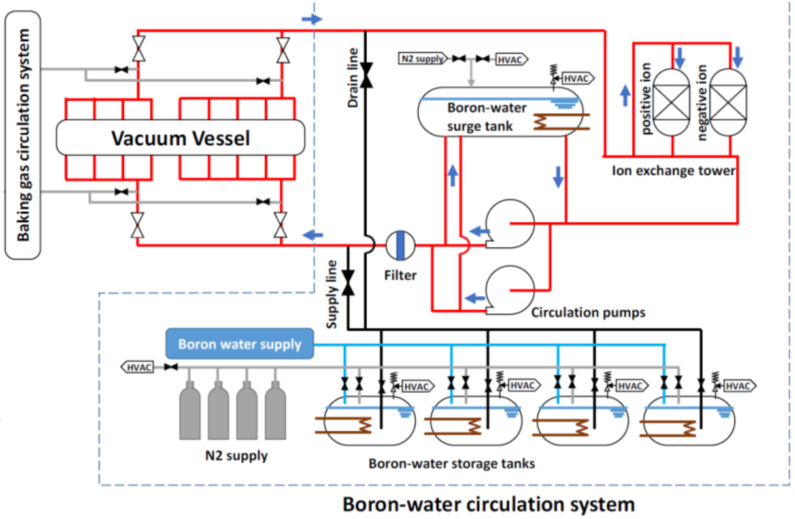
EU-DEMO FW/BLK PHTS working water chemistry specs [5]

Parameter	Value
pH_T (at 311 °C)	7.2 to 8.0 → pH@25°C 9.7
Li (as LiOH)	0–2 mg/kg
Dissolved hydrogen	10 to 50 cc/kg
Dissolved oxygen	< 10 µg/kg
Anion impurities (Cl, F, SO_4)	<10 µg/kg
Cation impurities (Mg, Na, Si)	< 50 µg/kg
Noble metal addition or zinc injection	To be determined

[5] Chemistry and corrosion research and development for the cooling water circuits of European DEMO
C. Harrington et al Fusion Engineering and Design 146 (2019) 478–481

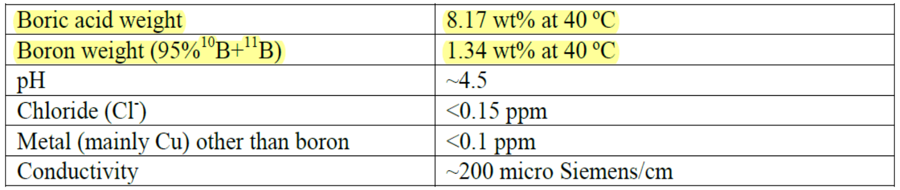
WCLL BB PHTS Design and Operating Parameters	BZ	FW
Reactor vessel inlet T (°C)	295	295
Reactor vessel outlet T (°C)	328	328
Pressure (MPa)	15.5	15.5
Flow rate per loop (kg/s)	3831	1136
Number of loops	2	2

JT-60SA VV PHTS



[6] JT-60 SA PID Plant Integration Document (V4.2)

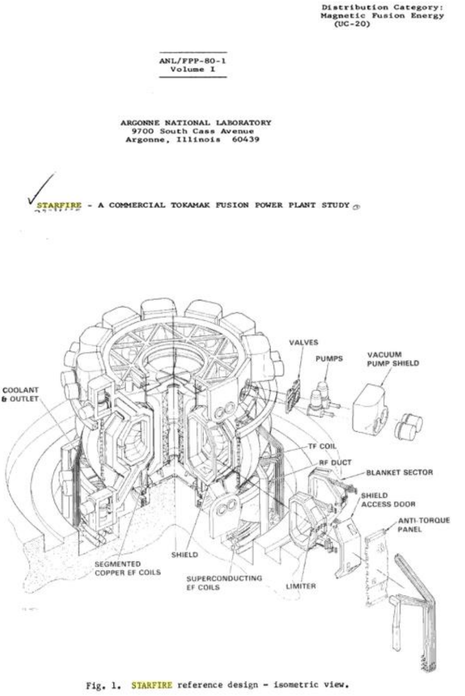
Inlet T for B water min, max	45, 50 ºC
DT	<1 ºC in the V
circulation pump pressure head	0.3 Mpa(g)
Nominal flow rate	100 m^3/h



Boric acid weight	8.17 wt% at 40 °C
Boron weight (95%^{10}B+^{11}B)	1.34 wt% at 40 °C
pH	~4.5
Chloride (Cl^-)	<0.15 ppm
Metal (mainly Cu) other than boron	<0.1 ppm
Conductivity	~200 micro Siemens/cm

Fusion phenomena not modelled in ACP codes

- The fusion environment is characterized by having strong magnetic fields.
- V x B Force (change in ion diffusion and in ion-solid state diffusion) ions are travelling in the bulk fluid
- Magnetostriction (inducing film stress)
- Induced Currents (acceleration of corrosion rate by induced current)
- Magnetic Field Gradients (increased deposition of coolant particles)
- Microstructure and Composition (corrosion rate alteration by change of film microstructure and by presence of ferritic steel produced in austenitic steel)
- Conclusion on Magnetic Effects (see APPENDIX G of Ref. [9])
  - Increased particles deposition in very low flow areas and oxide microstructure alteration
  - Advantages of magnetic filters may provide incentive to maximize the magnetization potential of coolant particles
  - Advantage to having Fe_3O_4 (magnetite) rather than Fe_2O_3 (ferrite) as stable phase (the chemical, hence magnetic, form of the coolant is controllable by water chemistry)



Distribution Category:
Magnetic Fusion Energy
(UC-20)

ANL/FPP-80-1
Volume I

ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

✓STARFIRE - A COMMERCIAL TOKAMAK FUSION POWER PLANT STUDY

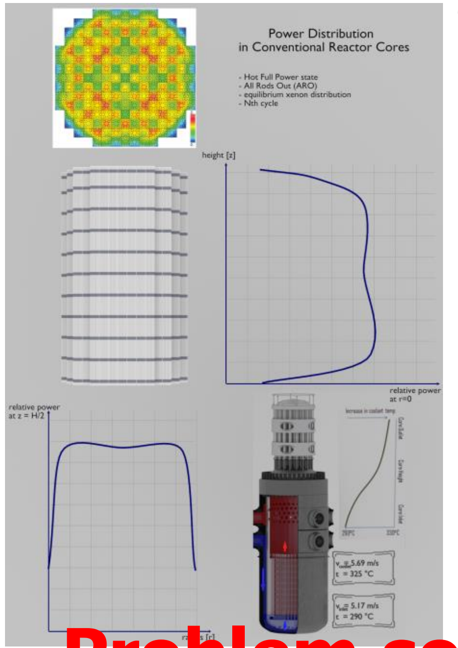
Fig. 1. STARFIRE reference design - isometric view.

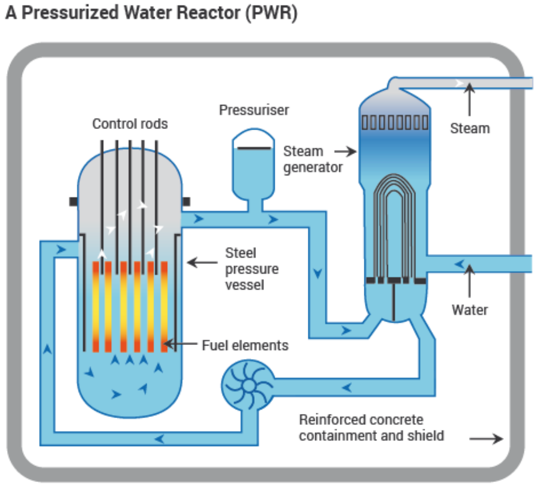
[9] STARFIRE – A COMMERCIAL TOKAMAK FUSION POWER PLANT STUDY ANL/FPP-80-1, 1980

Fusion phenomena not modelled in ACP codes

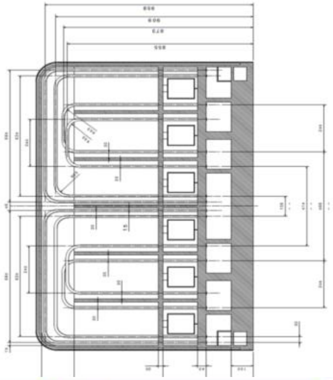
- Other difference: variability of n-flux on cooled materials

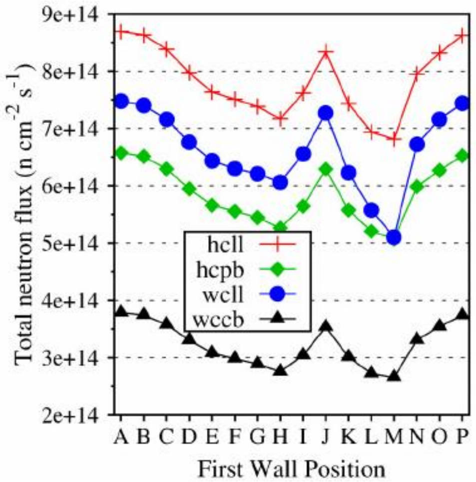
n-flux in LWR core quasi-uniform
Neutrons generated inside the core

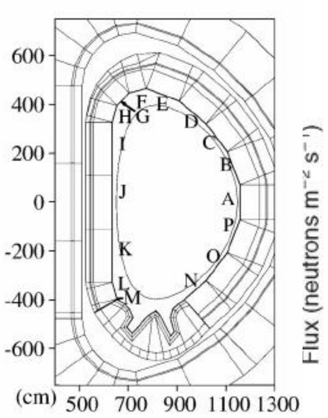


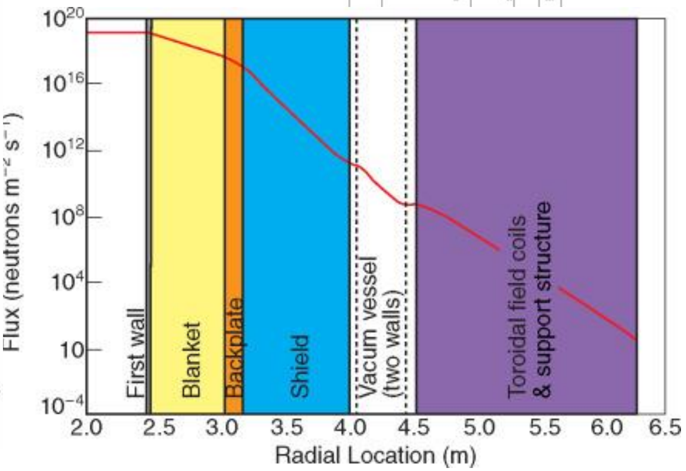


n-flux in Fusion Blanket extremely variable:
2-3 orders difference FW vs BP in r direction
Less pronounced in p direction,





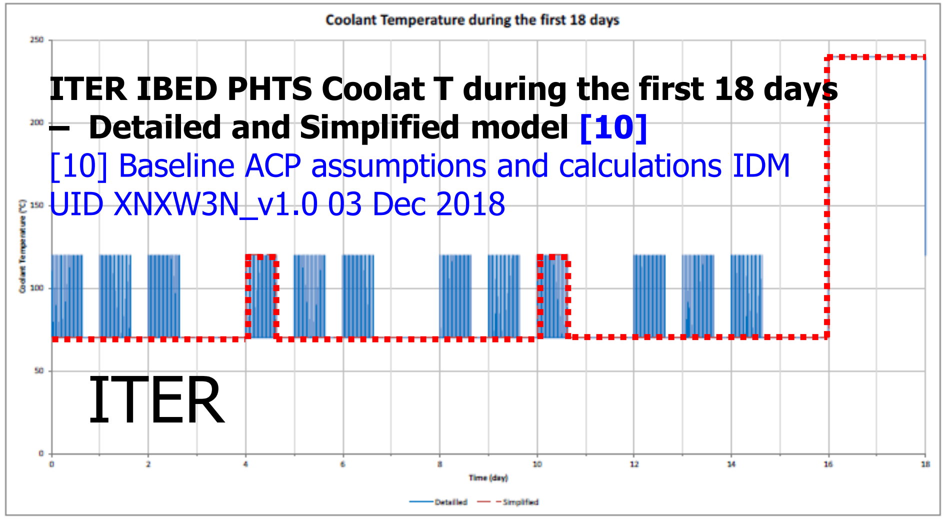




Problem solved by adapting the input (in PACTITER, OSCAR) but common approach still TBD how to calculate RRs

Fusion Phenomena not modelled in ACP codes

- Following pulsed operation coupling with neutronics and activation calculations

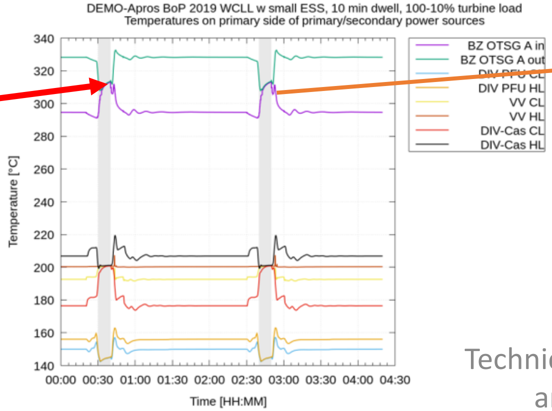


ITER IBED PHTS Coolat T during the first 18 days – Detailed and Simplified model [10]

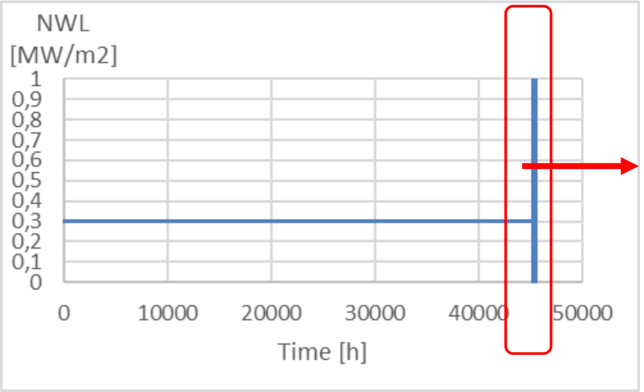
[10] Baseline ACP assumptions and calculations IDM UID XNXW3N_v1.0 03 Dec 2018

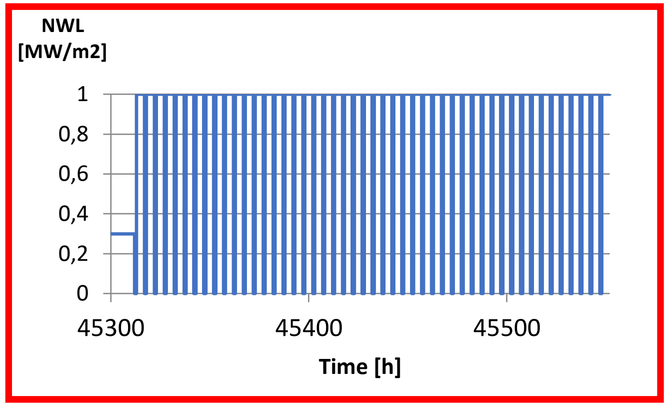
ITER

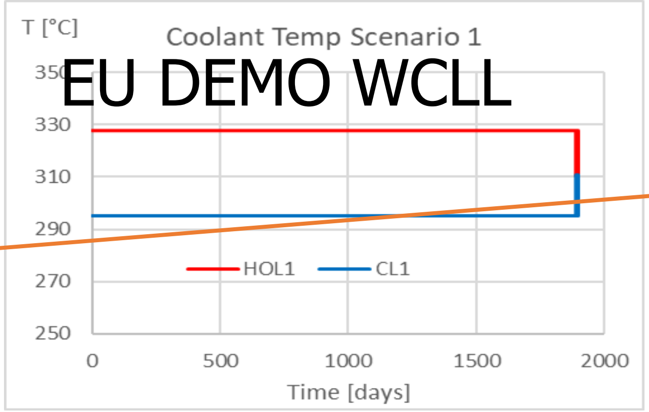
Figure 5.2-3 Coolant temperature during the first 18 days – Detailed and Simplified model



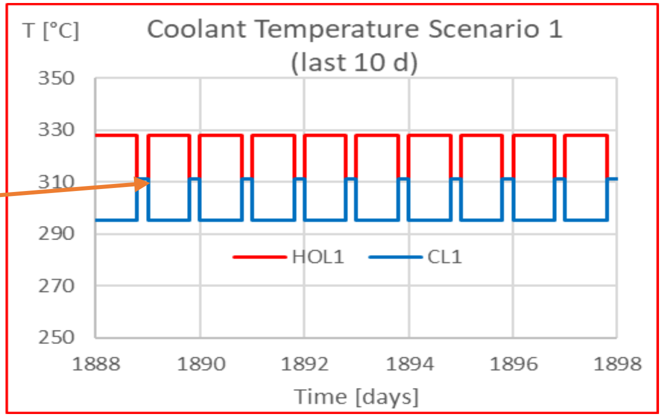
311 °C







EU DEMO WCLL



Computer codes for ACPs assessment in water

Code name	**Developed for**
Burrill's mechanistic model	CANDU PWR
Babcock&Wilcox model	*Specific PWR plant Oconee Unit 1, USA*
ACE-II code	Prediction of radioactivity level and evaluation of the effect of countermeasures in the primary circuit of *Japanese PWRs*.
CRUDTRAN code	Prediction of the corrosion products and radioactivity transport in the primary coolant system of PWR
MIGA-RT computer program	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*.
CORA-II code	Prediction of corrosion-product transport and radiation field build-up in PWRs, incorporating recent advances in scientific understanding of these processes.
DISER code	Prediction of corrosion products behaviour and radioactivity build-up on the *WWER* and *PWR* primary system surfaces
CRUDSIM code	Prediction of corrosion products in PWR primary coolant circuits
COTRAN-M code	The evaluation of radiation conditions in the vicinity of primary equipment in *WWER-1000*
CPAIR-P code	To simulate corrosion product activity build-up in reactor core, inner piping surface and primary coolant loop of PWRs, accounting for the effect of flow rate and power transients on corrosion product activity in primary coolant.
TRACT code	To simulate the flow and mass transport of isotopes inside a network of 1-D channel for **fusion power plants**.
PACTOLE code	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.
PACTITER code	For the prediction of contamination in the **ITER** Primary Heat Transfer System (PHTS). Analyze the behaviour of corrosion products, activated or not, to determine the fluid and the deposited activity of out-of flux surfaces. V3.3 is the fusion version of PACTOLE v3.2
OSCAR-Fusion code	For the prediction of contamination in the primary circuit of PWRs. OSCAR-Fusion v1.3 / v1.4 developed for **fusion reactor** (ITER). Used for EU-DEMO WCLL
CATE 2.0 code	Simulation of the production and transport of ACPs in the cooling loops of a **fusion power plants**, (CFETR of China in the future).

Gas Corrosion Codes

- There are no simulation codes of the generation and transport of ACPs in gas cooling loop of nuclear fusion reactors as the phenomenon is negligible. (Ref. [15]).

For fusion gas cooled reactors the only radioactive contamination of the cooling loop is due to the **sputtering** products. [SPUTTER code *→ UKAEA]

	CO_2	He
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	CO_2 has a high chemical reactivity above 650 °C (carburization of metals and graphite oxidation above this temperature). This reactivity increases further under exposure to radiation (due to the radiolytic decomposition of CO_2, which produces oxidizing and corrosive agents in response to gamma flux).	Chemically inert, regardless of temperature. No usage limitation under high temperatures.
Availability, resources	Abundant and very inexpensive	Available and inexpensive

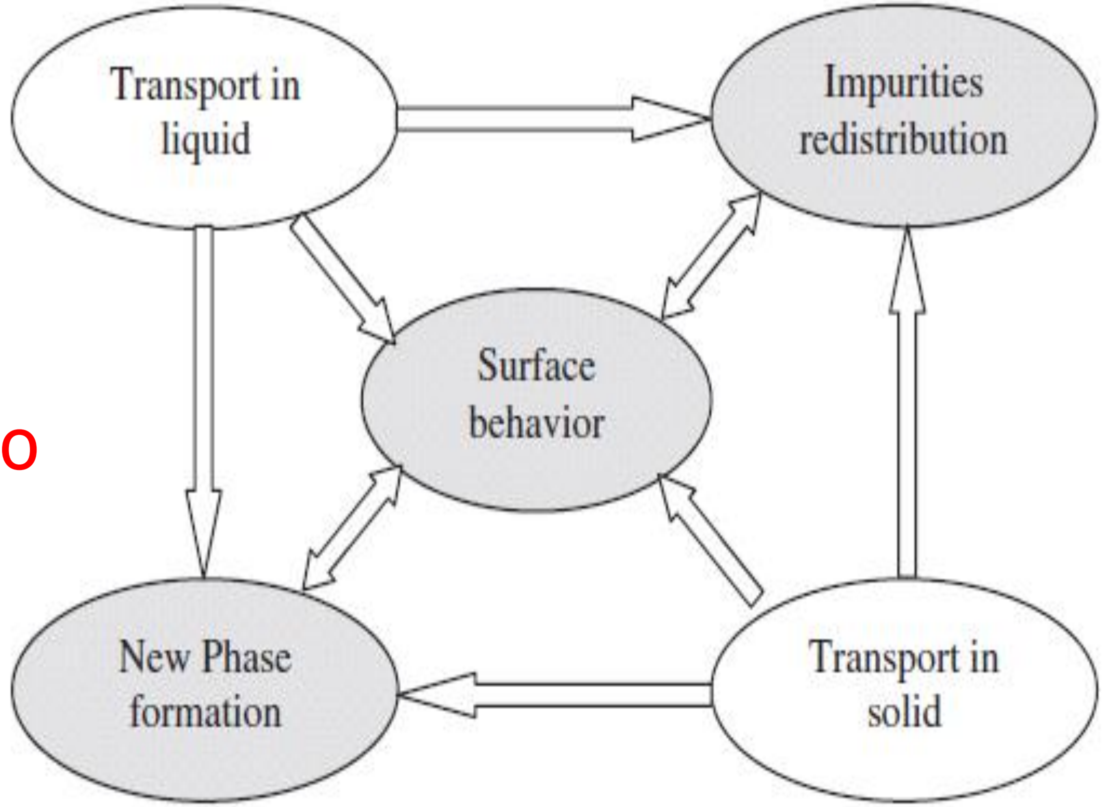
*P. J. Karditsas, *SPUTTER code,* CCFE GIT repository, git@git.ccfe.ac.uk:teade/sputter.git, 2002.

[15] L. Di Pace, Interim report on overview relating to ACP simulation codes suitable in fusion field, EFDA_D_2N3H96 v1.3 - Deliverable SAE-2.019-1-T001-D003, June 2018

Liquid Metal Corrosion Models

Main Models

- The description of main mathematical models for liquid metal corrosion phenomena is provided in Ref. [16], with several literature references. They are:
  1) transport in the solid (metal or alloy),
  2) dissolution of the steel constituents into the liquid, or mass exchange at the solid/liquid interface, and
  3) transport in the liquid of the corrosion products and impurities



[16] J. Zhang, P. Hosemann, S. Maloy; Models of liquid metal corrosion, Journal of Nuclear Materials 404 (2010) 82–96

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) For an ideal case of a loop with a hot and a cool zone, a heat exchanger and a heater	YES	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

[15] L. Di Pace, Interim report on overview relating to ACP simulation codes suitable in fusion field, EFDA_D_2N3H96 v1.3 - Deliverable SAE-2.019-1-T001-D003, June 2018

Liquid Metal Corrosion Models

- OSCAR-Na code [17]

OSCAR-Na developed by CEA, in order to calculate the mass transfer of CPs and related contamination in the primary circuits of sodium fast reactors (SFR). A solution/precipitation model & a modular mass transfer code up to now dedicated to PWRs. The key parameters of the model are:

1) diffusion in the steel, considered to be enhanced under irradiation;

2) diffusion through the sodium laminar boundary layer;

3) the equilibrium concentration of each element in the sodium; and

4) the velocity of the moving interface, due to bulk corrosion in hot parts (in relation to O_2 enhanced iron dissolution), and deposition in cold parts of the reactor.

Even with a simplified primary system description, simulation of the French reactor PHENIX by V1.3 of OSCAR-Na was able to assess correctly the amount of contamination and the contamination profiles on heat exchanger surfaces for Mn54, Co58 and Co60 radionuclides, compared with measurements.

[17] J.-B. Génin, L. Brissonneau, T. Gilardi, G. Bénier, OSCAR-Na V1.3: a new code for simulating corrosion product contamination in SFR reactors, Proceedings of International Conference; on Fast Reactors and Related Fuel Cycles: Safe Technologies and Sustainable Scenarios (FR13). COMPANION CD-ROM. Paris, France, 4–7 March 2013

Experimental loops – existing, *projected*

CIRENE & CORELE @CEA

qui permettent l'étude du transfert de la contamination dans les réacteurs en reproduisant des conditions thermohydrauliques agressives requises pour les tests de matériaux et de dispositifs.
https://www.cea.fr/energies/iresne/Pages/Nos%20plateformes%20de%20recherche/Qualification%20de%20dispositifs.aspx

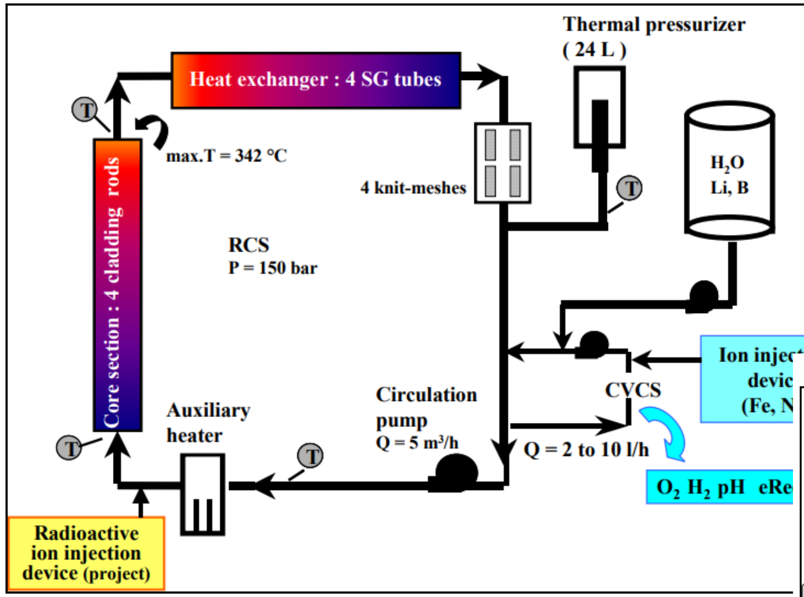


Figure 37: The CIRENE loop

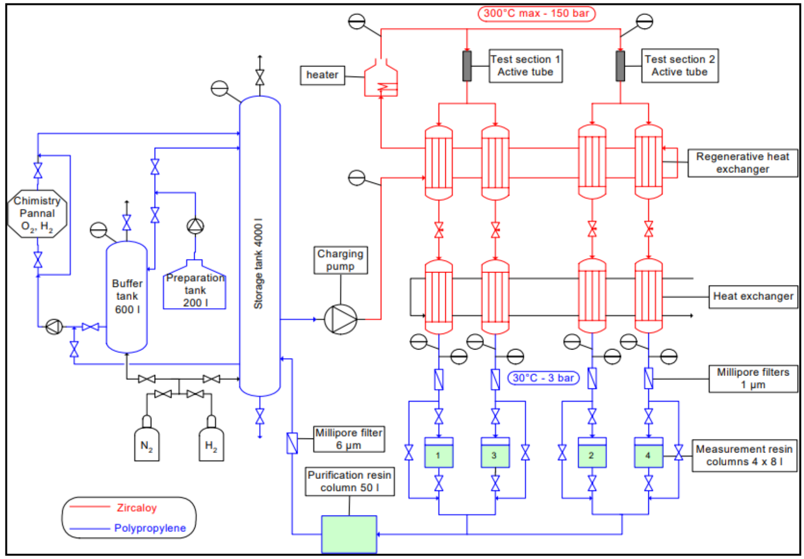
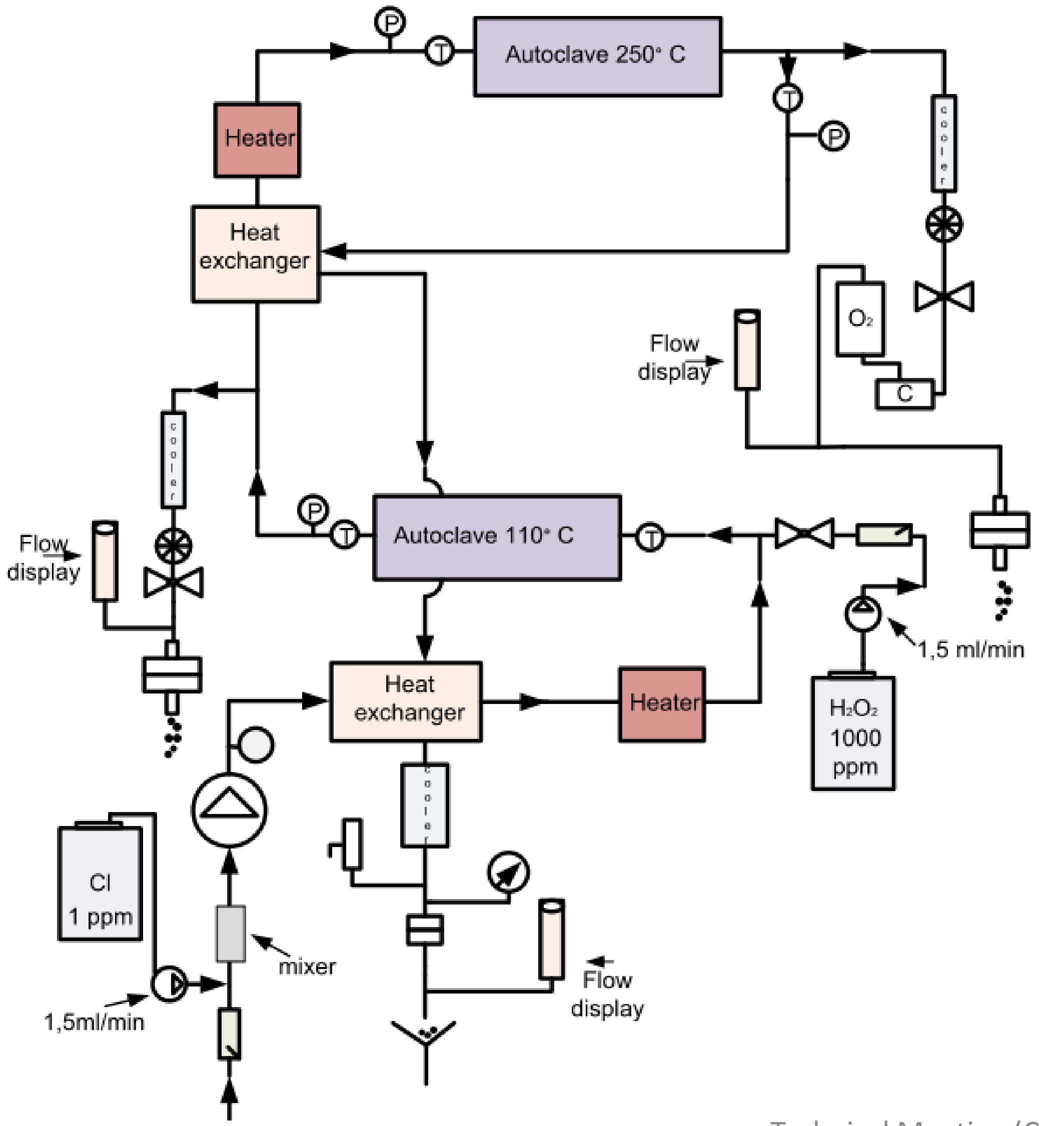


Figure 38: The CORELE loop

Figures from:

[from https://inis.iaea.org/collection/NCLCollectionStore/_Public/38/045/38045516.pdf](https://inis.iaea.org/collection/NCLCollectionStore/_Public/38/045/38045516.pdf)

Experimental loops – existing, *projected*

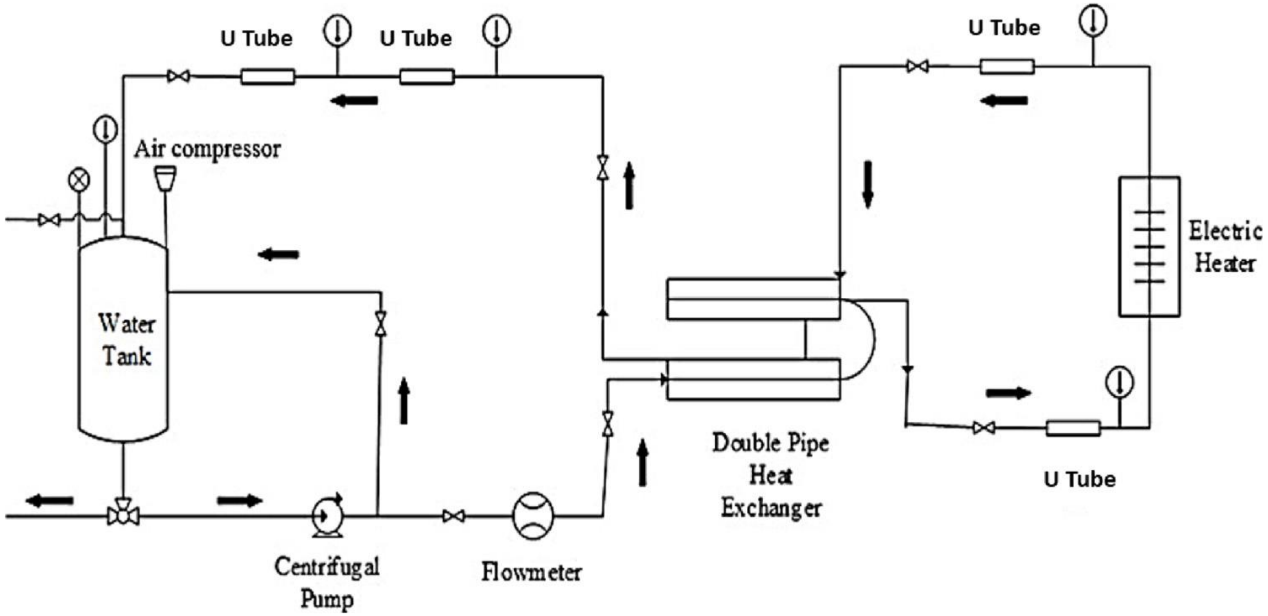


The test loop installed at Studsvik Corrosion and Water Chemistry Laboratory applied for exposure of the Cu alloy CuCrZr and joints between CuCrZr and 316L(N)-IG under simulated ITER conditions

Source:
Experimental Assessment of Erosion Corrosion Parameters of Copper Alloys and Copper to Steel Joints at ITER Operational Conditions
S. Wikman[1], C. Gustafsson[2], J. Öijerholm[2] and J. Eskhult[2]
[1] Fusion for Energy, Barcelona, Spain. Email: stefan.wikman@f4e.europa.eu
[2] Studsvik Nuclear AB, Nyköping, Sweden.

Experimental loops – existing, *projected*

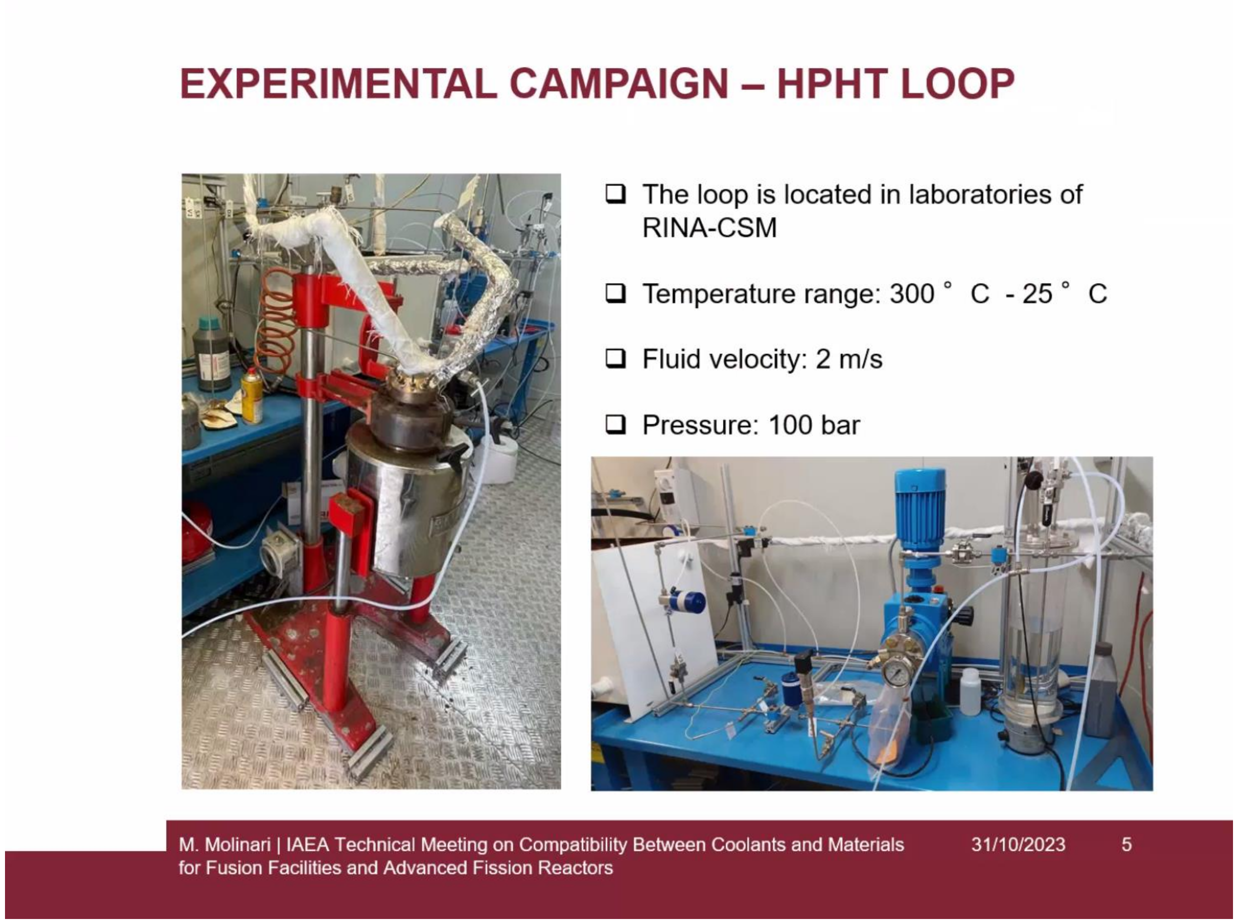
Experimental loop set-up by Laboratory of Passive Nuclear Power Safety and Technology, North China Electric Power University to study the deposition behavior of CPs in water cooling conditions as ITER



Reference: Deposition behavior of corrosion products in an ITER water-cooling experimental loop
https://doi.org/10.1016/j.fusengdes.2020.111883

Experimental loops – existing, *projected*

Courtesy: Martina Molinari, presentation this TM

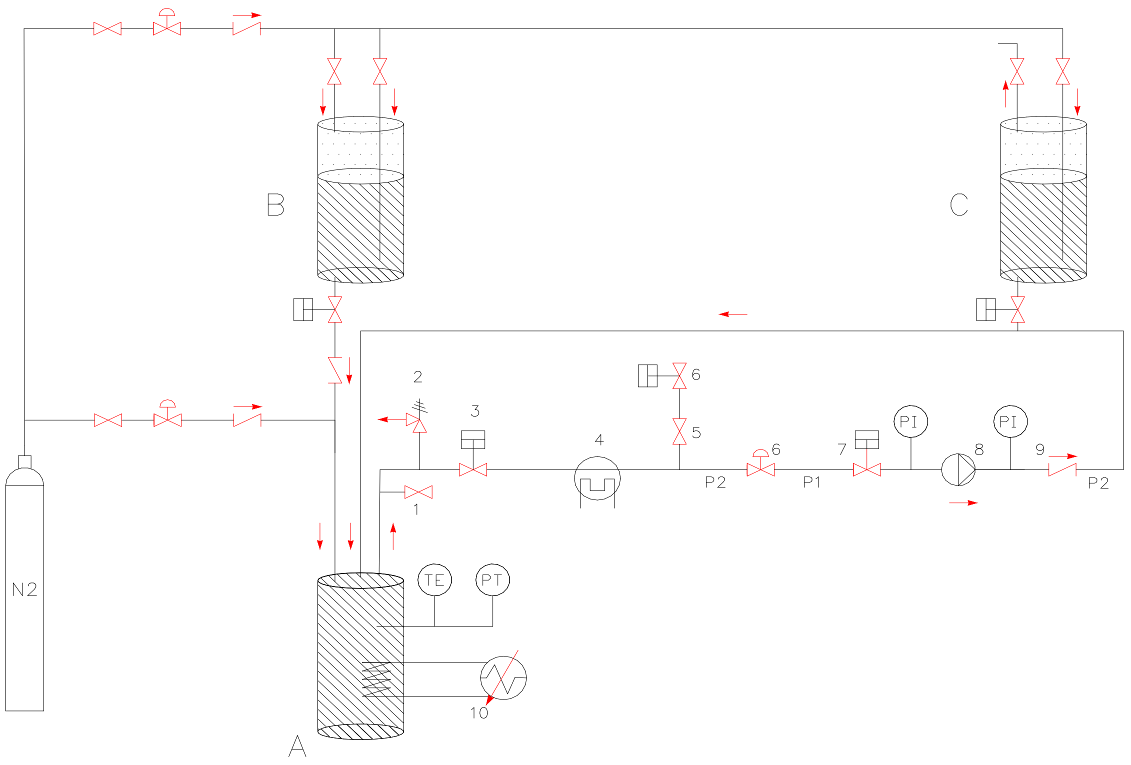


EXPERIMENTAL CAMPAIGN – HPHT LOOP

- ☐ The loop is located in laboratories of RINA-CSM
- ☐ Temperature range: 300 ° C - 25 ° C
- ☐ Fluid velocity: 2 m/s
- ☐ Pressure: 100 bar

M. Molinari | IAEA Technical Meeting on Compatibility Between Coolants and Materials for Fusion Facilities and Advanced Fission Reactors 31/10/2023 5

HPHT Loop @ RINA Consulting CSM



Courtesy: Raffaella Torella; RINA Consulting CSM

Experimental loops – *existing*, projected

Proposal for an integral validation experimental loop

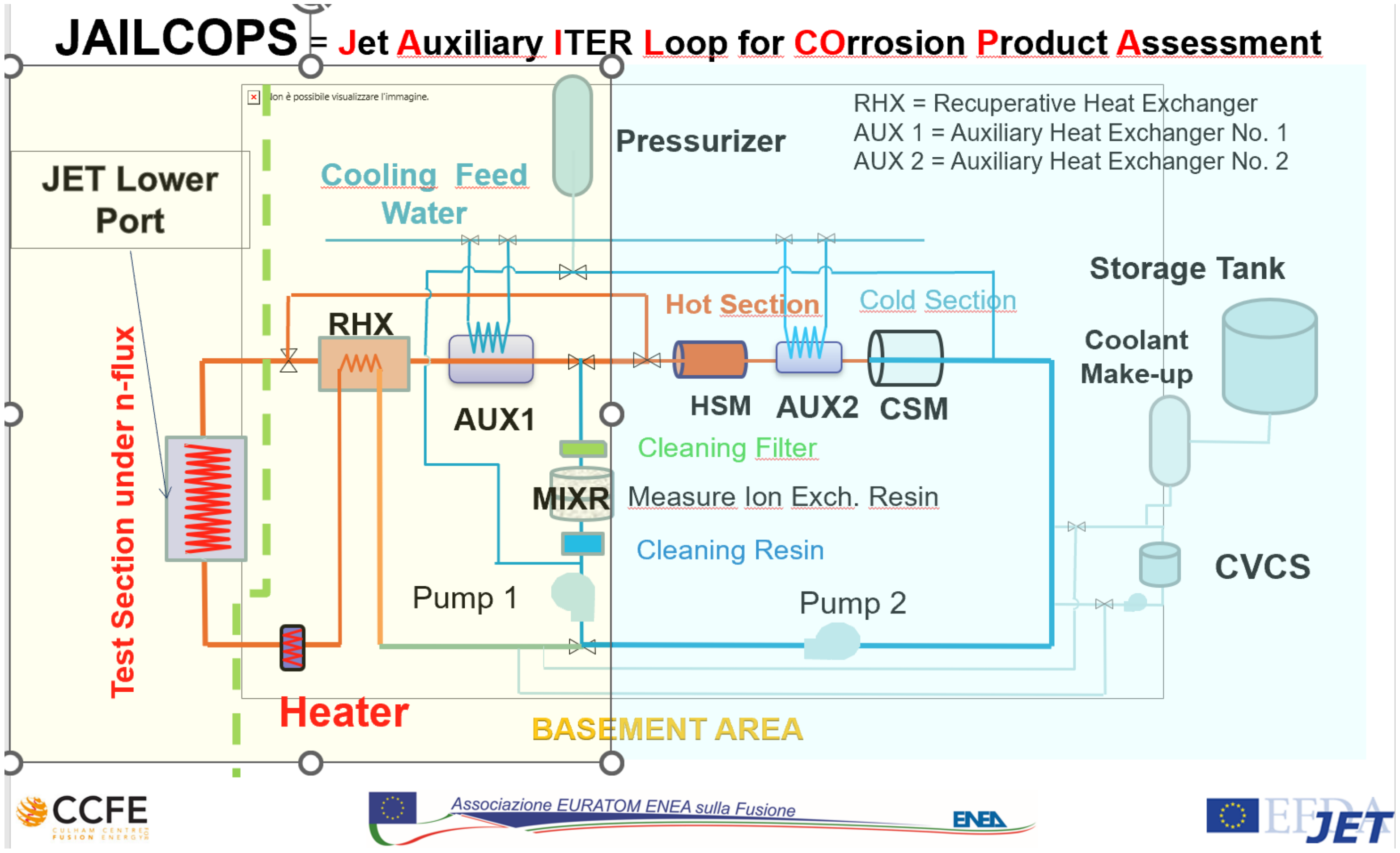
described in the paper

Feasibility Study of Validating Activation Corrosion Products Calculations in Cooling Water Loops at JET presented at the 25th SOFE, San Francisco (2013)

Issued in the Symposium Proceedings, IEEE Catalog Number: CFP13SOF-CDR; ISBN: 978-1-4799-0169-2

as outcome of the

EFDA JET Task: Fusion Technology JW12-FT-5.46

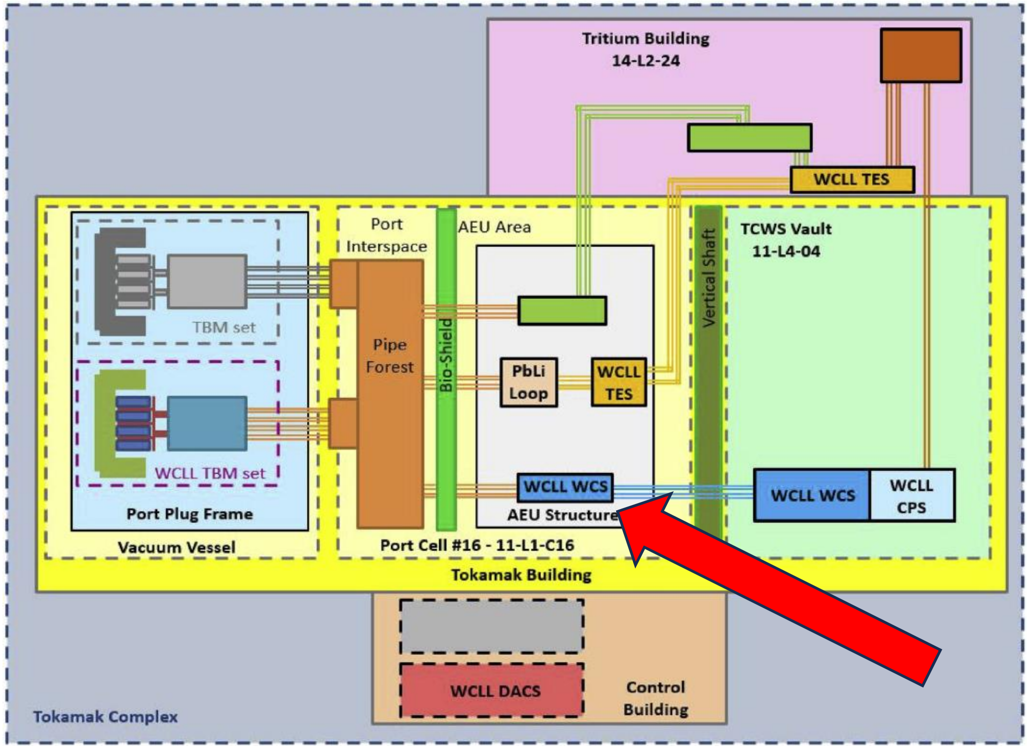


Experimental loops – *existing*, projected

What about to use CHIMERA @UKAEA?

Facility designed for testing fusion components under the unique combination of conditions with high heat flux with static and pulsed magnetic fields within a vacuum or inert atmosphere – conditions that will be faced in large fusion devices such as ITER, and in future commercial plants.
https://ccfe.ukaea.uk/divisions/fusion-technology/chimera/

What about to use the WCS of EU-DEMO WCLL TBS to perform ACPs code validation?



Reference Fig.1 of paper
Conceptual design of the main Ancillary Systems of the ITER Water Cooled Lithium Lead Test Blanket System
https://doi.org/10.1016/j.fusengdes.2021.112345

ITER SAFETY DEMONSTRATION:

what are the key uncertainties?

- Neutron transport calculations
- Activated Corrosion Products generation, impact on occupational radiation exposure (ORE)
- Mechanical and thermal loads on vessel and in-vessel due to plasma transients
- Superconducting magnets, reliability of insulation, impact on VV in case of failures
- Dust formation
- Hydrogen formation due to in vessel Loss-of-Coolant Accidents
- Tritium retention
- Effect of neutrons on electronics
- Reliability and maintenance requirements, impact on ORE
- Maintainability of in-vessel components and impact on hot cell
- Etc. ..

Conclusions #1

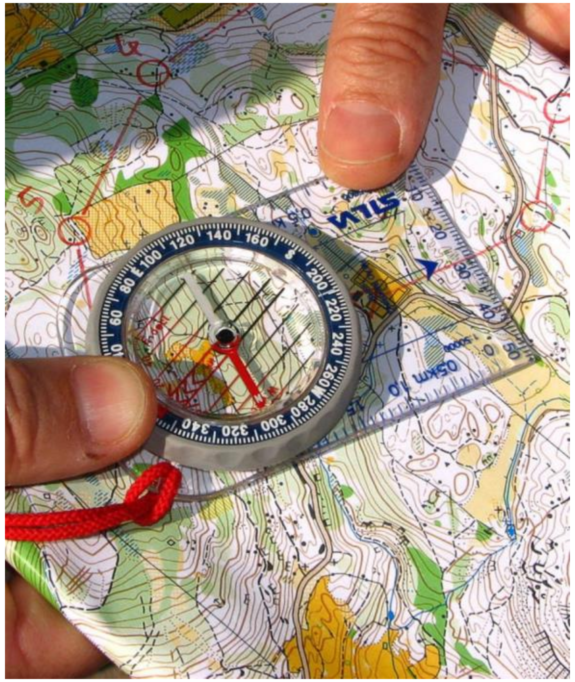
- Water corrosion codes reviewed focusing on fission and fusion reactors.
- Some codes developed for fission are specific plant relevant.
- Codes, developed for predicting ACP formation and transport in fusion facility cooling loops, are mostly derived from fission LWRs, as OSCAR-Fusion.
- OSCAR-Fusion is the most promising code, but its application to ITER and DEMO water cooling systems requires experimental validation for licensing purposes.
- Radioactive contamination in fusion facilities using He as coolant is due to sputtering products → gas corrosion codes (e.g. SPUTTER code)
- LM corrosion models and calculation tools, focus on the physical-chemical process of species dissolution & transport, chemical reactions, and new phase formation.

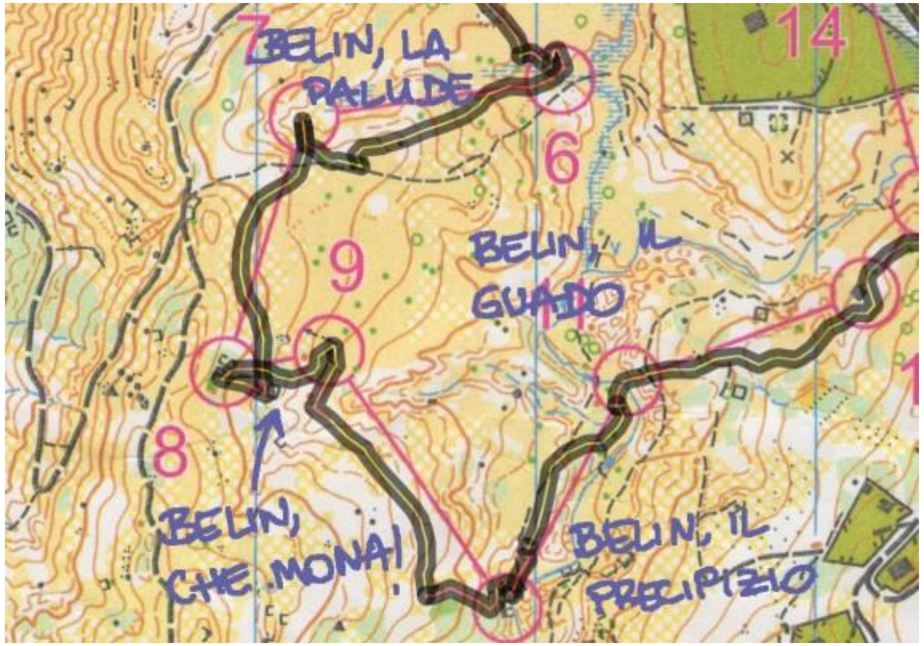
Conclusions #2

- Significance of experiments for the validation of computer code models, metal release and corrosion, oxide and particle dissolution, oxide and deposit erosion, particle dissolution and deposition, ion and particle convection. Need of an integral validation test loop for fusion codes
- Experiments also required to feed the codes data.
- Reach agreement in the approach to simulate n-transport and activation in fusion ACP assessments.
- Fission-derived experience indicates that variations in input conditions can cause discrepancies between model predictions and experimental data.
- Codes for ACPs in fusion facilities must consider uncertainties like coolant ΔT, pulsed operation, lack of boron, and strong magnetic fields.

Conclusions #3

Allow me this comparison: ACP assessment for fusion facilities is quite similar to navigating a partly unexplored territory with valid tools such as compasses, maps and even GPS





Thank you for your attention

Questions?

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