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IRSN
INSTITUT DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE

SEVERE ACCIDENT CODE ASTEC

PATRICK DRAI

Patrick.drai@irsn.fr

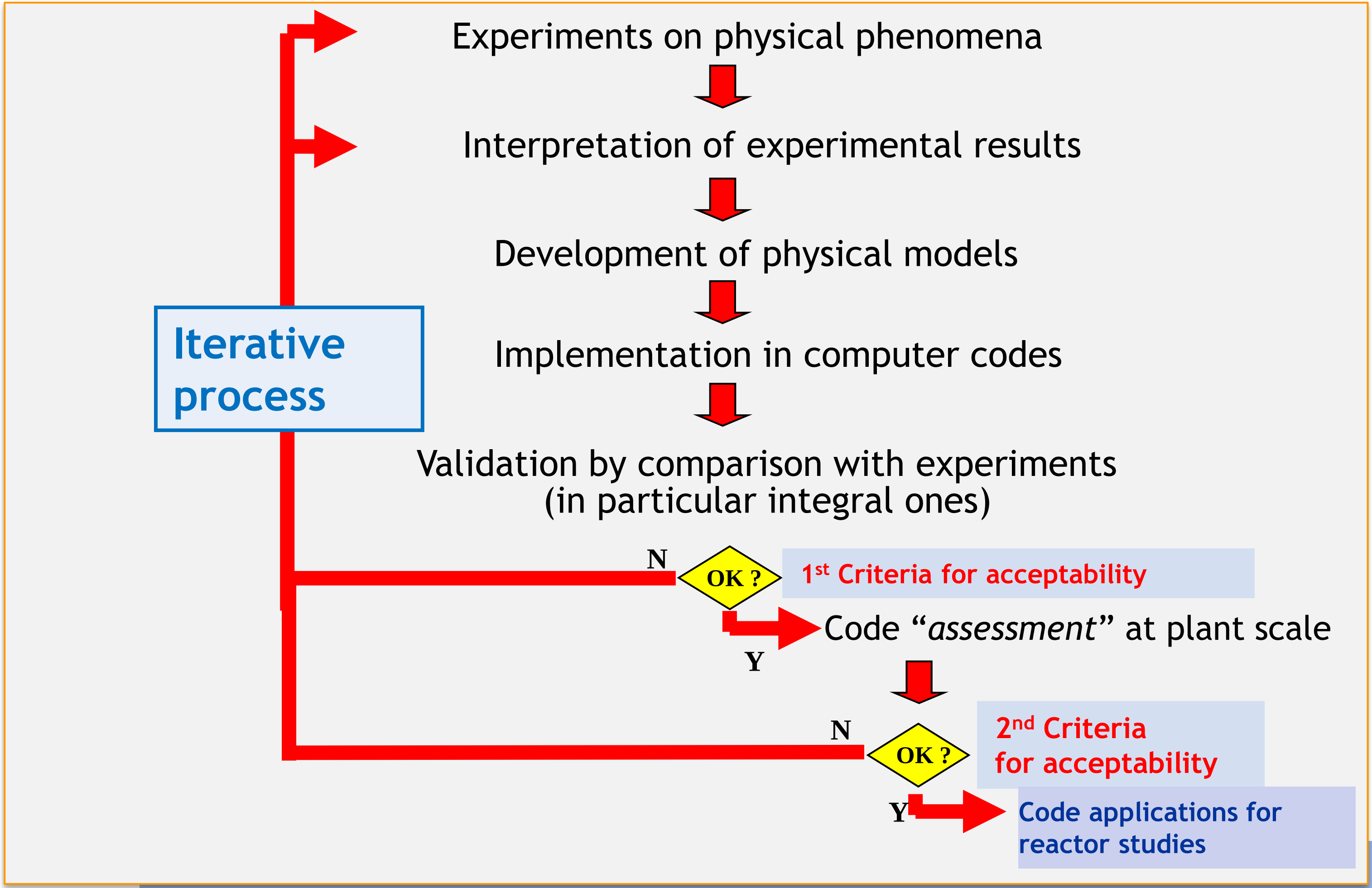
R2CA Short Course

MEMBRE DE
ETSON

Content

- General strategy for a code development
- The ASTEC code: context and objectives, current status
- ASTEC main physical models
- ASTEC validation vs. experiments
- ASTEC film
- Conclusion

General strategy for code development (1/2)



General strategy for code development (2/2)

Approaches for development of SA codes since many years

1. **Integral codes** (or code systems) such as **ASTEC (Europe)** or **MELCOR** and **MAAP (USA) codes** for:
   - Evaluation of source term,
   - Probabilistic Safety Assessment level 2 studies (PSA-2),
   - SA Management (SAM) evaluation,
   - Support of experimental programmes (preparation, interpretation).

2. **Mechanistic** (or detailed) **codes** such as **ICARE/CATHARE**, **ATHLET-CD**, **SCDAPSIM/RELAP5**, **MFPR…** for:
   - Detailed understanding of the phenomenology,
   - Detailed interpretation of experiments,
   - "Best-estimate" plant applications on specific parts of the scenarios,
   - And support to derive simplified modelling for the integral codes.

The ASTEC code: context and objectives and current status

- **ASTEC** (**A**ccident **S**ource **T**erm **E**valuation **C**ode) is being developed from the late 1990s **for simulation of severe accidents in present/future Water-Cooled Reactors** **(PWR**, incl. **SMR**, **VVER**, **BWR, CANDU)**, **from the initiating event until radioactive release out of the containment**

  - **ASTEC** has been jointly developed by IRSN (France) and GRS (Germany) up to 2015 and **is exclusively developed by IRSN today** (collaboration agreement with KIT (Germany) around the developments has been initiated) .

- ASTEC progressively **V3.1** has been released in November 2022

ASTEC context and objectives

Detailed codes for benchmarking or derivation of simplified models:

CATHARE2, MFPR, ICARE/CATHARE…

Experiments for validation, such as:

International Source Term Program (incl. Phebus.FP)

OECD/CSNI projects

EURATOM projects

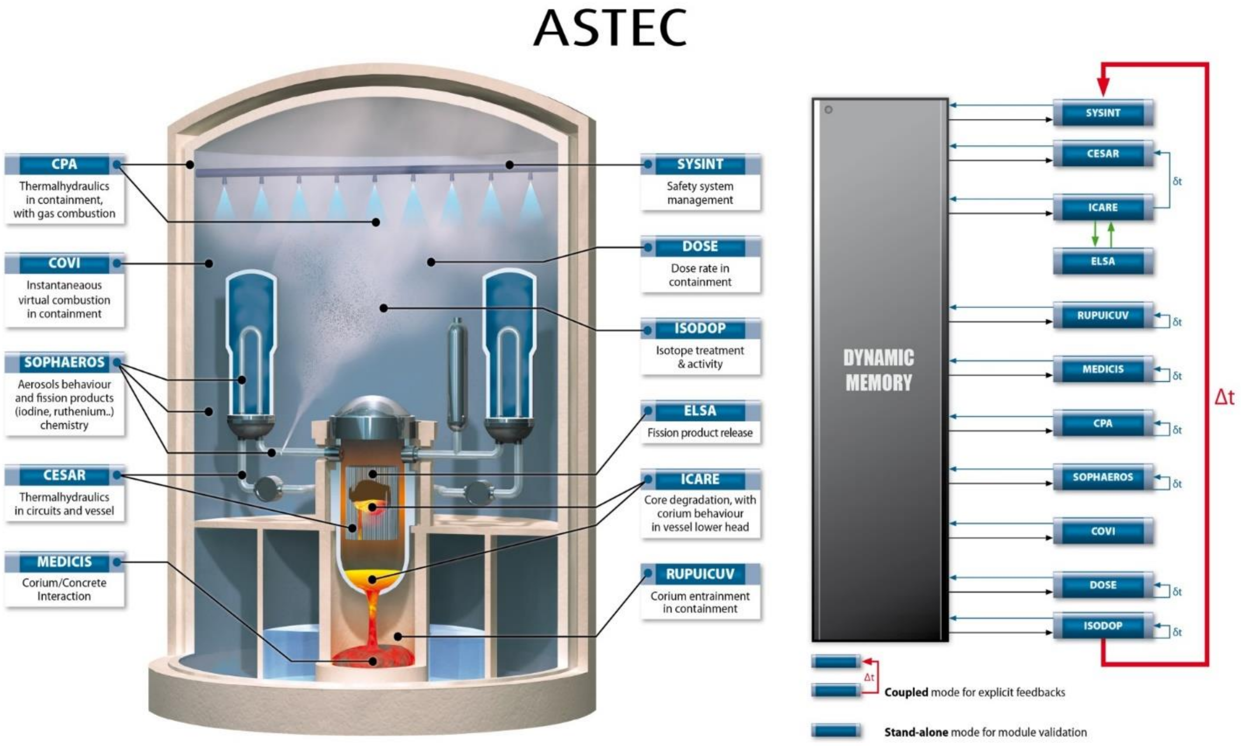
ASTEC

Modelling of physical phenomena

(including PhD, post-doctorates..)

NUCLEA European reference databank for material properties

ASTEC V3 general architecture



Structure of the V3.1 major version

Status of ASTEC code

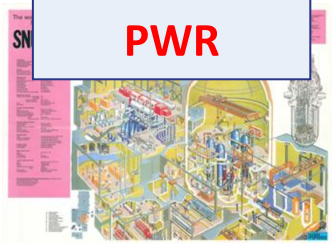
Main capabilities of ASTEC V3.1 (current **production version**)

- Physical models close to current State of the Art (notably FP models)
- Good enough results of extensive validation based on most available experiments worldwide (≈ 200 tests), in particular the Phébus FP integral experiments
- **Simulation of all SA scenarios on Gen.II reactors for normal power** and shutdown states in both **PWR** (incl. **VVER**-440 and VVER-1000) and **BWR**, and also of LCDA scenarios in **PHWR/CANDU**
- **Capability to simulate most safety systems and SAM measures** (*one can notably refer to CESAM project outcomes*):
  - In-vessel : RCS deliberate depressurisation; core reflooding (both early water injection in a "not too damaged" core or reflooding of a degraded core);
  - Ex-vessel : Containment spray, venting, hydrogen recombiners…
- Applicability to new Gen.III designs:
  - **EPR**, with its ex-vessel corium catcher,
  - **In-Vessel Melt Retention** concept by external cooling of vessel lower head.

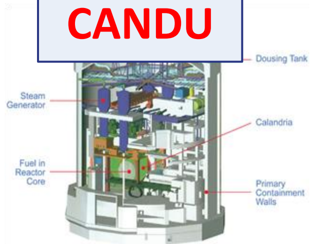
Status of ASTEC code

- **Achievement of “reference" ASTEC input decks**
  - Combine the best knowledge of the different teams using ASTEC in Europe and India for PWR, BWR, VVER and PHWR/CANDU with the advises of the IRSN ASTEC code developers
  - To serve as a **basis for** any **ASTEC V3.1** user to develop own **plant specific ASTEC input deck**

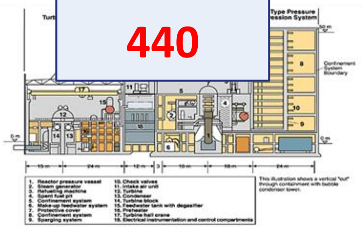
Western PWR



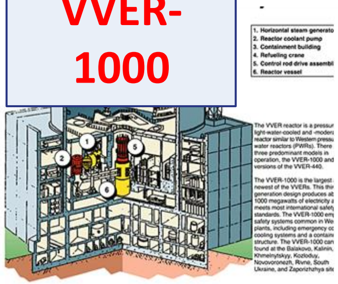
CANDU



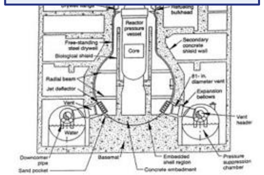
VVER-440



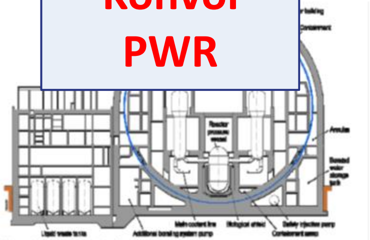
VVER-1000



BWR Mark 1



Konvoi PWR



Status of ASTEC code

- **Applicability of ASTEC V3.1 to other nuclear designs**:
  - Small Modular Reactors (**SMR**): Nuward, Nuscale, IRIS
  - Spent Fuel Pools (**SFP**)
  - **Gen.IV** reactors, in particular **SFR** but also **HTR**
  - Fusion installations, in particular to **ITER**

- **Other powerful features** of ASTEC V3.1 series:
  - **Coupling with the IRSN SUNSET tool** to make easier the realization by users of uncertainty and sensitivity studies
    - Functionality that is fully included in the ASTEC V2 standard package
  - **Interfacing of ASTEC with atmospheric dispersion tools** to enhance capabilities of direct comparison with on-site measurement
    - Significant progress towards a “diagnosis” version

Status of ASTEC code

- **Complete code documentation**:
  - Description of all physical models (theoretical manuals),
  - On-line HTML users manuals, with examples of input decks,
  - Users Guidelines,
  - Post processing manuals.
- Software structure:
  - 500 000 lines of standard Fortran, today use of Fortran 2003
- **Two main target computers**:
  - PCs with either **Linux®** or **MSWindows®**, **32** or **64bits**, **O**perating **S**ystems
- Graphical User Interface **XASTEC** (for pre- and post-processing)
- **Powerful on-line visualisation tool**
  - Along with the **possibility to look on-line at the transient database**
- **Computing time around accident real time**
  - But it depends of course on the nodalization and the selection of model options…
  - With a very coarse nodalization, a few modules can run as fast as 10 minutes for 1 day of accident (use for emergency response tools).

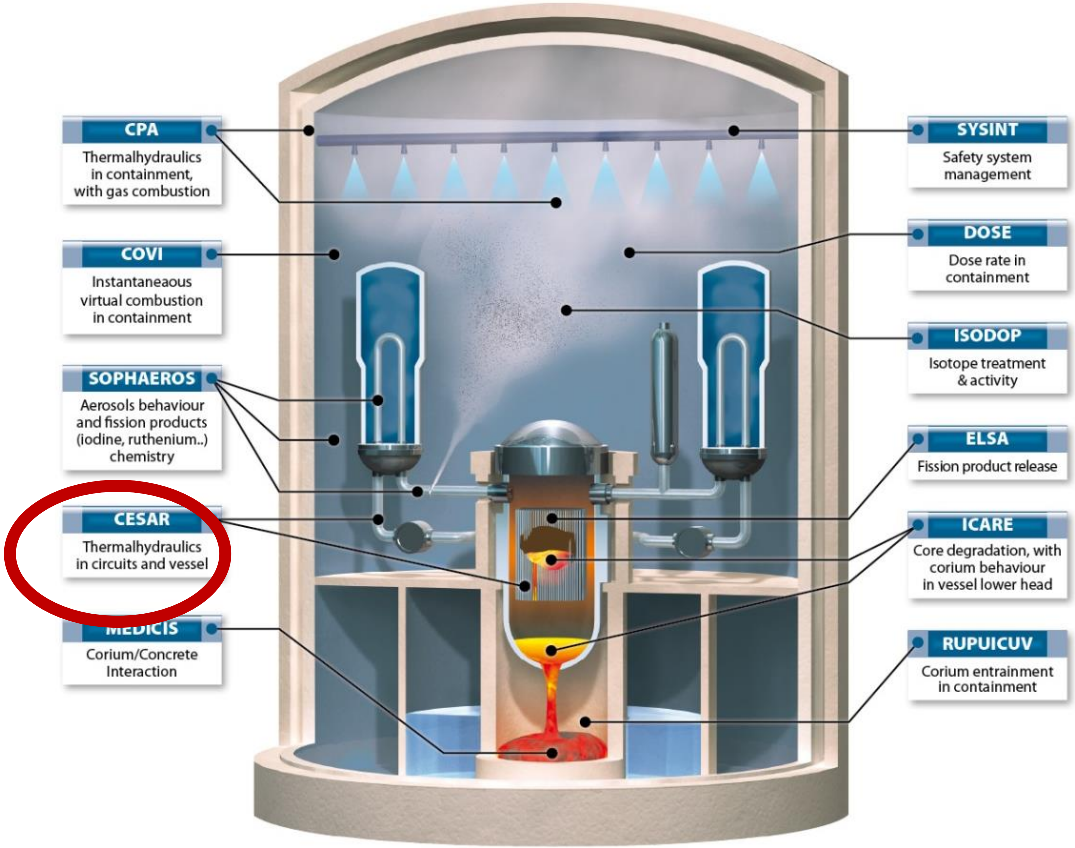
International collaboration

- **Large international collaboration**: almost 40 software agreements today
  - More than 30 European organisations
  - Out of Europe:
    - CNL and KINECTRICS (Canada), NPCIL (India), NSC ,CNPE and HFIPS-INEST (China), NUS (Singapore), IPEN (Brasil)

- **Intensive support to the users**:
  - Periodic organisation of **international Users' Club Meetings** (*roughly every 18 months*)
    - **Next one to be planned is 2024**
  - Periodic organisation of **1-week training courses for beginners** in code use
    - **Next one planned in january 2024 at Aix-en-Provence (France)**
  - Specific web site for downloading the code, documentation, examples…
  - **On-line web support** for treatment of anomalies or questions

3- ASTEC V3.1 main physical models (See Appendix 1)

ASTEC



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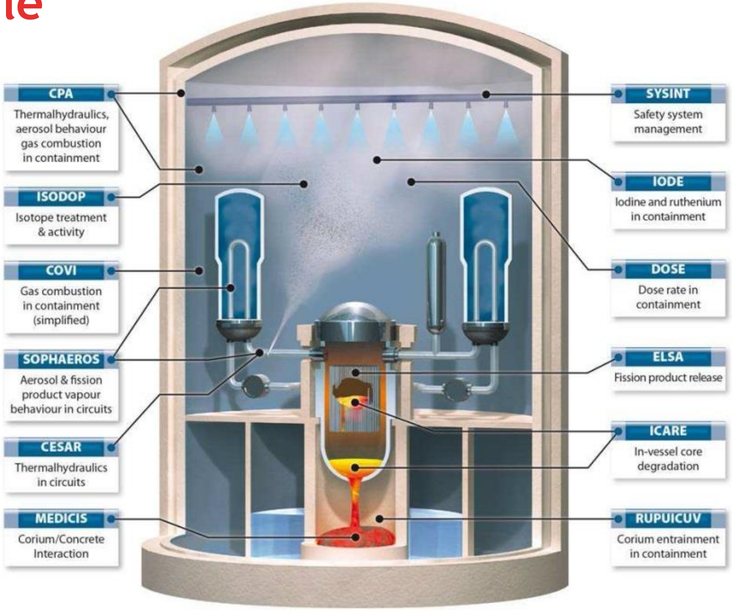
CESAR = Circuit Evolution during a Severe Accident in a Reactor

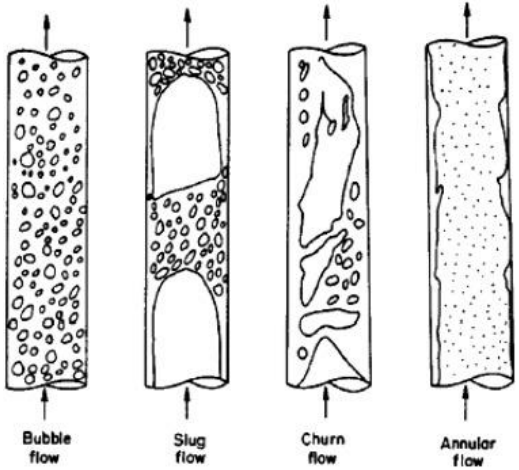
CESAR : ASTEC thermal-hydraulic module

- Primary and secondary circuit
- Intact and degraded core

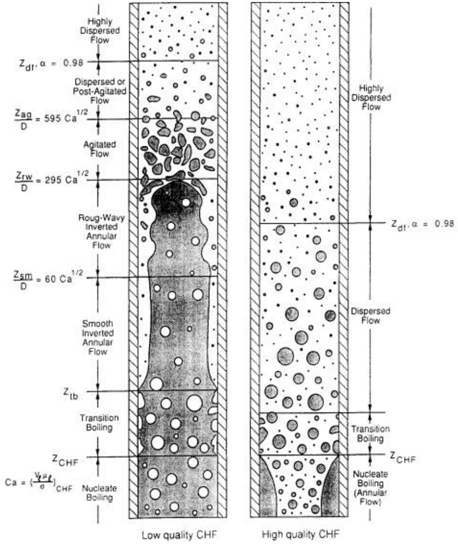


Thermal-hydraulics: not so simple

- Mix air/water: different flow topologies depending on Vliq, Vgas, pressure
  → different exchanges (heat and impulsion) between air/water



- In heated configurations, phase changes (ebullition, condensation)
  → even more topologies



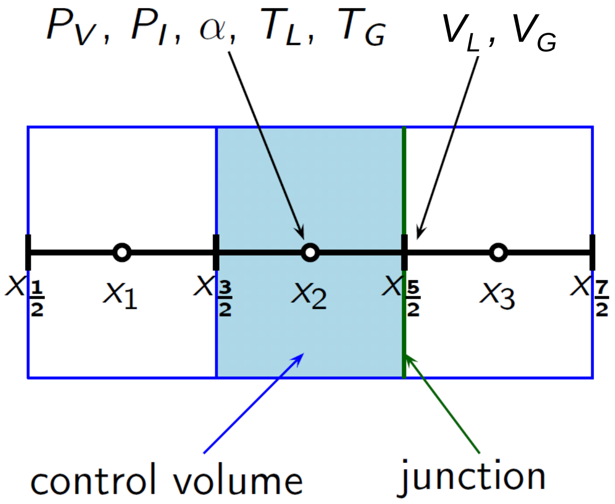
Nelson et al, 1992, Nucl. Eng. And Design

- + evolving geometry in the core!

Main objects: VOLUME and JUNCTION

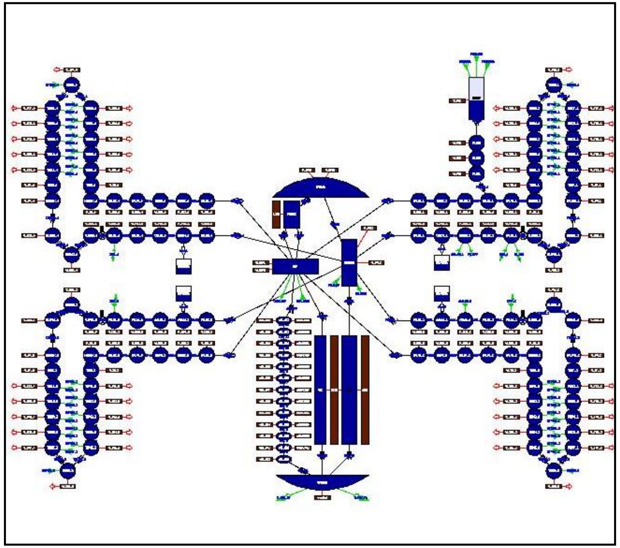
- Volume (or mesh) equations and *unknowns*
  - Mass conservation equations
    - Liquid → α *(void fraction=gas volume fraction in the mesh)*
    - Steam → *Pv (vapour partial pressure)*
    - Up to 5 non-condensable gases
      → P_{N2}, P_{H2}, P_{O2}, P_{CO}, P_{CO2}, P_{BHO2}, P_{He}, P_{Ar}
  - Energy conservation equations
    - Liquid → T_L
    - Gas (Thermal equilibrium of steam and non-condensable gas) → T_G

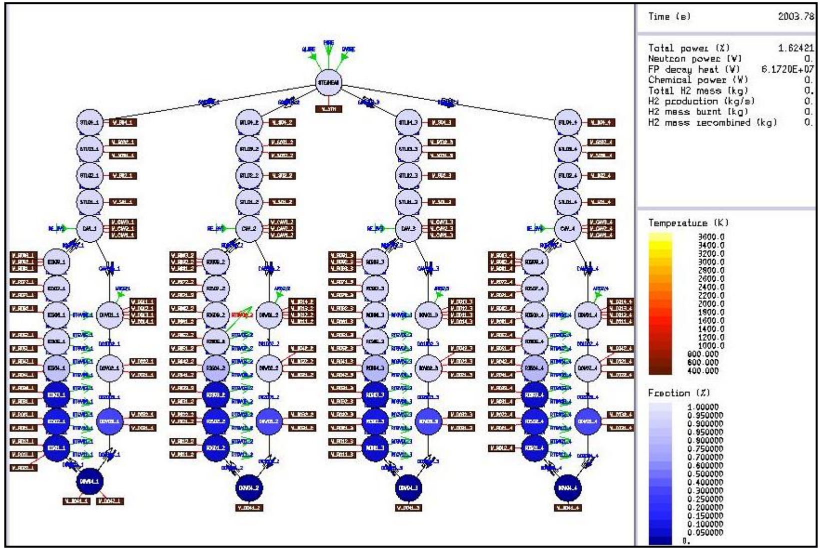
- Junction (or face)
  - Momentum conservation equations
    - Liquid → V_L
    - Gas → V_G



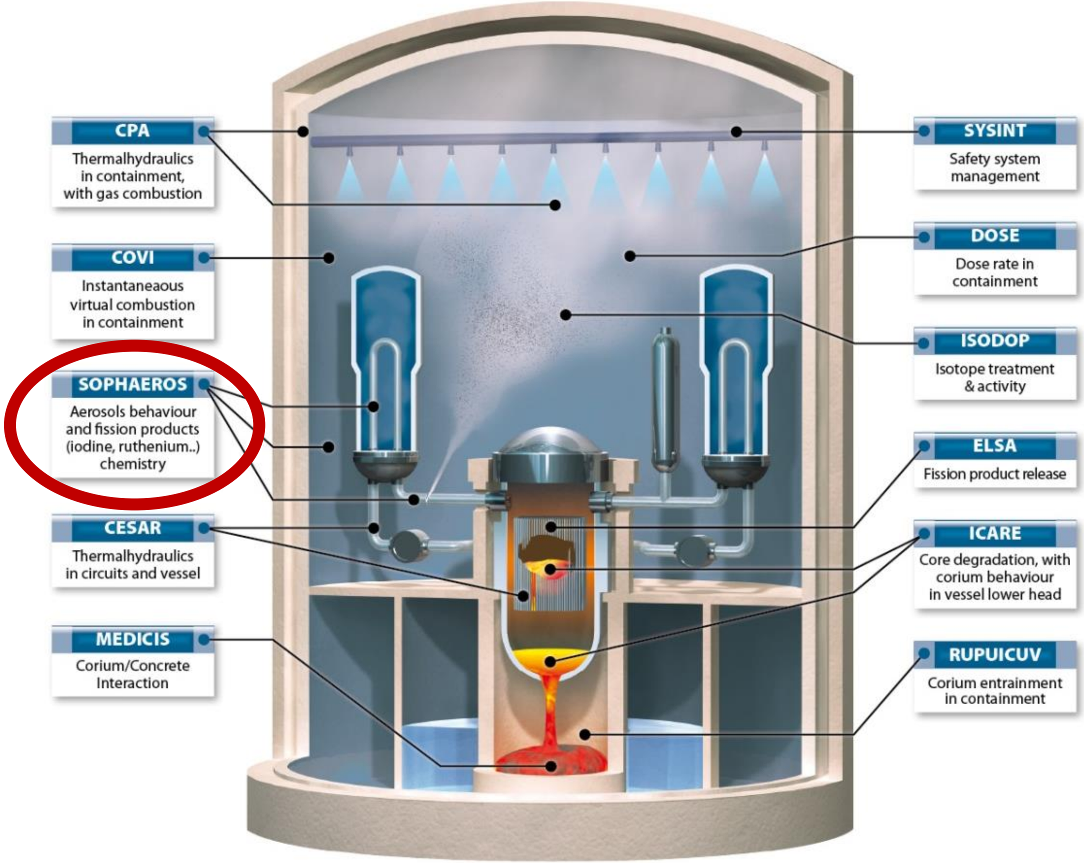
CESAR circuit definition

- The circuit of a NPP is modeled in CESAR using:
  - volumes (~100-300) or pipes (used to generate volumes)
  - junctions (~200-400)
  - walls (~200-400)
  - pumps (~50)
  - boundary conditions (e.g. injections, breaks)





ASTEC



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FP/aerosols transport models

- In the **ASTEC V3.1** new series, the **SOPHAEROS** module simulates transport and chemistry of FP vapours and aerosols in the whole reactor, i.e. **in both the RCS and the containment domains**

  ➔ *Nodalization scheme fits those of CESAR and CPA respectively*

- **For the RCS**, **6 different physical states are considered:**
  - Suspended vapour,
  - Suspended aerosol,
  - Condensed vapour on walls,
  - Deposited aerosol on walls,
  - Sorbed vapour in walls,
  - Liquid.
- **For the Containment**, **6 more physical states are considered:**
  - Species on painted dry walls,
  - Species on Steel dry walls,
  - Species on concrete dry walls,
  - Species on painted wet walls,
  - Species on Steel wet walls,
  - Species on concrete wet walls.
- **Carrier gas**: H_2O, H_2, O_2, N_2, He, Xe, Kr, Ar

Description of the containment iodine chemistry:

Family of chemical reactions taken into account

Thermal reactions:

- **Liquid phase**
  - hydrolysis of I_2 and CH_3I
  - decomposition of HOI
  - oxidation of I^- by O_2
  - reactions with Ag (3)
  - formation of CH_3I
- **Gaseous phase**
  - formation of IOx aerosols by oxidation of I_2 by air radiolytic products (O_3) => I_2O_5 aerosols
  - decomposition of IO_x into I_2
  - conversion of HOI/HI into I_2

Radiolytic reactions:

- **Liquid phase**
  - oxidation of I^- in I_2
  - radiolytic reduction of IO_3^-
  - formation/decomposition of CH_3I
- **Gaseous phase**
  - formation of air radiolytic products (O_3)
  - CH_3I and I_2 adsorption and release from paints
  - conversion of I_2 into CH_3I through organic pollutions (CH_3R)
  - decomposition of I_2 and CH_3I into IOx
  - decomposition of IO_x into I_2
  - decomposition of iodine aerosols (I_{aer})

Mass transfer :

- Liquid – gas (I_2, I_2O_5, CH_3I, HOI)
- Liquid – surfaces (I_2 : steel, paint, concrete)
- Gas – surfaces (I_2 : steel, paint, concrete + IOx and Iaer settling)

Iodine behaviour understanding in containment in 2022

Thermal reaction
Radiolytic reaction

% I_{aer}/I_{tot}
% $I_{gaseous}/I_{tot}$

Circuit

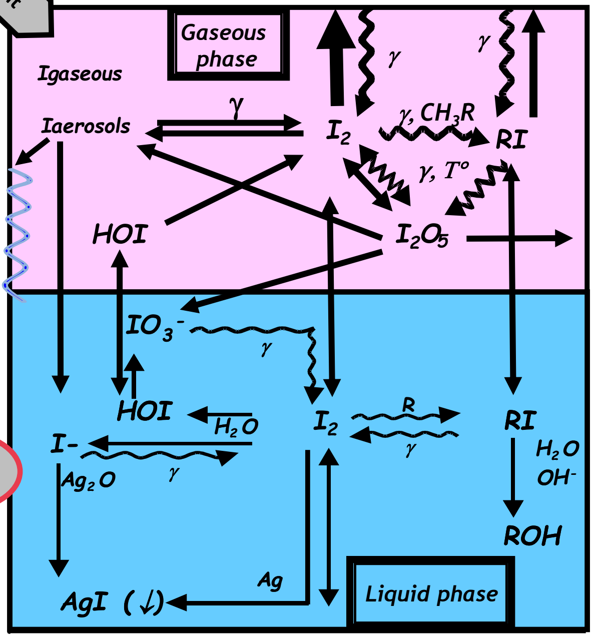
Air radiolytic products oxidize a fraction of I_2 and RI => formation of iodine oxides (considered as fines particles) that decompose back into I_2 by thermal and irradiation processes

DR, T°

$K_{ads(i)}/k_{rel(i)}$

Iodine aerosol sediment and settle on walls where they are decomposed under the effect of the irradiation.
If solubles (CsI…), they form iodides ions (I-) in the aqueous phase. The insoluble aerosols (AgI…) stay in the bottom of the sump

DR and aerosol type



I_2 reacts with surfaces (adsorption, desorption, RI release under radiation)

Gaseous I_2 is converted into RI in the gaseous phase by radiolysis through volatile organics (CH_3R…)

DR, T°

Iodides ions are oxidided by water radicals (OH°) and form I_2 that can be hydrolysed, adsorbed on immersed paint, or react with organics in solution to form organic iodides

T, pH

Iodine oxides sediment and settle on surfaces (walls + surface developed by aerosols in suspension)

τ ½

If Ag is present, iodides ions an I_2 can be converted into insoluble compounds (AgI…)

M_{Ag}/M_I

Volatile species are transferred to the gaseous phase (I_2, RI, HOI). HOI is instantaneously converted into I_2

Th. conditions of the sump

The competition between formation/decomposition phenomena governs the iodine volatility in the containment

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ASTEC V3.1 validation Vs Experimental data (See Appendix 2)

General approach for ASTEC validation

- <u>**Different level validation approach**</u> (benefits from ASTEC code modularity):
  1. **Separate-Effect-Tests** (SETs) focusing on only 1 physical phenomenon,
  2. **Coupled-Effect-Tests** (CETs) focusing on a set of physical phenomena,
  3. **Integral tests** (IT) to check the coupling of physical models and that no essential phenomenon was forgotten or neglected

     ➔ *Example of **Phébus FP** integral experiments at IRSN*
  4. **R**epresentative **simulations at plant scale** for few reference sequences

     ➔ not detailed hereafter, but very important too to check the reliability of any new version
- Very large validation matrix, covering all SA phenomena through more than 180 experiments:
  - Major (past, on-going) French, German and international exp. programs,
  - Continuous IRSN detailed interpretation of **Phébus FP** integral tests.
- At each major code release, application of a sub-set of the matrix for checking non-regression and model improvements:
  - Covering all the main phenomena,
  - ≈25 SETs/CETs (2-3/module) + 2 integral applications (**Phébus**, **TMI2**)

NOW, Let's have some fun!

6- ASTEC modelling perspectives

Towards future ASTEC versions

Continuous capitalization of international knowledge:

→ **Improvements of physical models** are expected **from the interpretation of experimental programmes that are underway or planned :**

- in international frame (e.g. **OECD** projects),
- European frame (e.g. **E.C** projects),
- or in French frame (e.g. **ANR** projects),

in priority on:

- **Reflooding of degraded cores** (**PEARL** at IRSN, **DEBRIS** at USTUTT),
- **Corium/debris behaviour in lower head** (**CORDEB** at NITI, **IVMR H2020**),
- **Corium coolability during MCCI** (**CCI** in ANL),
- **Hydrogen behaviour in containment** (**OECD-THAI2/THAI3**, **ANR-MITHYGENE**…),
- **Iodine and Ruthenium chemistry** (**OECD-STEM/STEM2**, **OECD-BIP2/BIP3**…),
- **Pool scrubbing and mitigation** (**IPRESCA**, **ANR-MIRE**…).
- **SMRs models and Passive systems**
- **ATF's modelling**

Thank you for your attention

Questions?

APPENDIX 1 – MAIN PHYSICAL MODELS

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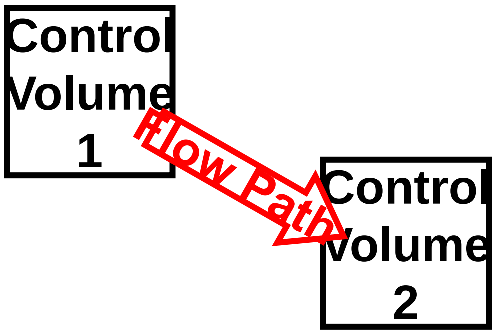
Hydrodynamics Basic Approach (1/4)

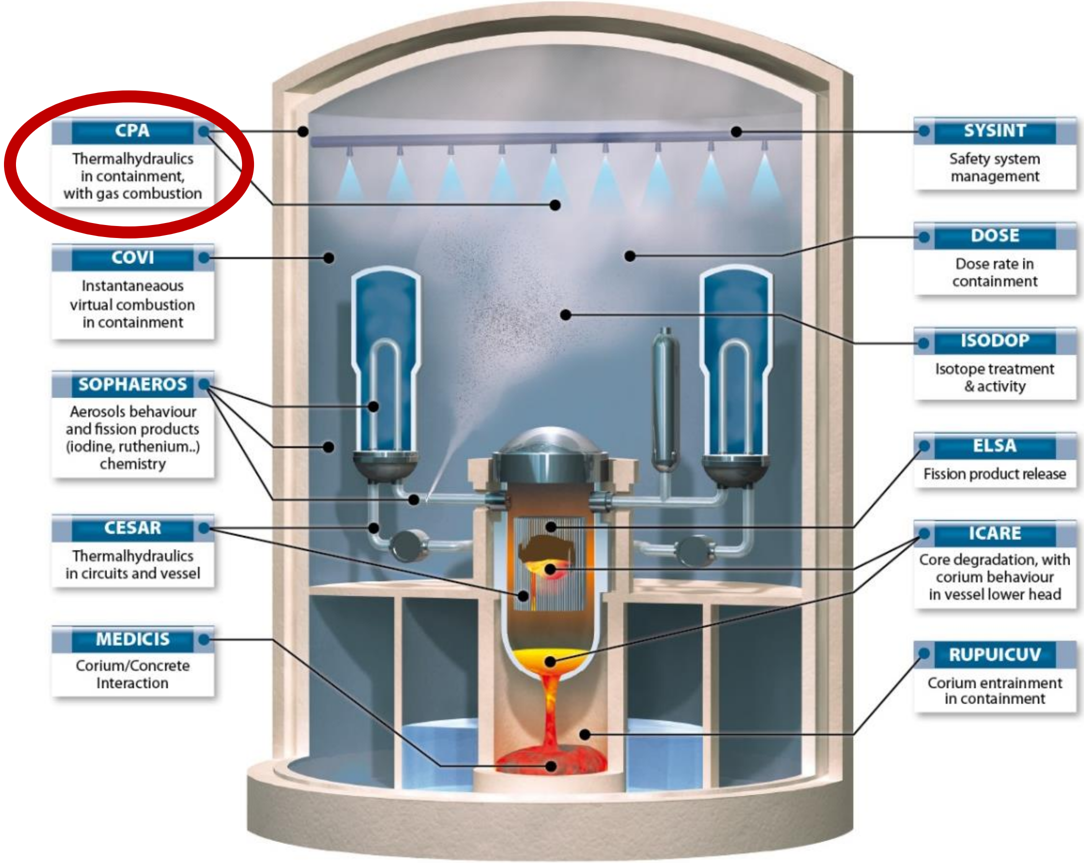
- **Space discretisation in control volumes, connected by flow paths:**
  - Provides maximum flexibility (but user's responsibility),
  - Allows building 1- 2- or 3-dimensional finite difference grids.



- In general, material can flow in either direction.
- Direction of the arrow defines the direction of positive flow.

- In general, **no predefined "components" in ASTEC**:
  - The user must build pipe, pressurizer, steam generator, etc... from control volumes, flow paths, and other elements
    - Users can rely for that on adequate documentation (Users Guidelines).

ASTEC



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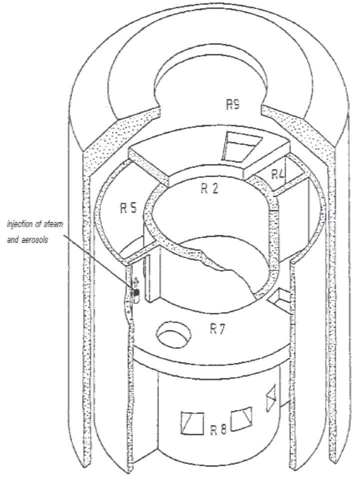
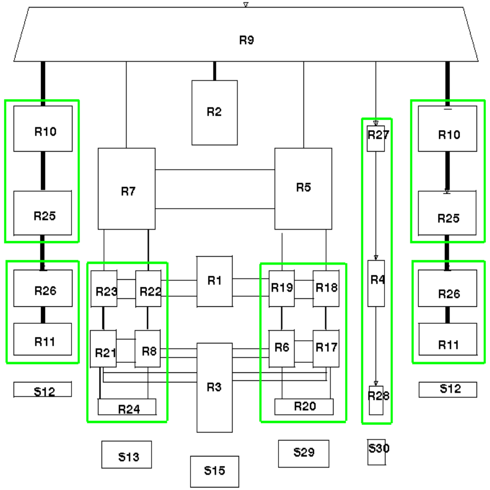
Hydrodynamics Basic Approach (2/4)

For the containment, Discretization through a “Lumped-Parameter” approach (0D zones connected by junctions and surrounded by walls):

- Control volumes represent the physical compartments such as dome, tunnels, cavity pit…
- May be subdivided in many zones to simulate local heterogeneities
- With possible leakages to the environment or to normal buildings and specified openings to the environment.

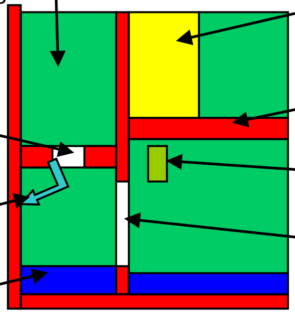




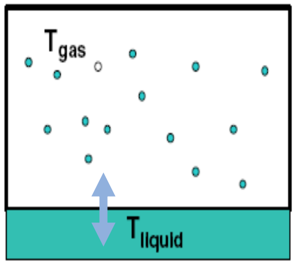
Example of VANAM-M3 experiment detailed nodalization

Hydrodynamics Basic Approach (3/4)

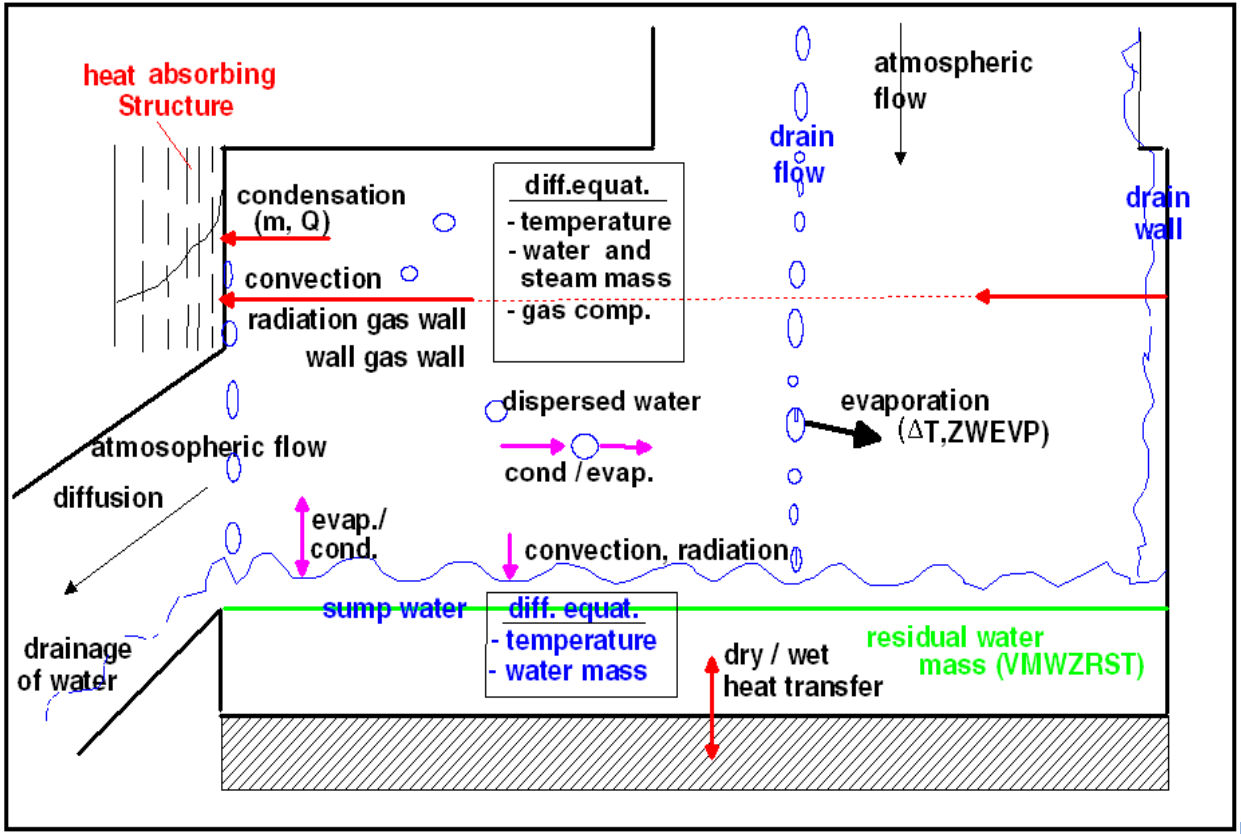
- **For the containment, any Control Volume of CPA module can contain a pool and an atmosphere:**
  - Non-equilibrium between pool and atmosphere (separate temperatures)
  - Pool can contain vapour bubbles, in equilibrium with liquid
  - Atmosphere can contain:
    - Liquid droplets, called “fog”, in equilibrium with water vapour
    - Several non-condensable gases in atmosphere: H_2, CO, CO_2, Air…
  - Pressure equilibrium between fields
  - Coupling between fields:
    - Pool and atmosphere exchange heat with structures
    - Mass-Energy exchange from condensation or evaporation



Control Volume example



Summary of basic th.hyd. phenomena simulated in the containment



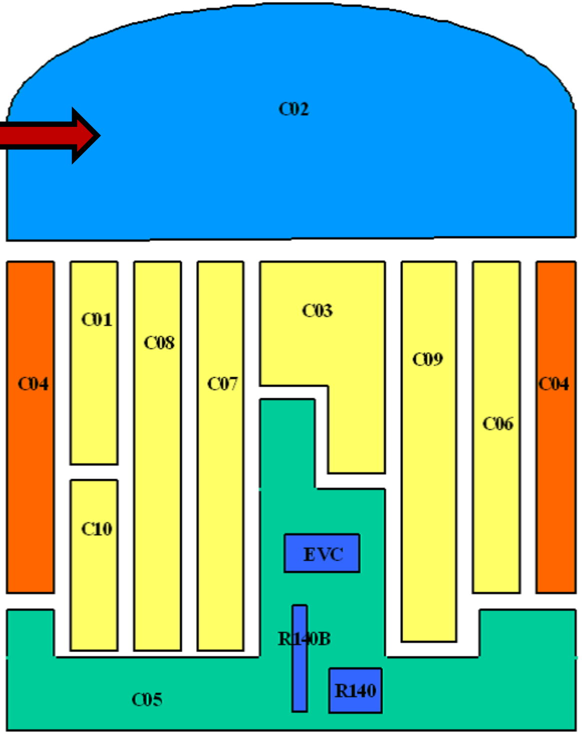
Example of ASTEC-CPA nodalization at plant scale

Example of a <u>"basic" ASTEC containment nodalization</u> for a French PWR 900 MWe

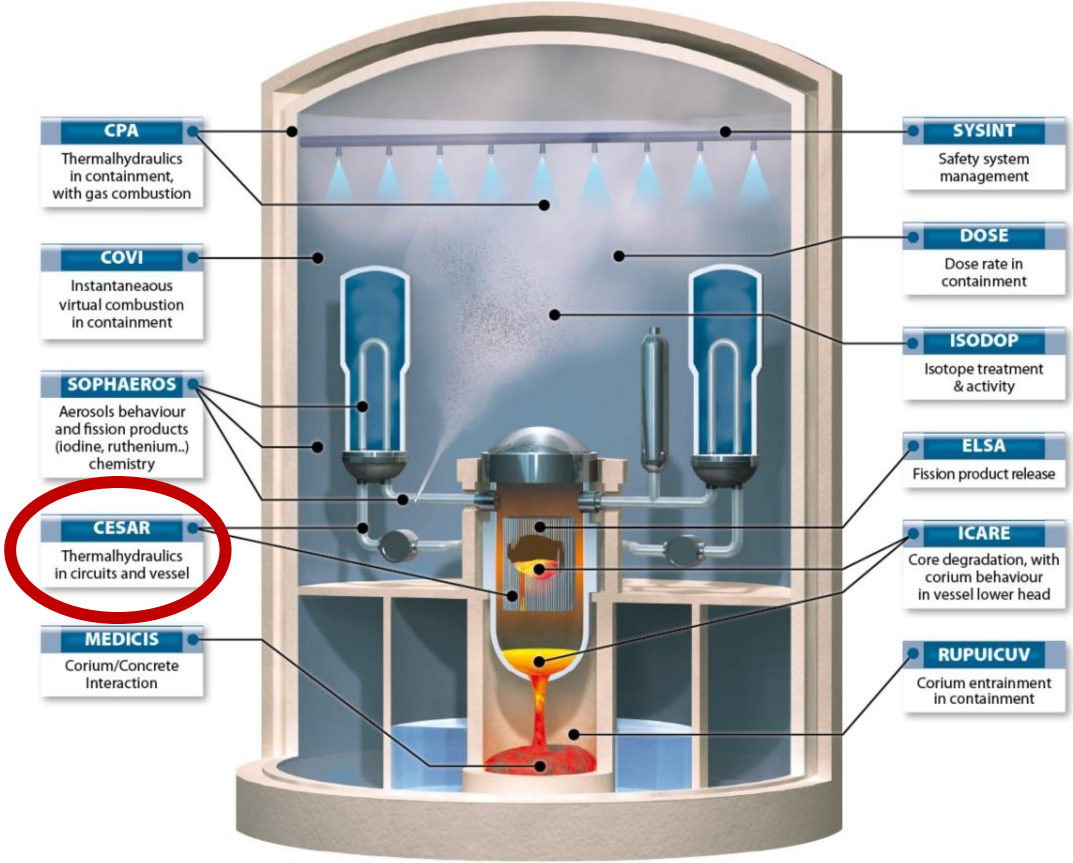
➔ 13-zones **CPA** model typically used for **complete SA simulations**, i.e. for transient calculations involving all ASTEC modules to work together

<u>For very detailed analyses</u> focussing only on one or few containment phenomena (*i.e.* ***detailed topical analyses*** *with boundary conditions supplied by user, such as e.g.* H_2 *risk studies*), **a much <u>more refined</u> <u>nodalization is often used</u>**

➔ 50-zones or 80-zones CPA models

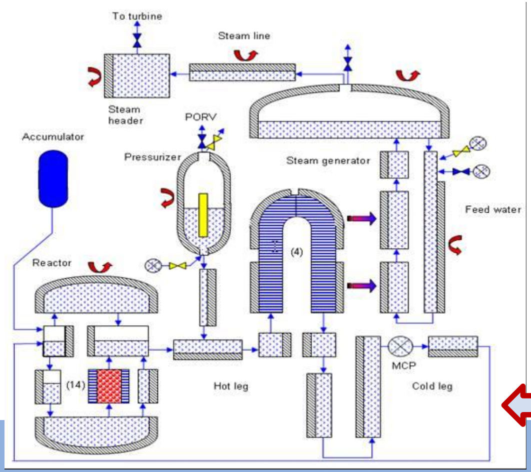


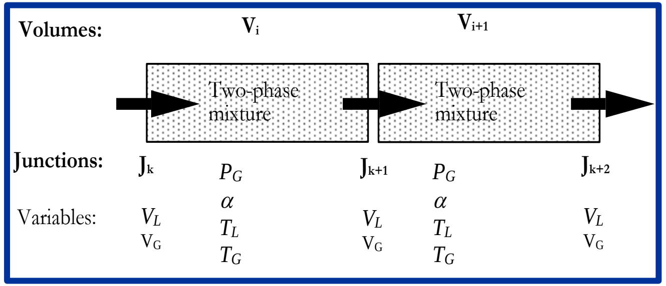
ASTEC


CPA
Thermalhydraulics in containment, with gas combustion
COVI
Instantaneaous virtual combustion in containment
SOPHAEROS
Aerosols behaviour and fission products (iodine, ruthenium..) chemistry
CESAR
Thermalhydraulics in circuits and vessel
MEDICIS
Corium/Concrete Interaction
SYSINT
Safety system management
DOSE
Dose rate in containment
ISODOP
Isotope treatment & activity
ELSA
Fission product release
ICARE
Core degradation, with corium behaviour in vessel lower head
RUPUICUV
Corium entrainment in containment

Hydrodynamics Basic Approach

- Different approach **for the RCS (primary/secondary circuits)**
- Discretisation: volumes, axial modules (pipes), junctions, walls.
- 2-phase thermal-hydraulics:
  - Water and gas ➔ *gas = steam + non condensable gas (any number of gases)*
  - 6-equation approach: water and steam mass, water and steam energy, water and steam momentum:
- Numerical scheme: staggered grid, implicit scheme, Newton method.



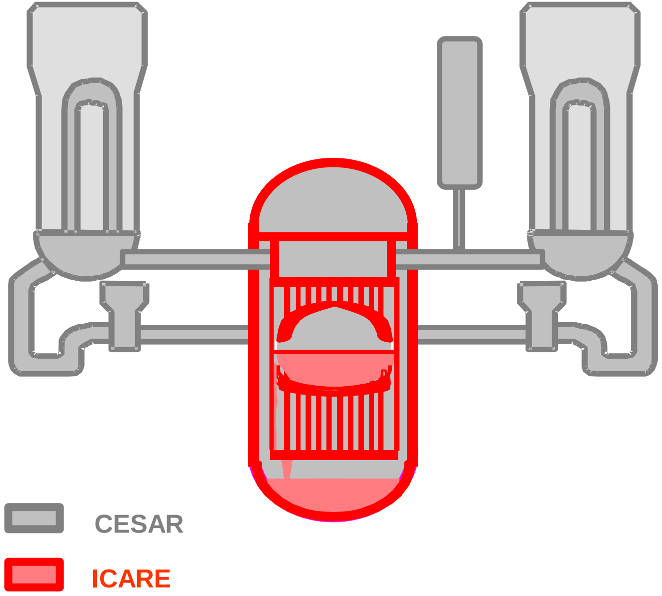


Example of 2-phase basic volumes (P, α, T_L, T_G) with junctions (V_L, V_G)

Example of discretization of the RCS in a French PWR 1300 MWe

CESAR/ICARE coupling scheme in ASTEC V2.1

- The coupling between the RCS thermalhydraulics module **CESAR** and the core degradation module **ICARE** was deeply reengineered in the **ASTEC V2.1** new major version



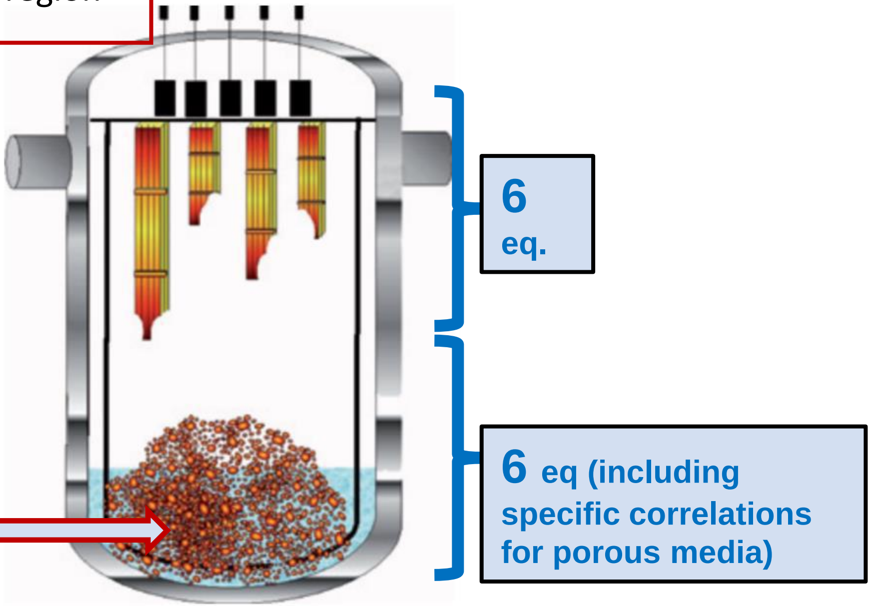
- Such a new CESAR/ICARE coupling concept was needed **to** notably **answer specific modelling requirements for adequately dealing with late phase core quenching**

New hydrodynamics model in the vessel

- Specific modelling approach **for the vessel region**
  → 2D (r-z) discretization applied in the core region

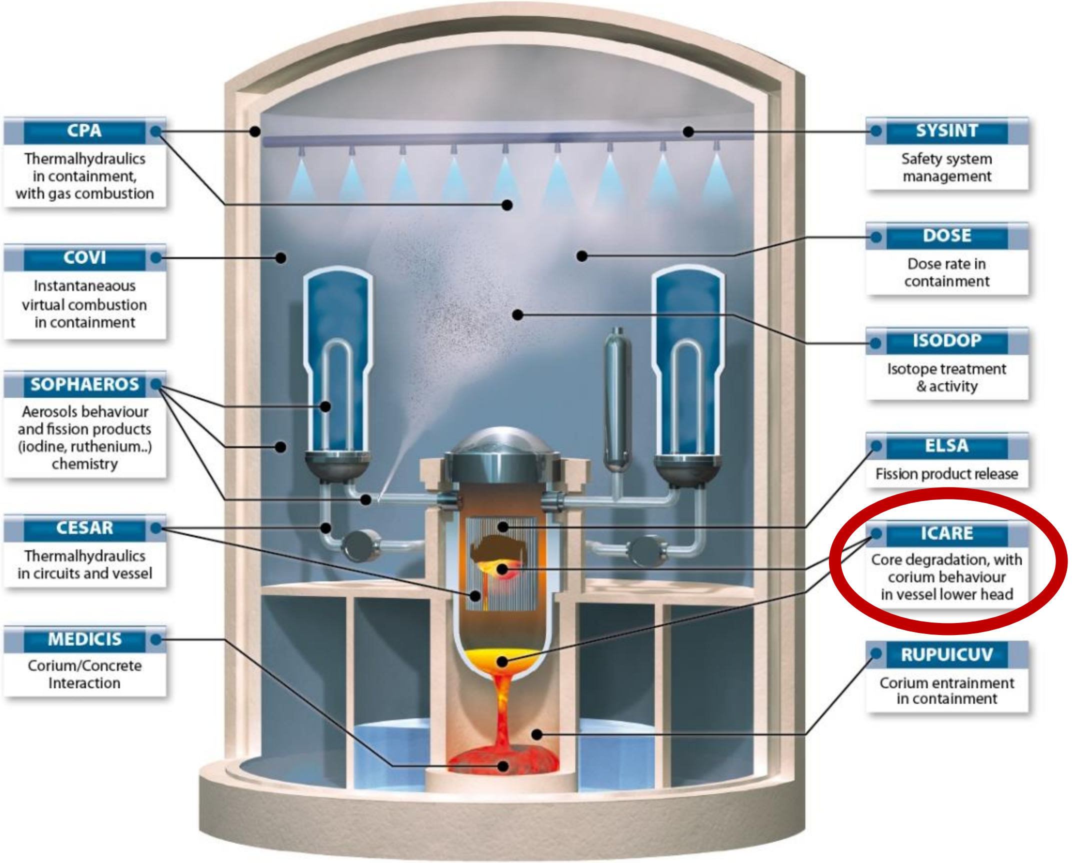
- During the core degradation phase, particulate debris are expected to form in the vessel

- **6-equation model in porous media**
  mliq, mgas, Tliq, Tgas, Vliq, Vgas



→ Automatic switch in **CESAR** from a classic to a porous thermal-hydraulic"
→ Triggered on criterion $S_{debris} > S_{rods}$

ASTEC



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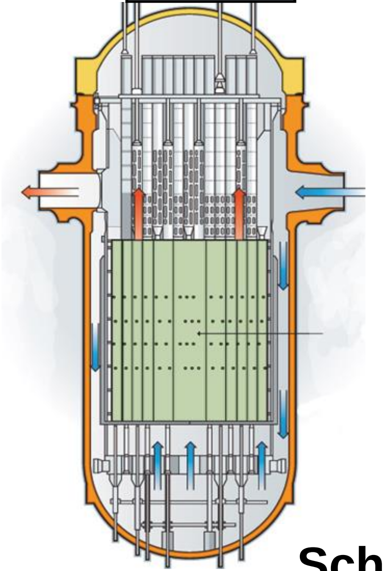
Introduction to core degradation modelling

Core degradation = Multiphysics phenomena and changing geometry

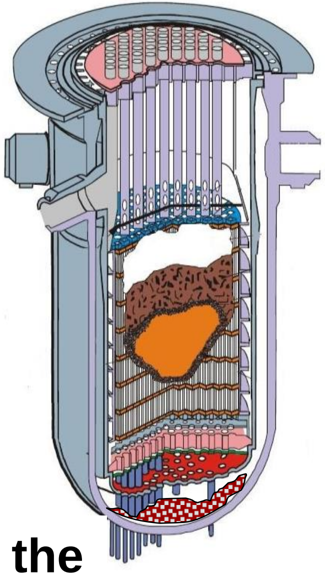
intact



Continuous transformations

Complex coupled phenomena

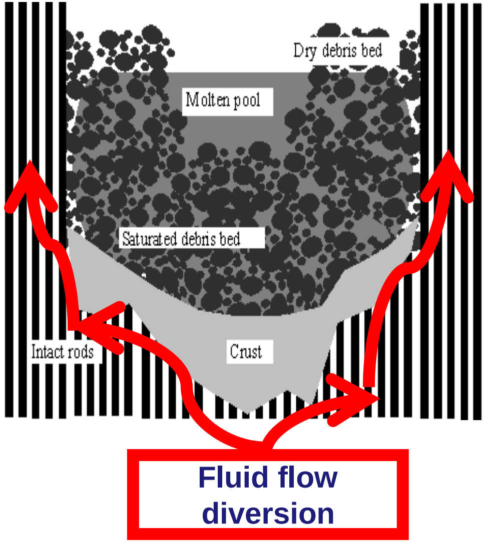
degraded



Schematic view of the TMI2 vessel

Core degradation models (1/5)

- **Complex heterogeneous geometry of degraded cores**:
  - Vertical rod bundles, including spacer grids (intact or partly damaged),
  - Peripheral and lower/upper core structures (e.g. plates, barrels..), also partly or totally molten,
  - Channels blocked with molten/frozen mixtures,
  - Debris beds and corium molten pool (with crusts),
  - Etc…



A dynamic management of these core and vessel components is needed

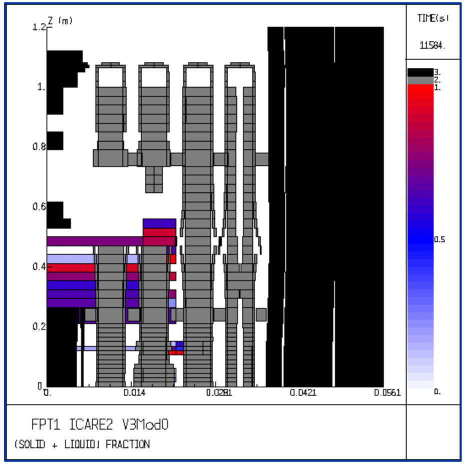
Powerful modelling features are required to properly handle the extreme complexity of phenomena and geometry.

- **Appearance and disappearance of a large number of components in each control volume** (chemical reactions, failure, melting, relocation, etc…)

Core degradation models (2/5)

Early degradation phase

- Account for most physical phenomena occurring in "rod-like" geometry
  - **Thermal behaviour** (conduction, convection, radiation)
  - **Mechanical behaviour** (ballooning, creep, burst)
  - **Chemical interactions** (oxidation and dissolution processes on fuel rods and control rods, according to reaction kinetics at the state of the art)
  - Fuel rod and control rod **melting**, and degradation (1D candling **relocation**)



- Novelty since **V2.1**: New description in **ICARE** module for **BWR** and **PHWR** cores
  - Was required to overcome modelling limitations coming from the ASTEC in-vessel original concept that was designed to address the axisymmetric structure of PWR cores
  - New ASTEC version allows now properly describing BWR and PHWR core geometries with the so-called **multi-channels modelling**
    - **New components to represent square canisters and crossed control blades**

Core degradation models (3/5)

Late degradation phase

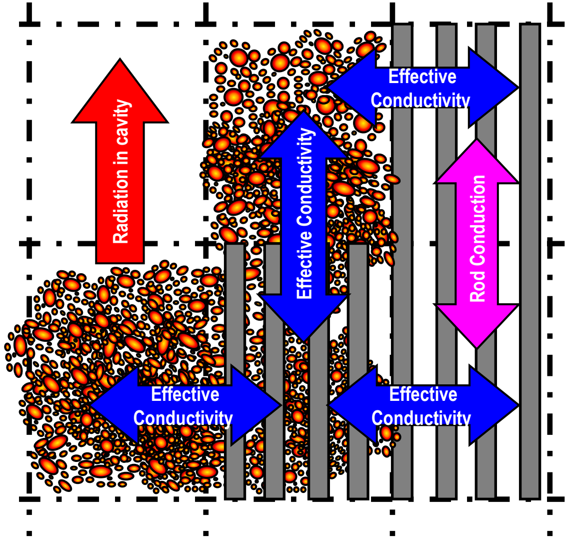
Modelling of a degraded core : "porous media" approach in **ICARE**

- Heat and mass balances are solved on a 2D meshing,
- Medium is supposed homogeneous with specific features in both **r** and **z** directions (porosity, permeability, heat conductivity, ..).

- Heat transfers within the "porous medium" are evaluated with an effective conductivity

  Main advantage of this method:
  ➔Continuous account for geometrical variation from intact rods to debris beds.

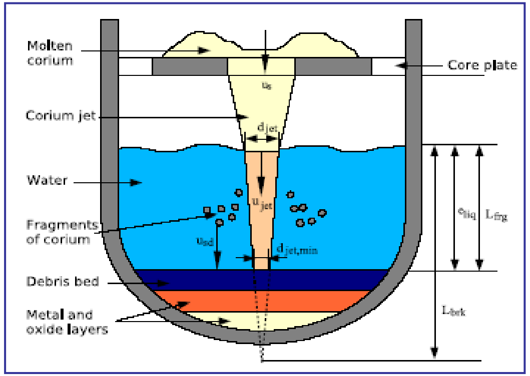
- 2D model for corium relocation based on a **generalization of the Darcy's law** :
  - The liquid materials flow through a solid matrix (rods, particles, grids, plates…),
  - The wall friction is averaged and expressed as a permeability,
  - Non uniform porosity properly considered (melting, geometrical evolution).



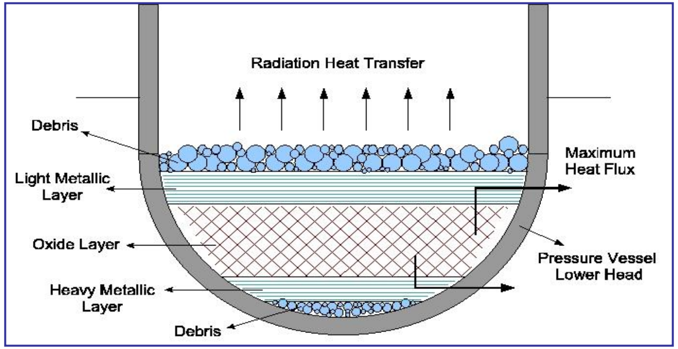
Core degradation models (4/5)

Modelling of corium in Vessel Lower Head

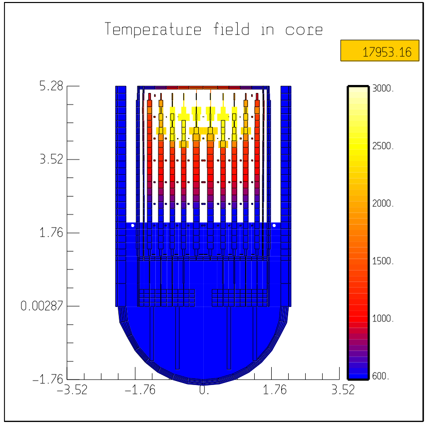
- **Fragmentation of molten corium slumps** into particles of different sizes:
  - Analytical model on jet break-up/fragmentation
    ➔ Correlations from Namiech for jet break-up length and particle diameter
- **Vaporisation of residual water**

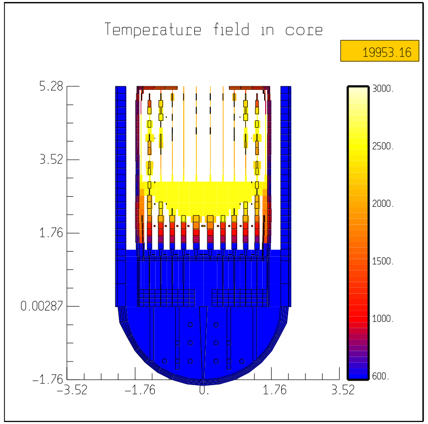


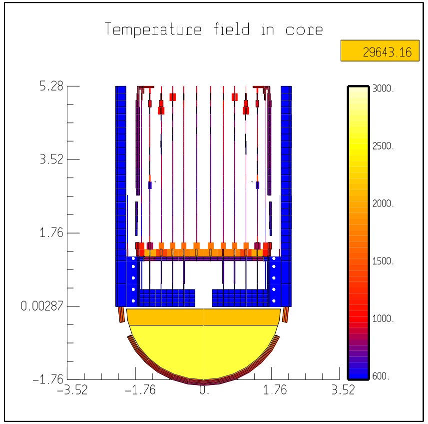
- **Formation/Stratification of corium layers in lower plenum**:
  - 0-D approach with **3 possible liquid layers** (light metal, oxide, heavy metal) and up to **2 possible debris layers**,
  - Possible evolution of layers position due to chemical interactions
    - Model of stratification based on the outcomes of **MASCA** experiments
      ➔ Both thermochemical and hydrodynamic phase separation processes are considered



Core degradation models (5/5)

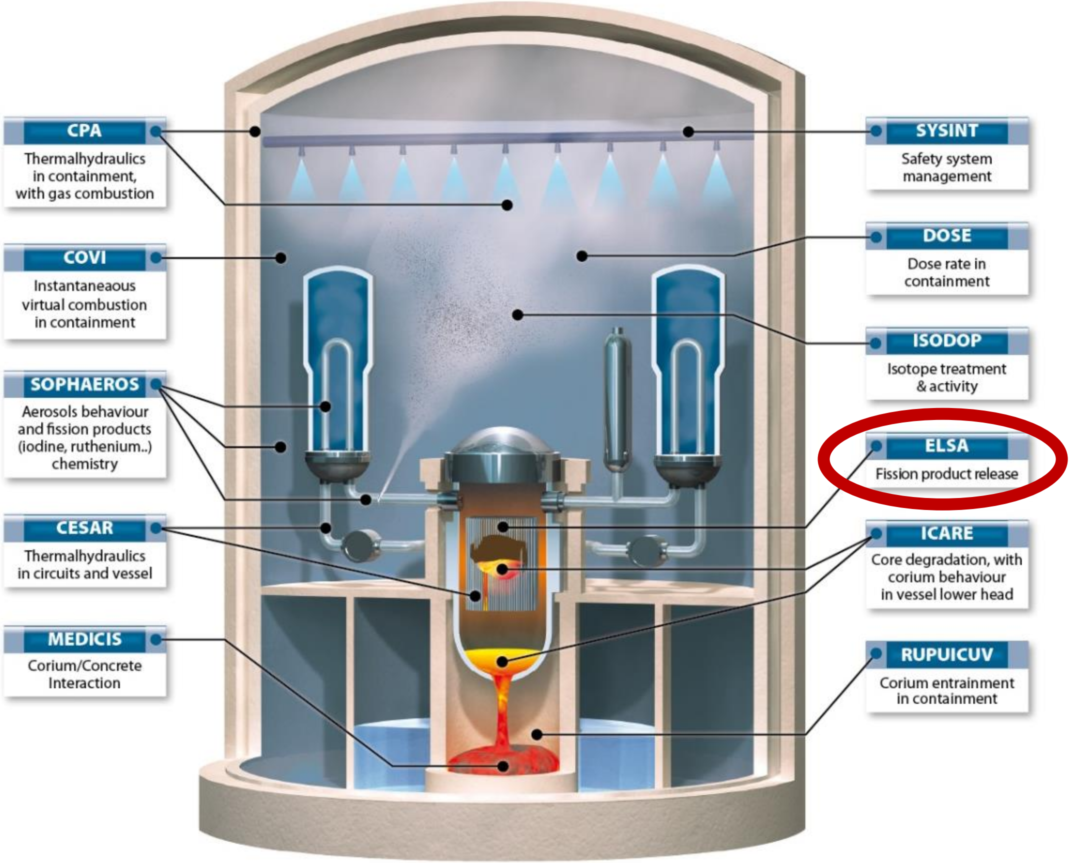






Example of ASTEC in-vessel degradation results for a LFW sequence applied to a French PWR 900 MWe

ASTEC



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Models of fission product release from fuel (1/4)

- **Main modelling concepts** (applied in **ELSA** module) are as follows:
  - FP behaviour depends on the degree of the FP volatility ➔ **3 categories** are distinguished : **volatile FP**, **semi-volatile FP**, **low volatile FP**
  - **Semi-empirical approach** : for each category, only the **main mechanism governing the release** and **identified as the dominant limiting phenomenon is modelled**

Models of fission product release from fuel (1/4)

Category	Species treated	Modelling
Volatile FP	Xe, Kr, I, Br, Cs, Rb, Cu, Se, Te, Sb, Ag	Limiting phenomena : **Solid-state diffusion through grains of UO_2 fuel matrix,** accounting for **fuel oxidation (UO_{2+x})** • For some species (**Te**, **Se** and **Sb**), their possible trapping in the oxidised cladding (that depends on temperature and the degree of clad oxidation) is taken into account • 100% of the remaining species are released at the fuel melting point • Debris bed geometry: *same modelling as above* (S/V ratio is adapted for spherical particles)

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Models of fission product release from fuel (3/4)

Category	Species treated	Modelling
semi-volatile FP	Ba, Ru, Sr, La, Eu, Ce, Mo	Limiting phenomena : **Evaporation in porosities and mass transfer processes at the fuel surface** Governed by the FP equilibrium partial pressures in the gas phase at the vicinity of the fuel ➔ *Those equilibrium pressures are based on thermodynamic data given by correlations mostly obtained by minimization of Gibbs free energy*
non-volatile FP	Rh,Pd,Tc,Nb,Zr,Np,Pu,Nd,Pm,Gd,Tb,Dy,Ho,Er,Tm,Yb,Pr,Am,Cm,Sm,U,Zn,AsCd,Sn,Ga,Ge,In,Y	Limiting phenomena : **UO_2 volatilisation treated as the vaporisation of UO_3** Debris bed geometry: *same modelling as fuel rods* (S/V ratio is adapted for spherical particles)

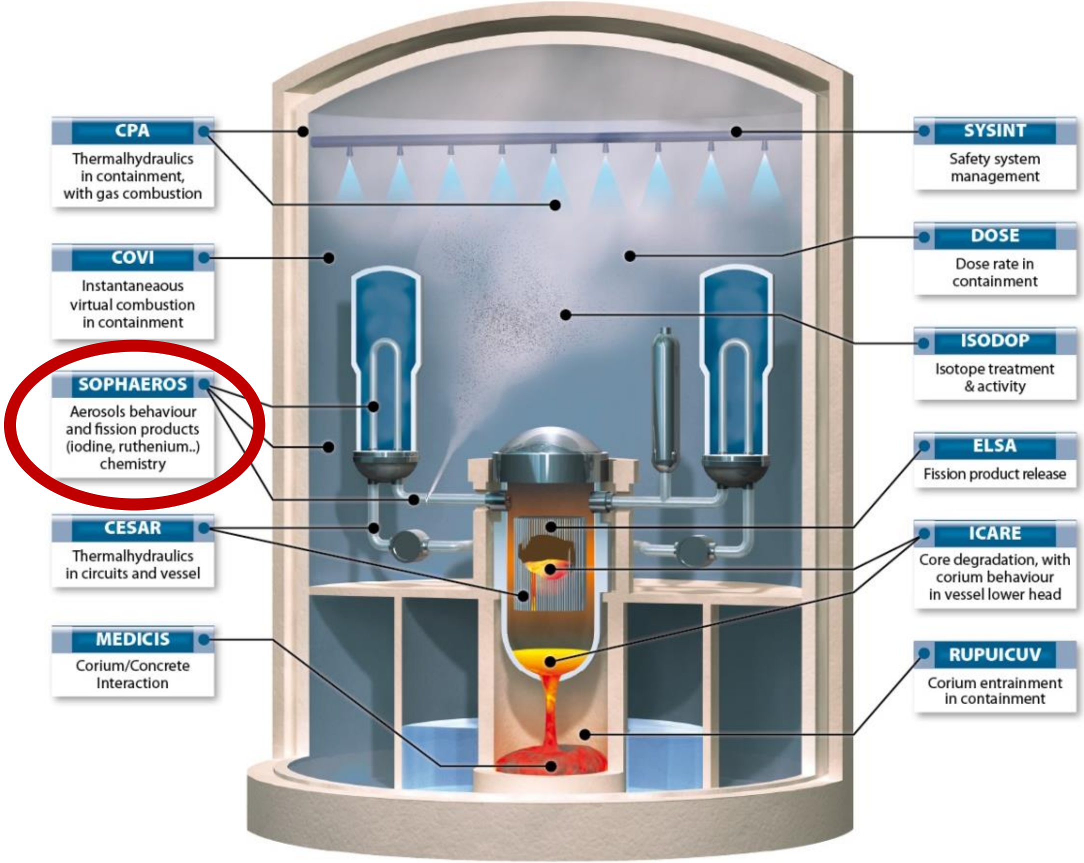
Models of fission product release from fuel (4/4)

- **Release from Corium molten pools** : Modelling based on evaporation and mass transfer processes at the free surface of the pool.
  - Vapour pressures of species are determined by considering an ideal solution chemistry but a non-ideal solution for phase distribution

    → **Strong coupling with core degradation** (**ICARE** module)

- Release of **control rod materials** (“SIC” or B_4C absorber) and **structure materials** (Sn, Zr, Fe, Ni, Cr) from core structures and from molten pool

ASTEC



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FP/aerosols transport models

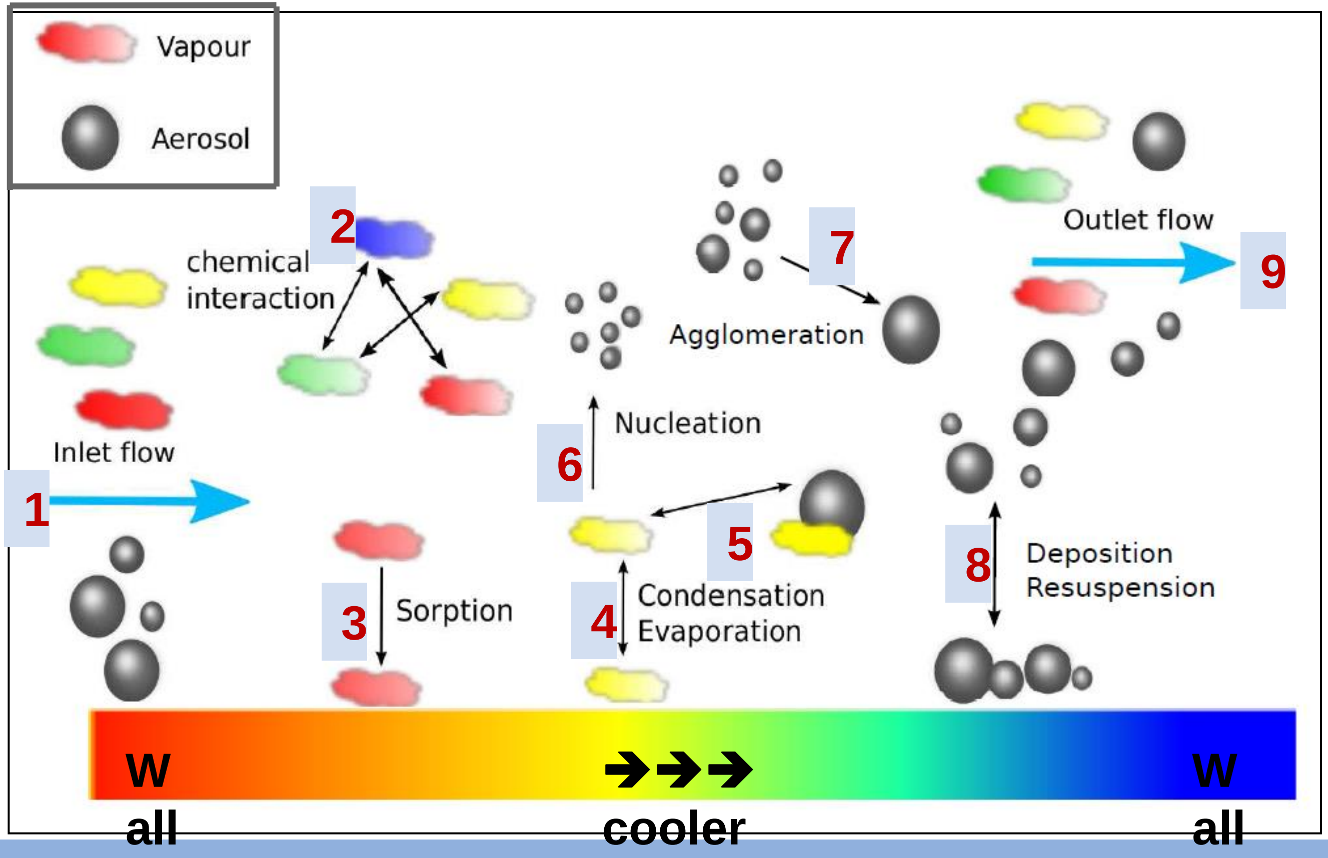
- In the **ASTEC V3.1** new series, the **SOPHAEROS** module simulates transport and chemistry of FP vapours and aerosols in the whole reactor, i.e. **in both the RCS and the containment domains**

➔ *Nodalization scheme fits those of CESAR and CPA respectively*

- **For the RCS, 6 different physical states are considered:**
  - Suspended vapour,
  - Suspended aerosol,
  - Condensed vapour on walls,
  - Deposited aerosol on walls,
  - Sorbed vapour in walls,
  - Liquid.
- **For the Containment, 6 more physical states are considered:**
  - Species on painted dry walls,
  - Species on Steel dry walls,
  - Species on concrete dry walls,
  - Species on painted wet walls,
  - Species on Steel wet walls,
  - Species on concrete wet walls.
- **Carrier gas: H_2O, H_2, O_2, N_2, He, Xe, Kr, Ar**

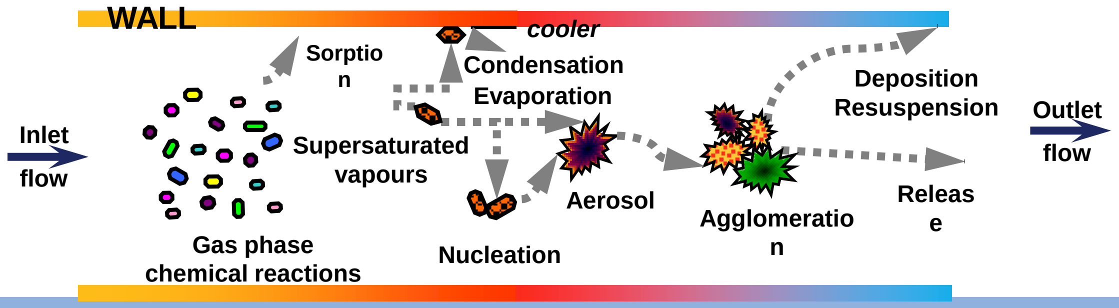
FP transport models **in RCS** (1/2)

Legend

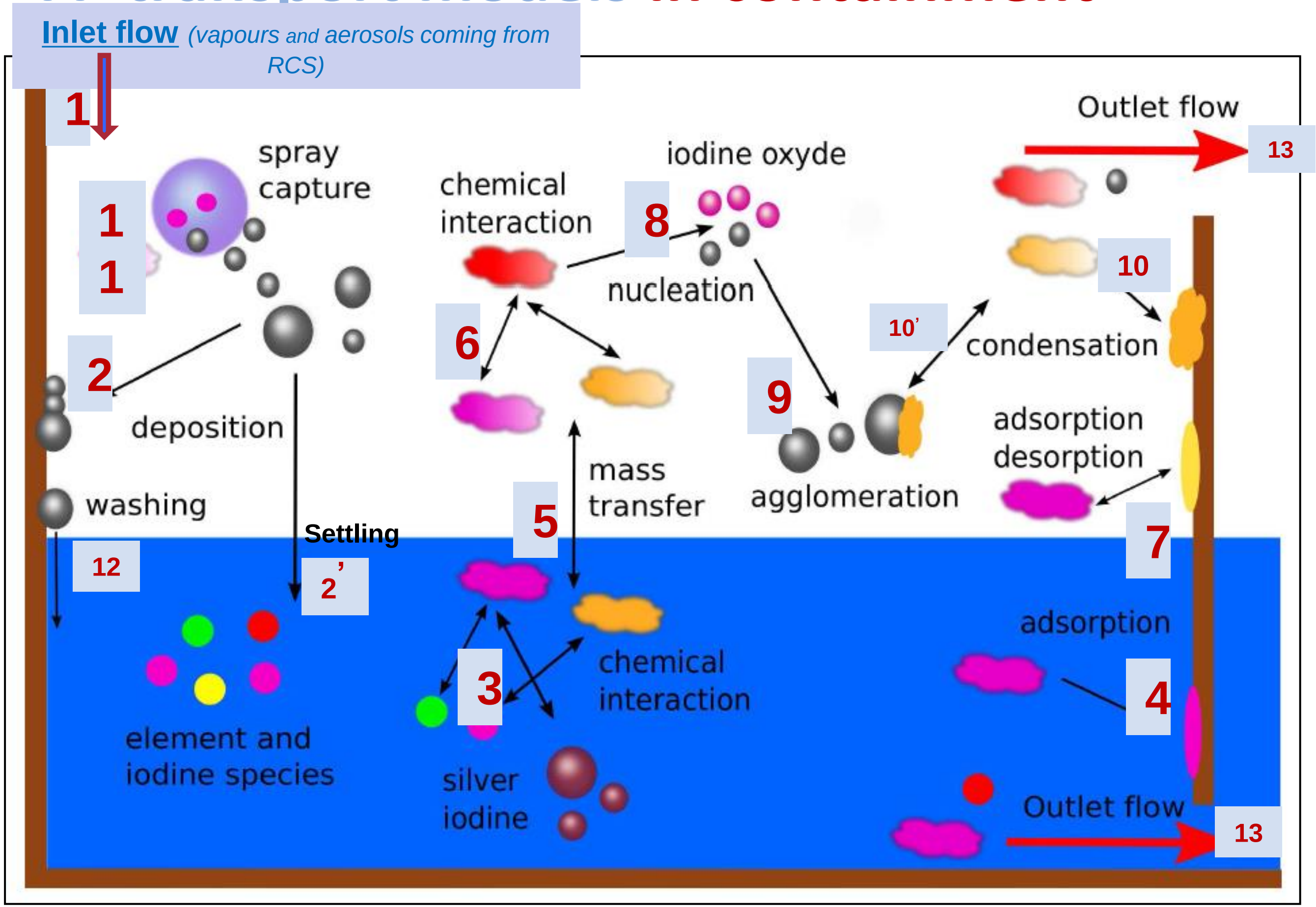


FP transport models in RCS (2/2)

- **Aerosol phenomena (up to 50 classes for aerosol size):**
  - Agglomeration : gravitational; Brownian diffusion; turbulent diffusion,
  - Deposition: sedimentation; thermophoresis; diffusiophoresis; Brownian or turbulent diffusion; impaction (eddy, in bends),
  - Re-mobilisation of deposits: re-vaporisation; mechanical resuspension.
- **Vapour-phase phenomena:**
  - Gas equilibrium chemistry or **kinetics chemistry**
    - Databank of ≈ 800 species to give final FP speciation
  - Chemisorption of vapours on walls,
  - Nucleation,
  - Condensation and revaporisation on/from aerosols and walls.



FP transport models in containment



FP chemistry models in containment

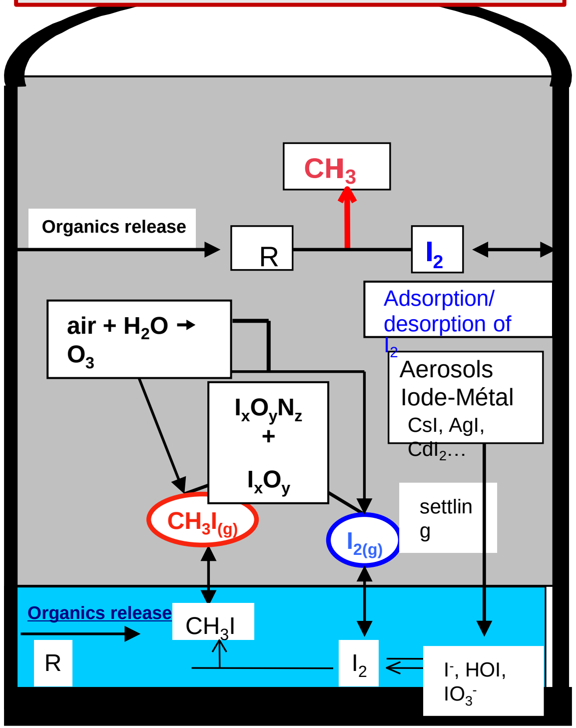
- **Chemical reactions (kinetics) in sump** and **gas phase in each containment zone**
  - ➔ **SOPHAEROS** module computes the transport of **Iodine** and **Ruthenium** species in containment zones using junction flow rates given by the **CPA** thermal-hydraulics module

❑ Reactions in **liquid phase**:
- Hydrolysis of molecular iodine,
- Radiolytic oxidation of I^- into I_2,
- HOI dissociation,
- Silver iodide (AgI) formation ……

❑ Reactions in **gas phase**:
- Adsorption / Desorption of molecular iodine on walls,
- Oxidation of molecular iodine by air radiolysis products,
- Radiolytic decomposition of iodine oxides and multi-components aerosols coming from the circuit
- Formation of organic iodine (CH_3I) from painted walls,
- Radiolytic destruction of organic iodide (ICH_3),
- O_3 formation, …….

❑ **Mass transfers** between sump and gas phase

***As to Iodine**, around **40 phenomenological models are considered** in ASTEC V2.1, that focus on the predominant chemical reactions in sump, gas phase and at the interface with surfaces*

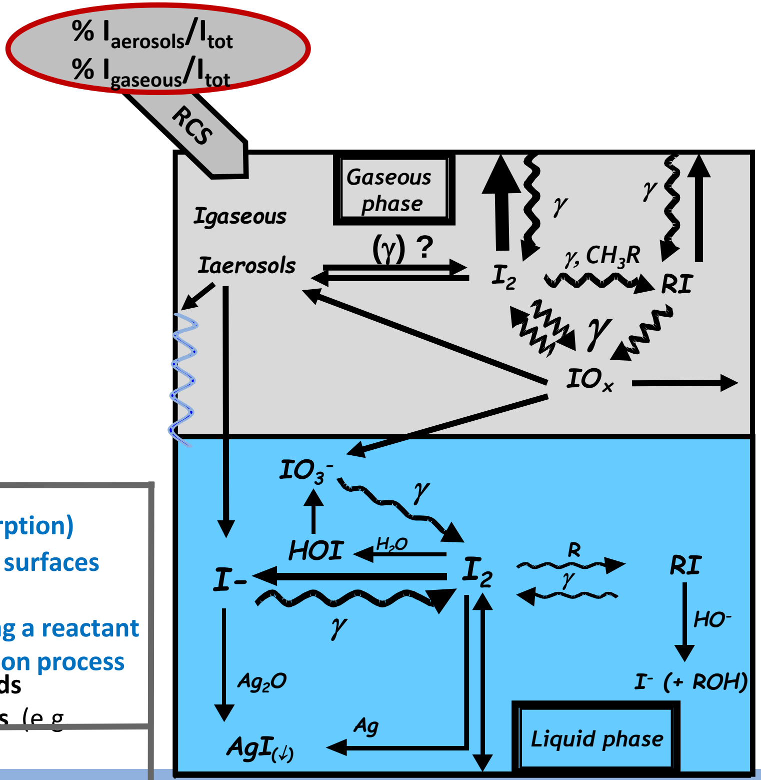


Summary of iodine models in containment

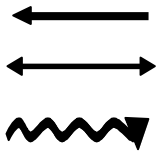
The competition between formation/decomposition processes of Iodine species governs the Iodine volatility in the containment (**short term ≠ long term**)

Main parameters likely to driving the iodine physical behaviour are:

- Sump and gas temperature
- Sump pH
- Dose rate in sump and gas
- Adsorption and desorption parameters (onto/from walls)
- Thermal-hydraulics conditions
  - such as e.g. humidity
- Aerosols solubility



Legends for the right figure



Thermal reaction (and adsorption)

Adsorption / desorption on surfaces (thermal reaction)

Radiolytic reaction converting a reactant into a product by an irradiation process

"R" represents volatile organics compounds

"RI" represents organic iodides compounds (e.g. CH_3I)

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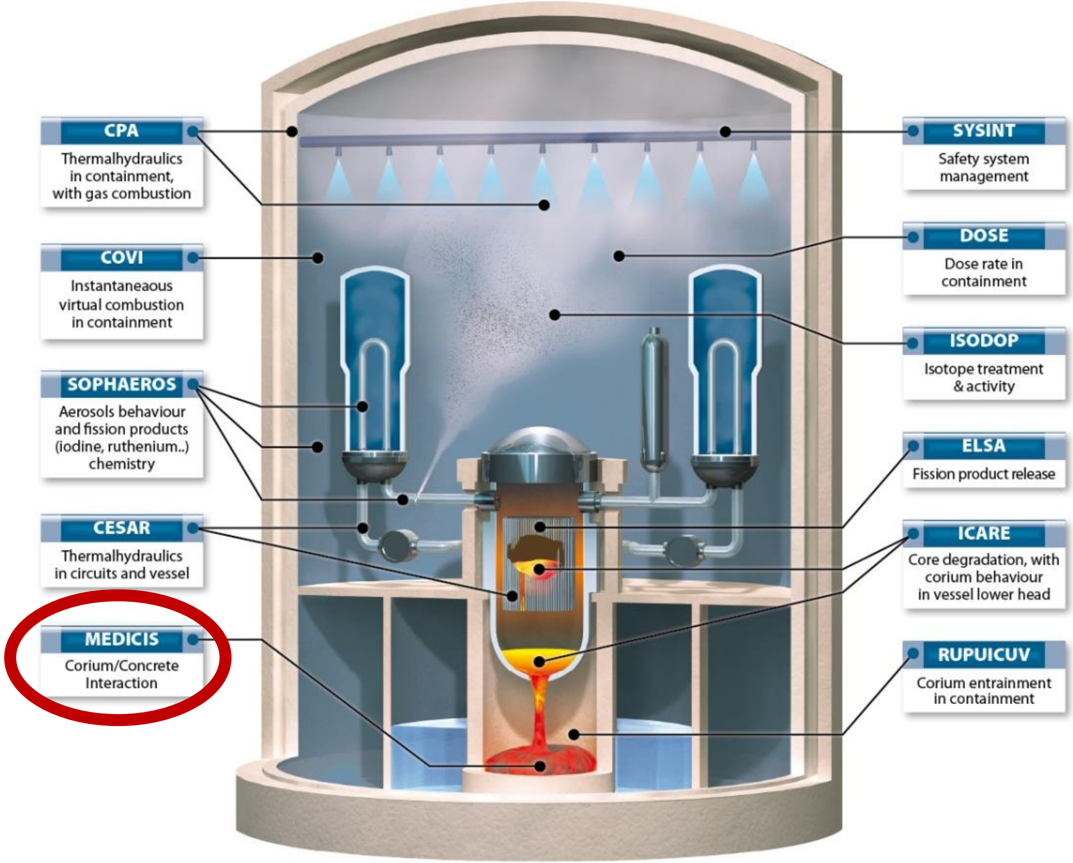

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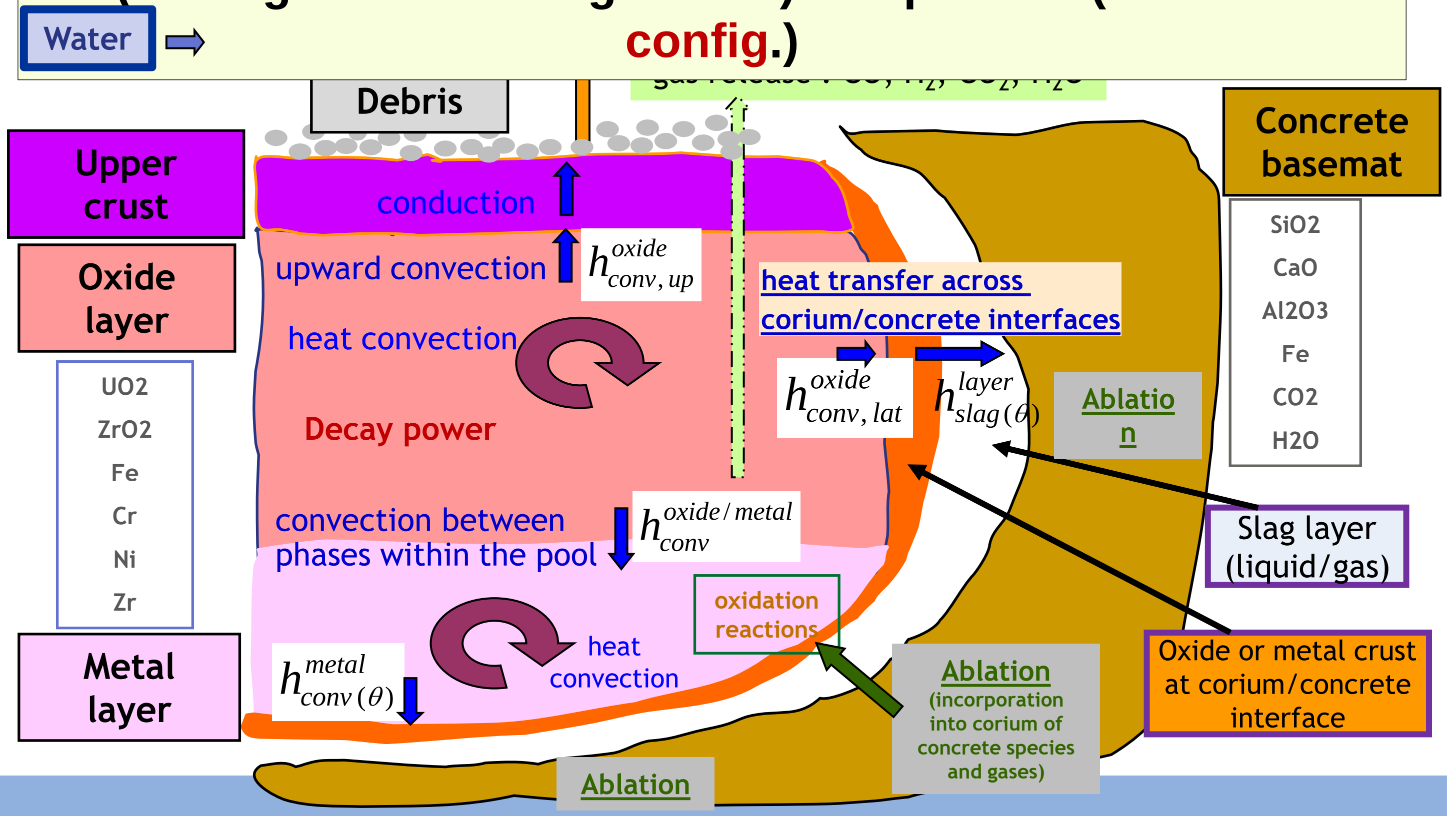
Molten-Core-Concrete-Interaction models (1/2)

In MEDICIS module, the corium is described by layers made of oxide species and metal species that can be mixed together (homogeneous configuration) or separated (stratified config.)



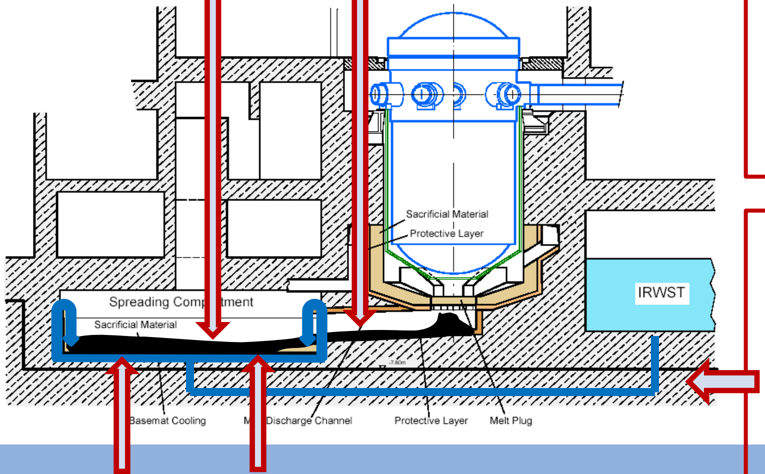
IRSN

Molten-Core-Concrete-Interaction models (2/2)

ASTEC specific models related to the EPR core catcher design

- Corium pouring kinetics from cavity towards the spreading chamber:
  - Simple model based on Bernoulli flow approach and corium properties

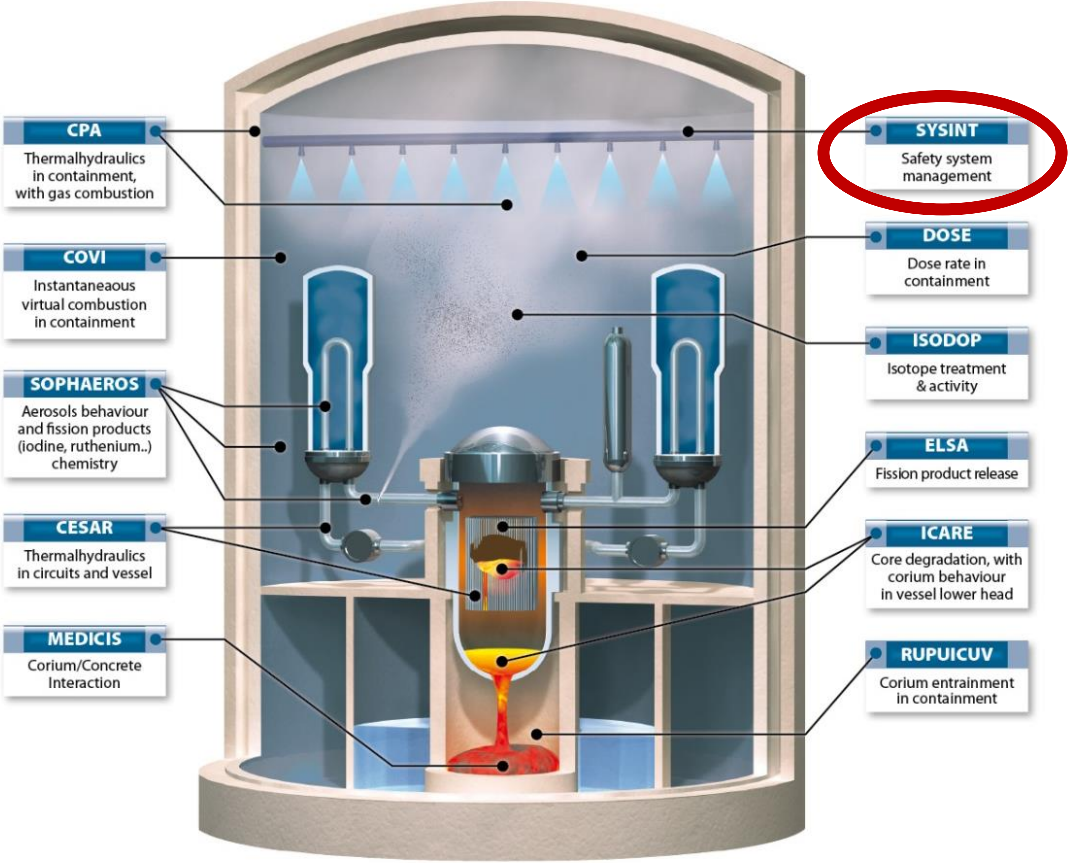
- Corium spreading in the spreading chamber:
  - Spreading radius versus time is evaluated with an analytical model for axisymetrical geometry in viscous or inertial regime,
  - Thickness of the solidified corium front is evaluated using a simple energy balance (accounting for the radiative heat losses at the upper corium interface).



- Thermal behaviour of the steel structures below the spread corium:
  - Heat conduction, possible melting

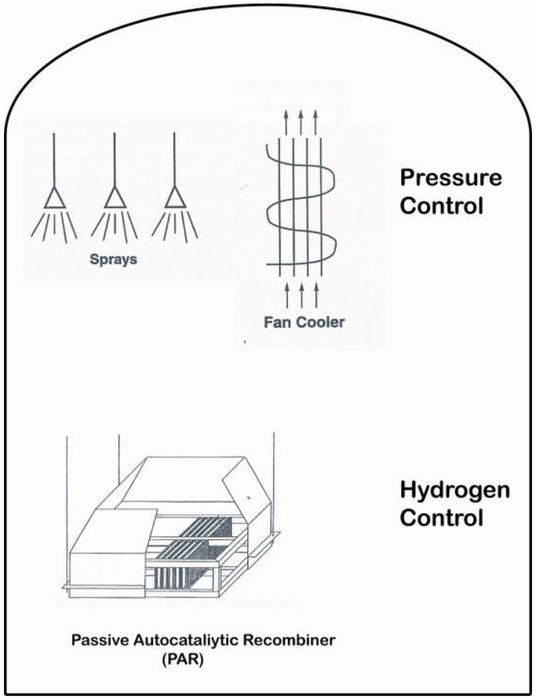
- Complete modelling of the cooling circuit after corium spreading phase
  - Gravity fluid flow from the IRWST to the spreading chamber, with account for the 2-phase circulation below the steel structures

ASTEC



CPA
Thermalhydraulics in containment, with gas combustion
COVI
Instantaneaous virtual combustion in containment
SOPHAEROS
Aerosols behaviour and fission products (iodine, ruthenium..) chemistry
CESAR
Thermalhydraulics in circuits and vessel
MEDICIS
Corium/Concrete Interaction
SYSINT
Safety system management
DOSE
Dose rate in containment
ISODOP
Isotope treatment & activity
ELSA
Fission product release
ICARE
Core degradation, with corium behaviour in vessel lower head
RUPUICUV
Corium entrainment in containment

Models for Safety System Features



- **In RCS:**
  - Hydro-accumulators, HPIS, LPIS
  - Pressuriser spray/heaters,
  - Valves (Pressuriser, SG)…

- **In containment:**
  - **Pump systems**,
  - **Fan coolers**,
  - **Valves**, **doors**, **rupture discs**, …
  - **Filters**,
  - **Spray systems**: droplet size evolution, interaction droplets-walls, …
  - **PAR** (passive autocatalytic recombiners) of different types (Siemens, AECL, NIS):
    - Simplified correlations,
    - or detailed model

Material properties Data Bank

- **MDB** : A sustainable tool for the **integration of recent research on the nuclear material properties**
  - From **EC Projects** (for FP) ➔ CIT, ENTHALPY
  - From **OECD Projects** (for corium) ➔ RASPLAV, MASCA 1, MASCA 2

- **MDB** : Reference Databank of Material Properties for Water-Cooled NPPs, providing not only the **physical properties of the individual substances**, but providing also approaches to evaluate the **corium properties** for SA applications
  - Based on European **NUCLEA database** for corium thermochemistry
    ➔ More than 25 years of development
  - MDB library associated to a very large and continuous data review process
    ➔ To get a critically evaluated material property database for thermodynamic and thermophysical properties

- **MDB** : A tool which was originally devised for the ASTEC needs, but due to its general design, can be used by any code studying nuclear reactors (**water-cooled reactors**, **Gen.IV SFR**, **ITER**…).

Material Data Bank : General data contents

Major material groups

Chemical Elements

Ceramics-Oxides

Absorber materials (B_4C, SIC)

Metallic alloys (AISI-304, …)

Isotopes

Iodine chemistry

Mixtures

Major material properties

Thermochemical properties

Gibbs energy, Cp, S, ΔH_f …

Thermophysical properties

Thermal conductivity, density, viscosity …

…

APPENDIX 2 – ASTEC V3.1 validation Vs Experimental data

General approach for ASTEC validation

- **Four-tier validation approach** (benefits from ASTEC code modularity):
  1. **Separate-Effect-Tests** (SETs) focusing on only 1 physical phenomenon,
  2. **Coupled-Effect-Tests** (CETs) focusing on a set of physical phenomena,
  3. **Integral tests** (IT) to check the coupling of physical models and that no essential phenomenon was forgotten or neglected

     ➔ *Example of **Phébus FP** integral experiments at IRSN*
  4. **R**epresentative **simulations at plant scale** for few reference sequences

     ➔ not detailed hereafter, but very important too to check the reliability of any new version
- Very large validation matrix, covering all SA phenomena through more than 180 experiments:
  - Major (past, on-going) French, German and international exp. programs,
  - Continuous IRSN detailed interpretation of **Phébus FP** integral tests.
- At each major code release, application of a sub-set of the matrix for checking non-regression and model improvements:
  - Covering all the main phenomena,
  - ≈25 SETs/CETs (2-3/module) + 2 integral applications (**Phébus**, **TMI2**)

Overview of the ASTEC validation matrix (1/3)

- **Most OECD/NEA/CSNI ISPs were already calculated**
  - **27** (**BETHSY**): Thermal-hydraulics in PWR RCS
  - **33** (**PACTEL**): Thermal-hydraulics in VVER RCS
  - **31** (**CORA**): Core degradation/reflooding of a PWR-type rod-bundle
  - **36** (**CORA**): Core degradation of VVER-type rod-bundle
  - **45** (**QUENCH**): Core reflooding
  - **34** (**FALCON**): Gas chemistry in RCS
  - **35** (**NUPEC**), **37** (**VANAM**): Containment Spray and H_2 distribution in containm.
  - **39** (**FARO**): Corium slump and fragmentation
  - **40** (**STORM**): Aerosol resuspension
  - **41** (**ACE-RTF**, **CAIMAN**): Iodine behaviour
  - **44** (**KAEVER**): Aerosol depletion and th.hydraulics in containment
  - **47** (**TOSQAN-MISTRA-ThAI**): Th.hydraulics in containment with spray operation
  - **49** (**ThAI-ENACEFF**): Hydrogen combustion in containment
  - **46** (**Phébus-FPT1**): Integral test
  - …

Overview of the ASTEC validation matrix (2/3)

Other experiments belonging to the ASTEC validation matrix:

- VVER-specific experiments
  - **PACTEL**, **CORA-W**, **QUENCH**, **EREC**, **PSAERO-HORIZON**,…
- OECD projects
  - **LHF-OLHF**, **RASPLAV/MASCA**, **ThAI**, **PANDA SETH II**, **STEM2**, **BIP**, **OECD-CCI**…
- Most of the other recent or on-going key-experiments
  - All **Phébus-FP** integral tests
  - **QUENCH** on core reflooding
  - **PRELUDE**, **PEARL**, **DEBRIS** on severely degraded core reflooding
  - **EPICUR** & ISTP/**CHIP** on iodine
  - **STEM** on Source Term mitigation
  - **ThAI** (Germany) on containment th.hydraulics, e.g. hydrogen behaviour (hydrogen distribution, combustion, recombination…)
  - **LIVE** on corium pool behaviour in vessel lower head
  - **CORDEB**, **CORDEB2** on corium/debris behaviour in vessel lower head
  - **VULCANO** and **CCI** on MCCI
  - …

Overview of the ASTEC validation matrix (3/3)

Illustration of a detailed validation matrix *(here for* CESAR ***module)***

Validation of the physical laws: Separate Effect tests

Main phenomena	Experiment	Mechanical Transfer	Interfacial Heat Flux	Wall Heat Flux
Critical flow rate	SMD long nozzle	Yes	Yes	
	SMD short nozzle	Yes	Yes	
	REBECA	Yes	Yes	
Reflooding 1D	PERICLES Reflooding	Yes	Yes	Yes
Swollen water level volume	PERICLES boil up			Yes
Wall friction	MD	Yes		
Wall heat flux	COTURNE	Yes	Yes	Yes
Condensation	COSI (Accu)		Yes	

Component validation

Component	Experiment
Steam Generator	PATRICIA GV1 GV2
	Comparison with CATHARE
Pressurizer	Comparison with plant results

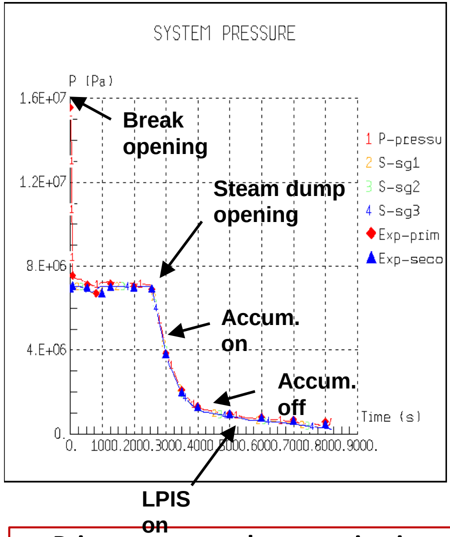
Integral tests

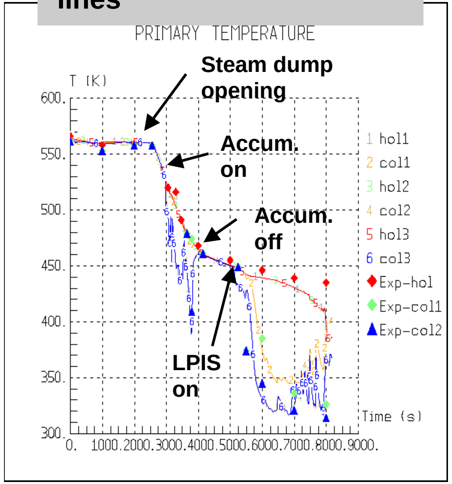
Experiment	Scenario
BETHSY	LOCA (2 inches break): 9.1b
	SGTR (6 tubes): 4.3b
	Total loss of Feed-Water: 5.2e

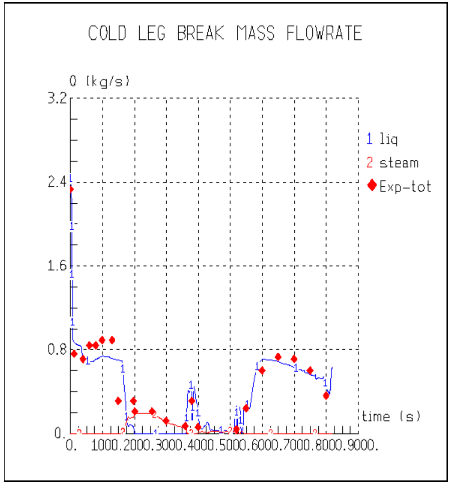
Validation of circuit thermal-hydraulic models

ASTEC V2.0 (*CESAR module*) validation on **BETHSY** (CEA) **test 9.1b**
simulating a 2'' Cold Leg Break without HPIS

ASTEC results are **in solid lines**







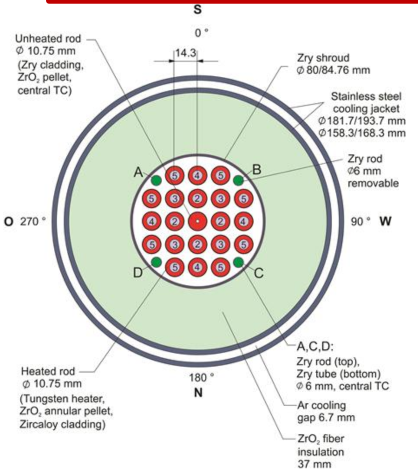
- **Primary system depressurization after break opening well predicted by ASTEC**
- **Primary and secondary pressure decrease and primary temperature reduction after steam dump opening is well simulated.**

- **Cold leg temperature decrease after cold water injection by safety systems is rather well reproduced**
- **Break mass flow rate is well estimated**
- **The clad maximum peak temperature (~ 995 K) is well reproduced**

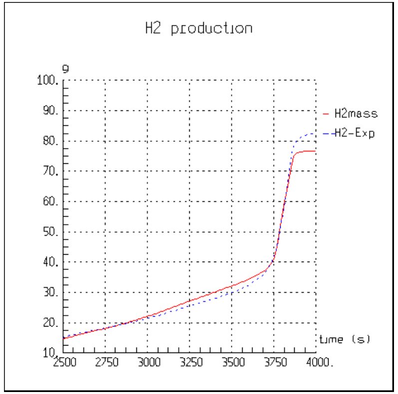
Validation of core degradation models (1/2)

Early degradation phase

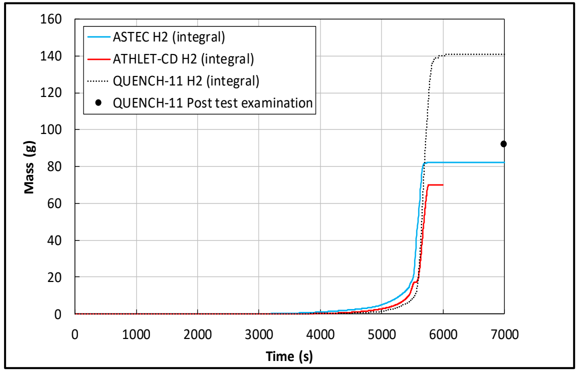
- **ASTEC V2.1** (*ICARE module*) validation on **QUENCH-08** and **QUENCH-11** (KIT experiments) up to the final quenching occurrence
  ➔ *Validation **tasks in CESAM** performed respectively by **KIT-INR** and **RUB***
  - Overall good agreements on water level and bundle temperature evolutions
  - Some underestimation of H_2 production (oxidation) during quenching period



QUENCH rod-bundle



QUENCH-08 test



QUENCH-11 test

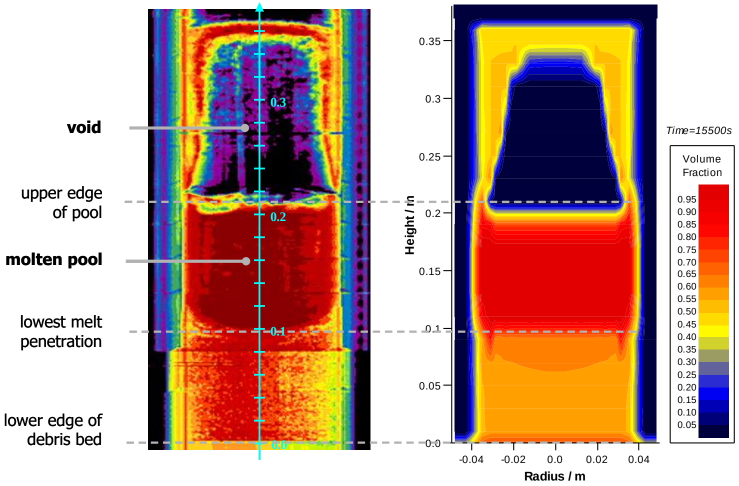
Cumulated hydrogen

(**ASTEC** and **ATHLET-CD** results are **in solid lines**)

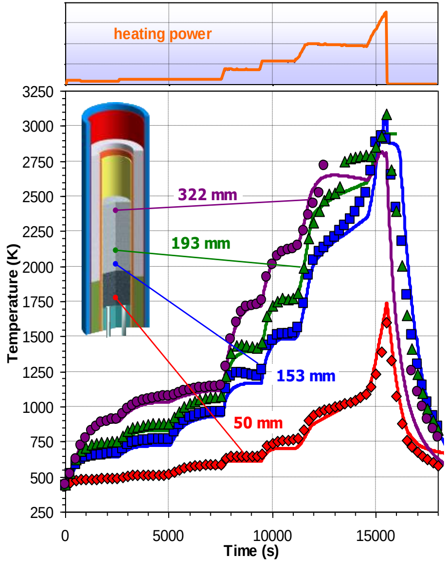
Validation of core degradation models (2/2)

Late degradation phase

- **ASTEC V2.0** (*ICARE module*) validation (*IKE work in SARNET*) on **Phébus FPT4** late-phase experiment (IRSN)
  - Good agreement as illustrated by: ***1)*** comparison of calculated final state of UO_2-ZrO_2 debris bed degradation with post-test radiography; ***2)*** comparison of calculated temperatures with measurements



Material distribution after the test
Comparison of post-test radiography of the test section (left) with ASTEC V2 calculated volume fraction of material (right)



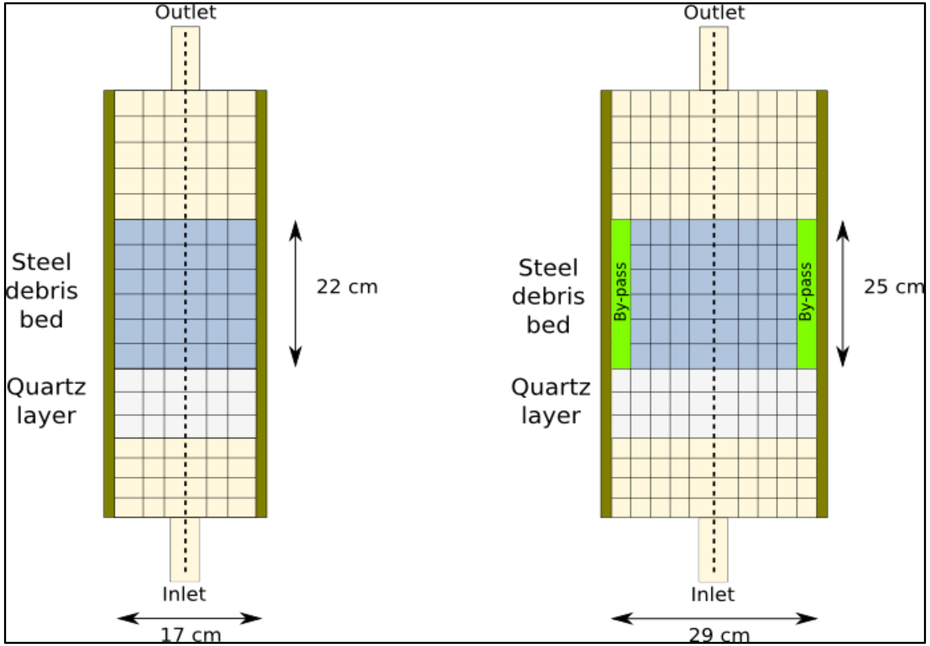
Comparison of temperatures at the bed centreline

(**ASTEC** results are **in solid lines**)

Validation of late phase core reflooding models (1/2)

- **ASTEC V2.1** (*ICARE/CESAR modules*) validation by *IRSN* on **PRELUDE 1D**, **PRELUDE 2D** and **PEARL** experiments (IRSN)

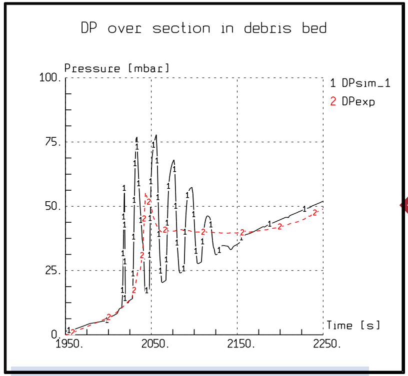
Prelude facility



ASTEC meshing of the PRELUDE facility: 1D (*left*) and 2D (*right*) configurations

Validation of late phase core reflooding models (2/2)

- **PRELUDE 1D**: **- Flat quench progression in ASTEC, in contrast to experiment**
- **PRELUDE 2D**: **- Steam flow is deviated to the bypass** (higher passability)
  - Faster quench progression in bypass in agreement with experiment

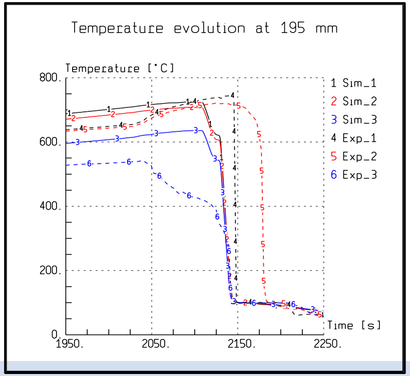


Pressure drop evolution in the steel debris bed

PRELUDE-1D (test 73)

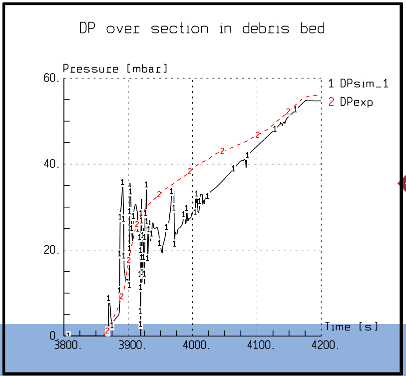
T_{debris} at reflood time : 700°C

Injection velocity : 5 m/h



Temperature evolution near the top of the steel debris bed, at 3 radial locations (centre, medium, periphery)

(**ASTEC** results are **in solid lines**)

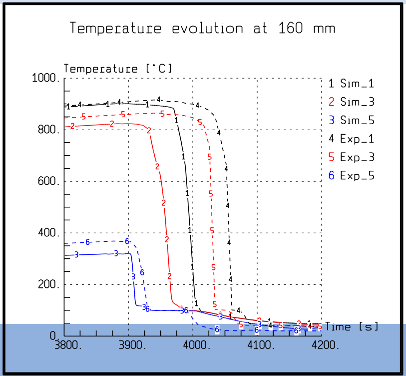


PRELUDE-2D (test 215)

T_{debris} at reflood time : 900°C

Injection velocity : 5 m/h

Bypass thickness : 4 cm

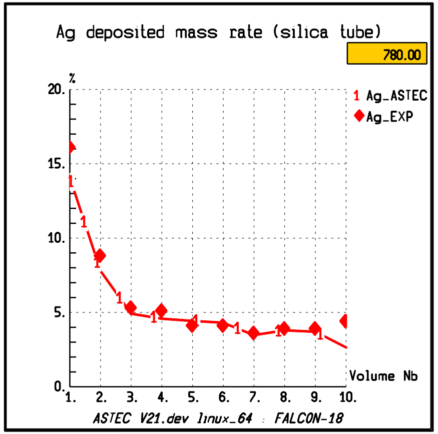


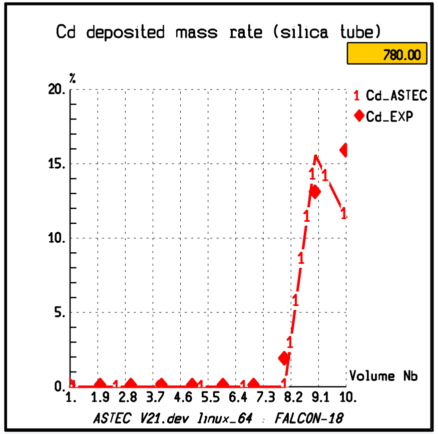
IRSN

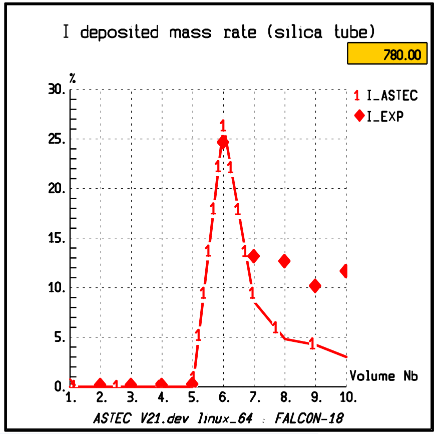
Validation of models for FP transport & chemistry in RCS (1/2)

- **ASTEC V2.1** (*SOPHAEROS module*) validation on **FALCON-18** (AEA-T) experiment on transport and deposition of FPs in presence of SIC control rod material (*IRSN task*)
  - ➔ **Good agreement on deposits in the RCS**
    - Deposition peaks are in particular well reproduced for Ag, Cd and I
    - but iodine deposited fraction is a bit underestimated

Elements	Ag	Cd	In	Cs	I
Exp. measure	57%	31%	57%	55%	75%
ASTEC V2.1	54%	28%	53%	47%	48%







Ag, Cd and I deposited mass fraction in each volume of the silica tube

Validation of Direct Containment Heating models

- **ASTEC V2.0** (*RUPUICUV module*) application to **ANL-IET1RR** (ANL)
  - **Test conditions**: simulation of **HPME** (High Pressure Melt Ejection) using simulant material to represent core melt
    - ➔ Reasonable agreement on pressure build-up in cavity and containment

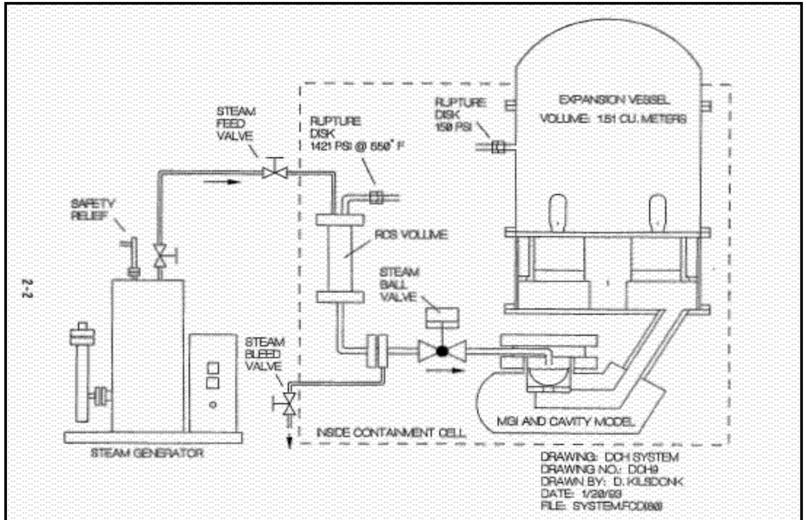
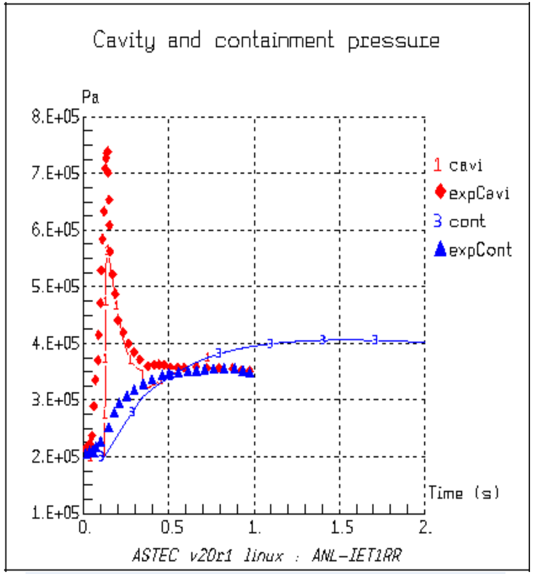


Figure 2.1 The Corium Ex-Vessel Interaction (COREXIT) Facility.

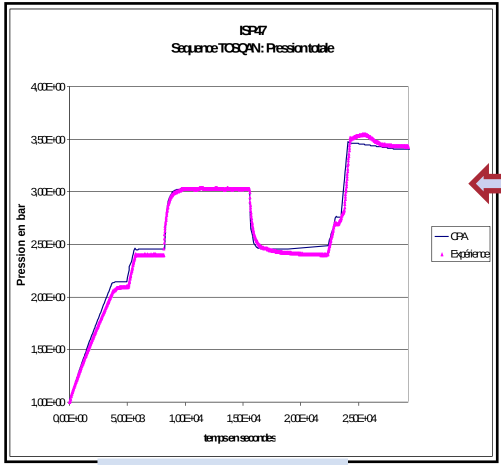


Comparison ASTEC/experiment on Cavity and Containment pressure

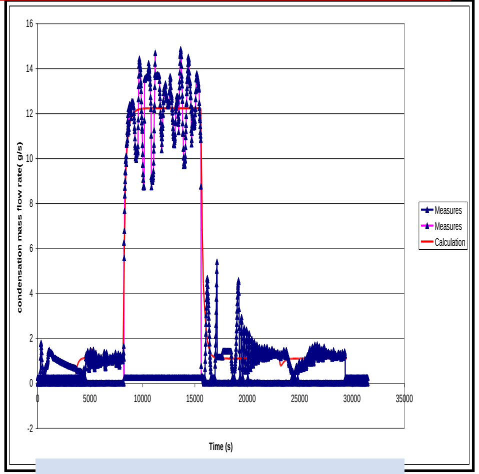
(**ASTEC** results are **in solid lines**)

Validation of Containment thermal-hydraulics models

- **ASTEC V2.0** (*CPA module*) assessment by *IRSN* through different scales



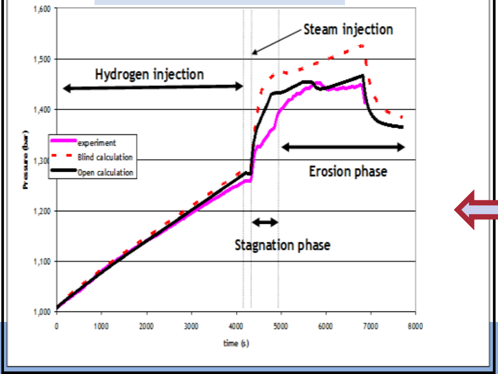
TOSQAN ISP47 (7 m^3 test facility)



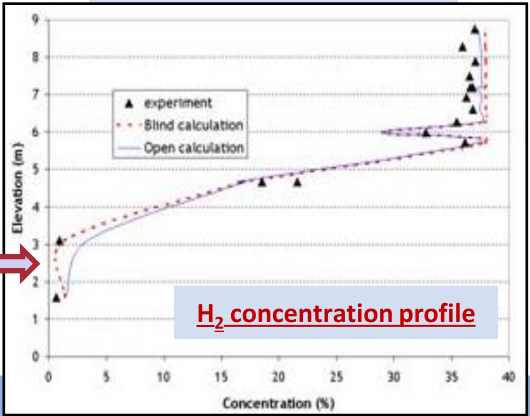
Condensation mass flow

Pressure evolution

ASTEC results in solid lines



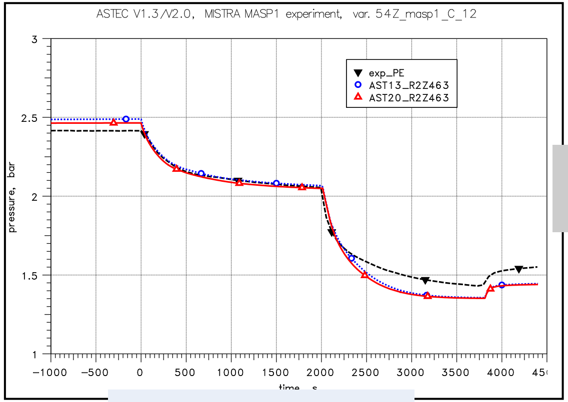
THAI-HM1 (60 m^3 test facility)



H_2 concentration profile

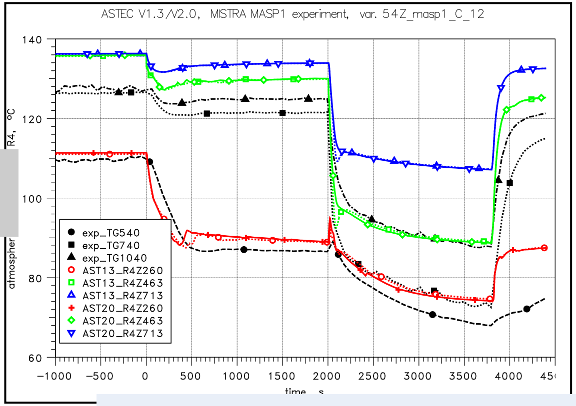
Validation of Containment thermal-hydraulics models

- **ASTEC V2.0** (*CPA module*) validation (*GRS work in SARNET*) on **MISTRA MASP1** (CEA large scale experiment ➔ *100m³ test facility*)
  - Main thermal-hydraulics effects of spray (pressure, atmosphere drops) are well matched by ASTEC-CPA
    - ➔ But temperature stratification is overestimated by ASTEC

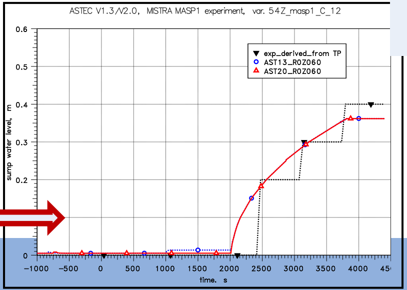


Containment Pressure

ASTEC results in solid lines



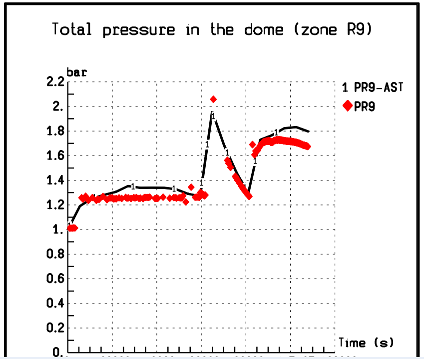
Atmosphere temperature in radius R4



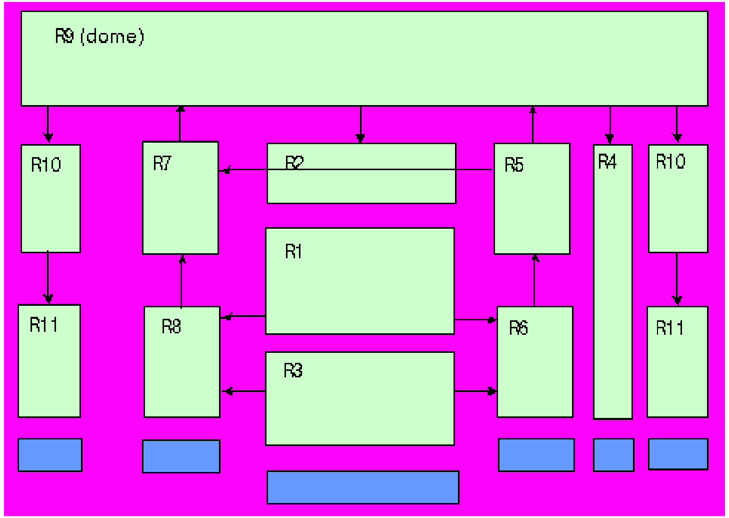
Sump water level evolution

Validation of Containment (Th.hyd/FP) models

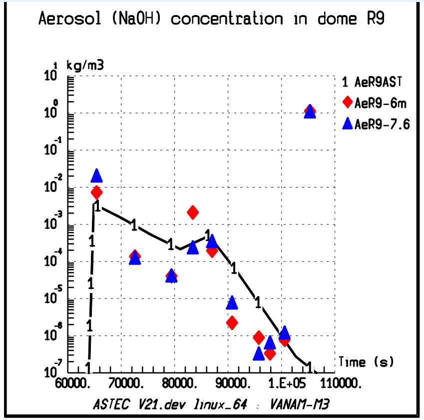
- **ASTEC V2.1** *(CPA/SOPHAEROS coupled modules)* validation by ***IRSN*** on **VANAM-M3** (Battelle) large scale experiment
- **Test conditions**: injection into a multi compartment volume of NaOH aerosols suspended in a steam-air mixture



Total pressure in room R9 (dome)
(**ASTEC** results **in black solid line**)



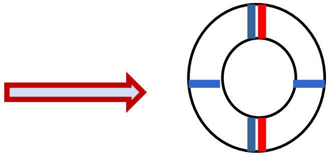
ASTEC nodalisation of the Battelle model containment

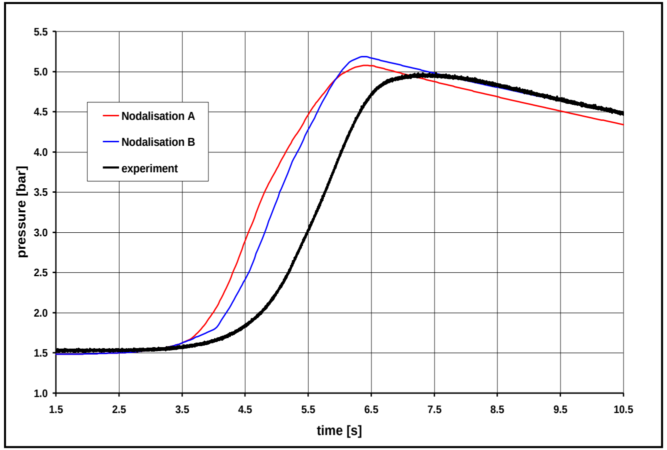


Aerosol (NaOH) concentration in room R9 (dome)

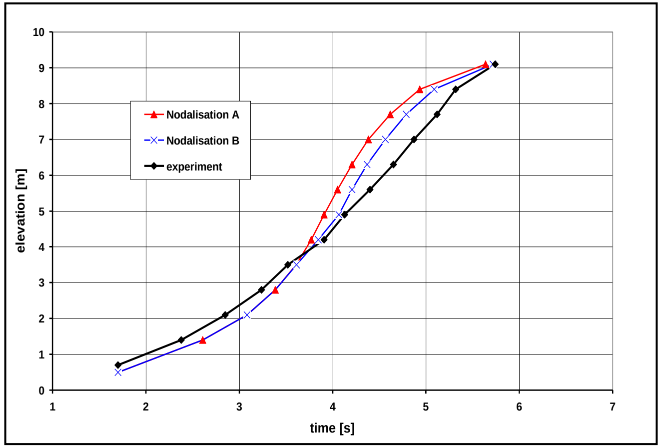
Validation of models for H_2 combustion in containment

- **ASTEC V2.0** (*CPA-FRONT model*) application on **ThAI-HD-12** (Becker Technologies)
  - ➔ *ISP-49 open post-test calculation performed by **RUB** in **SARNET***
    - Sensitivity study on the nodalization scheme :
      1. Nodalization **A** : 2 ring zones with an angle of 180°
      2. Nodalization **B** : 4 ring zones with an angle of 90°





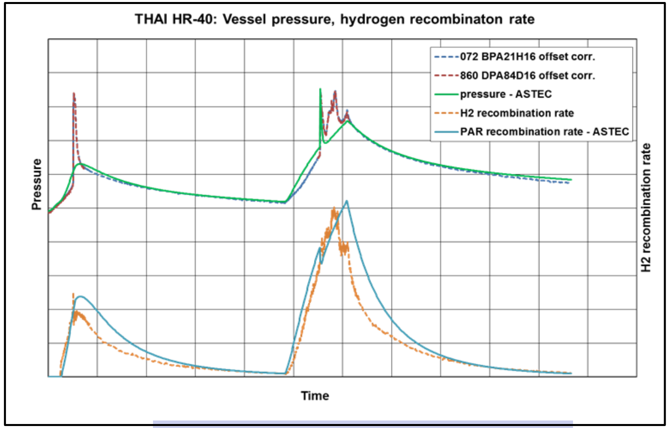
Pressure



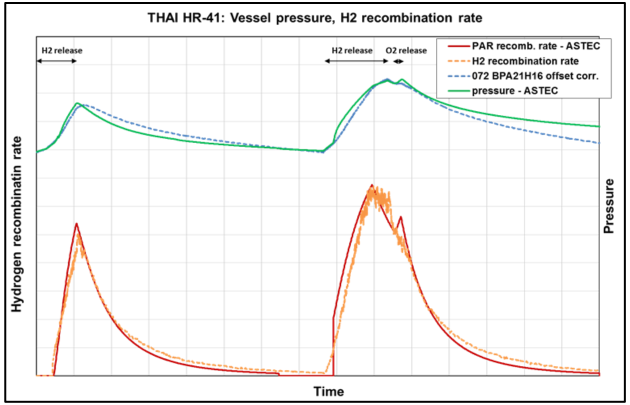
Flame front propagation

Validation of models for H_2 recombination in containm.

- **ASTEC V2.1** (*CPA-FRONT model*) validation (***NUBIKI*** *work in* ***CESAM***) on **OECD-NEA ThAI-2 HR** (Becker Technologies) experiments
  - **HR-40 test :**
    - First burning not calculated by ASTEC (calculated H_2 concentration was too low to trigger burning). So, the calculated recombination rate in the 1st phase is higher than measured because the inlet concentration is higher (owing to no 1st burning achieved).
    - Second burning was calculated with FRONT model. Peak pressure matches well the measured value.
  - **HR-41 test** : The calculated recombination rate agrees well with the measured value.



HR-40 test - (Pinit=1.5 bar **)**



HR-41 test - (Pinit=2 bar **)**

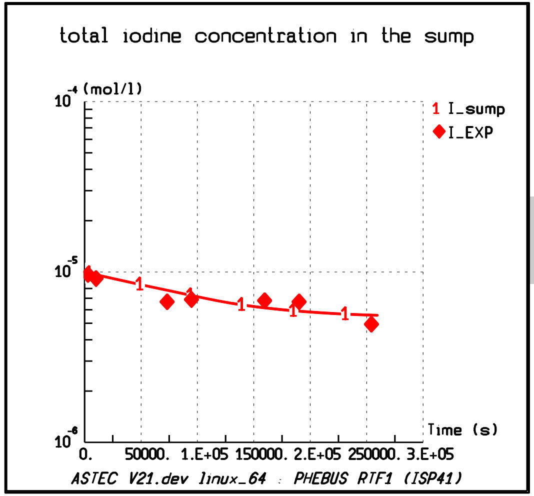
Vessel pressure and H2 recombination

(**ASTEC** results are **in solid lines**)

Validation of models for iodine behaviour in containment

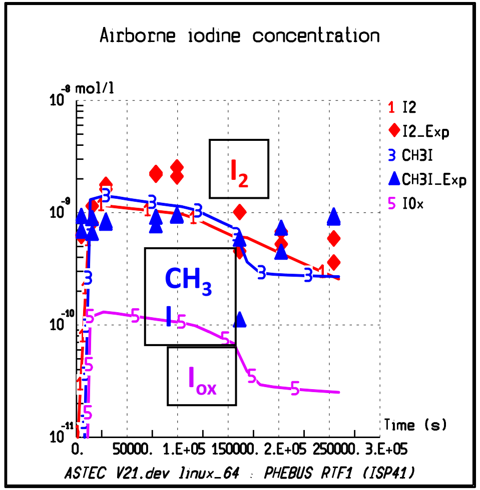
- **ASTEC V2.1** (*SOPHAEROS module*) validation by ***IRSN*** on **PHEBUS RTF3** experiment (AECL)
  - Volume 300 l with painted and steel surface
  - Semi integral test used to validate all the reactions under radiation (Co^{60} source)
  - **Test conditions**: Injection of I^- in presence of epoxy paints and on-line measurement of Iodine speciation in gas and liquid

➔ **Overall good agreement of iodine concentrations in sump and in atmosphere**



Concentration of total aqueous iodine

ASTEC results in solid lines

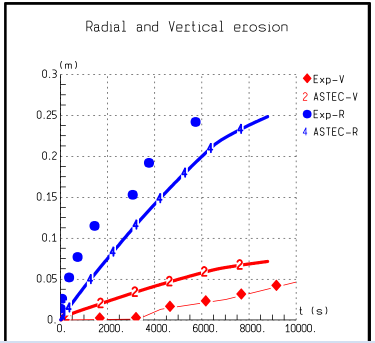


Concentration of iodine species in gaseous phase

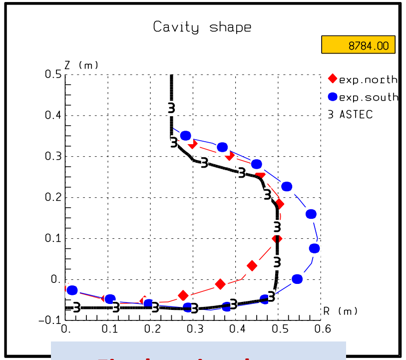
Validation of MCCI models

- **ASTEC V2.1** (*MEDICIS module*) validation by ***IRSN*** on **CCI** experiments (ANL)
  - Illustration of ASTEC results on MCCI **dry tests** for 2 different types of concrete
- ➔ Overall good enough agreement on ablation kinetics and final cavity shape

CCI-3 test with Siliceous concrete



Lateral and axial ablation kinetics

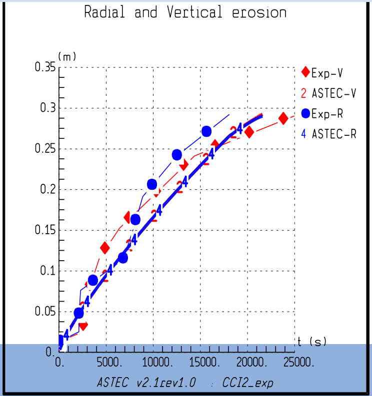


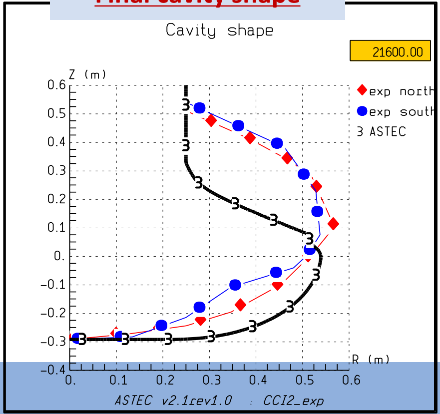
Final cavity shape

ASTEC results in solid lines

CCI-2 test with LCS concrete

(limestone / common sand)





Summary of the ASTEC V2.1 assessment (1/2)

Thermalhydraulics in circuits

- Good results on SETs and reasonable results on integral tests (including CESAR-to-CATHARE detailed benchmarks on SGTR scenarios)

Core degradation

- Good results for both early-phase models (heat-up, H_2 production, …) and late phase models (2D relocation, molten pool, corium in lower head, …)
- Promising results using the new "porous media" modelling in case of reflooding of a degraded core
  - *But still need to be further consolidated at different scales*

FP release

- Very good results for volatile and semi-volatile FPs and reasonable results (slight underestimation) for the low-volatile FPs

FP/aerosol transport in RCS

- Reasonable results on FP transport and chemistry
- But the importance of the gas chemistry kinetics with respect to the final Source Term has been underlined by **Phébus FP** post-test simulations (for instance, iodine partition at the break)

➔ *Further improvements are underway on the basis of **CHIP+** experimental data*

Summary of the ASTEC V2.1 assessment (2/2)

DCH

- Reasonable results could be often achieved, but current models are considered as still too parametric and too geometry-dependent
- Suitable new correlation to predict the corium dispersion in containment

Containment response

- Reasonable results on both thermal-hydraulics (including hydrogen combustion) and aerosols behaviour
- But need for model improvements on pool-scrubbing phenomena

Iodine and ruthenium chemistry

- Modelling at the State of the Art ➔ Global trends are well reproduced

MCCI

- Basic relevance of the set of models and assumptions
- Good enough results obtained under MCCI dry conditions
- Promising results obtained vs. CCI latest experiments using the new coolability models in case of corium top quenching during MCCI

➔ *But still need to be further consolidated under various transient conditions*