Development of an external routine using External Data Files for fusion modeling needs

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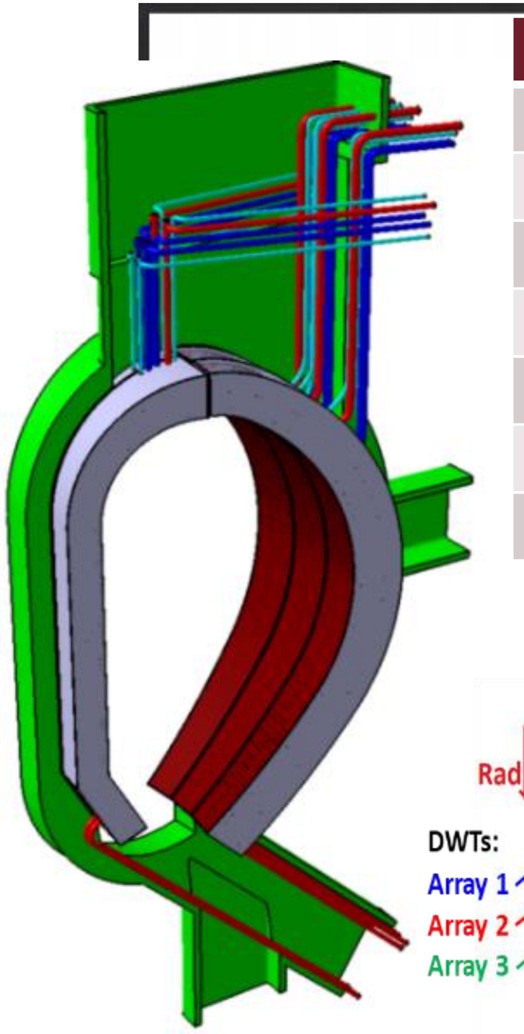
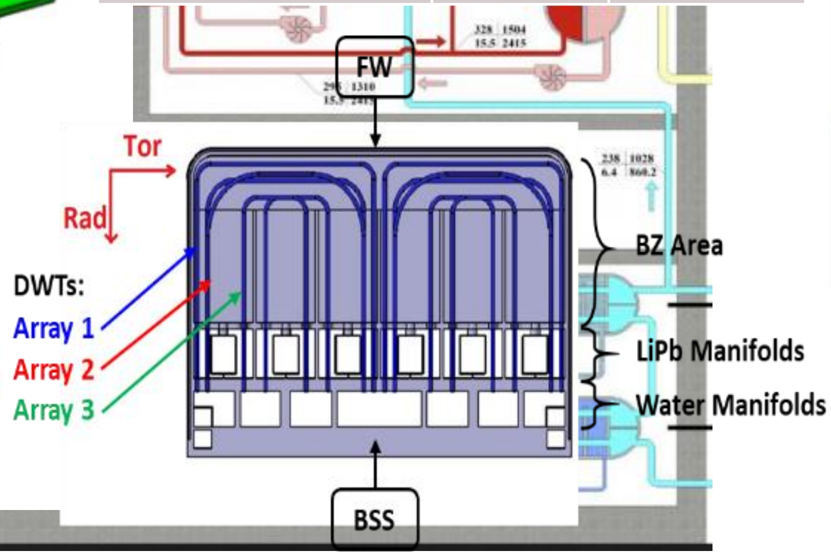
- MELCOR modeling of EU-DEMO reactor
- Fusion specific models present in MELCOR
- EU-DEMO Safety Analysis
- Python external model coupled with MELCOR
- Main Results

1. MELCOR modeling of EU-DEMO reactor

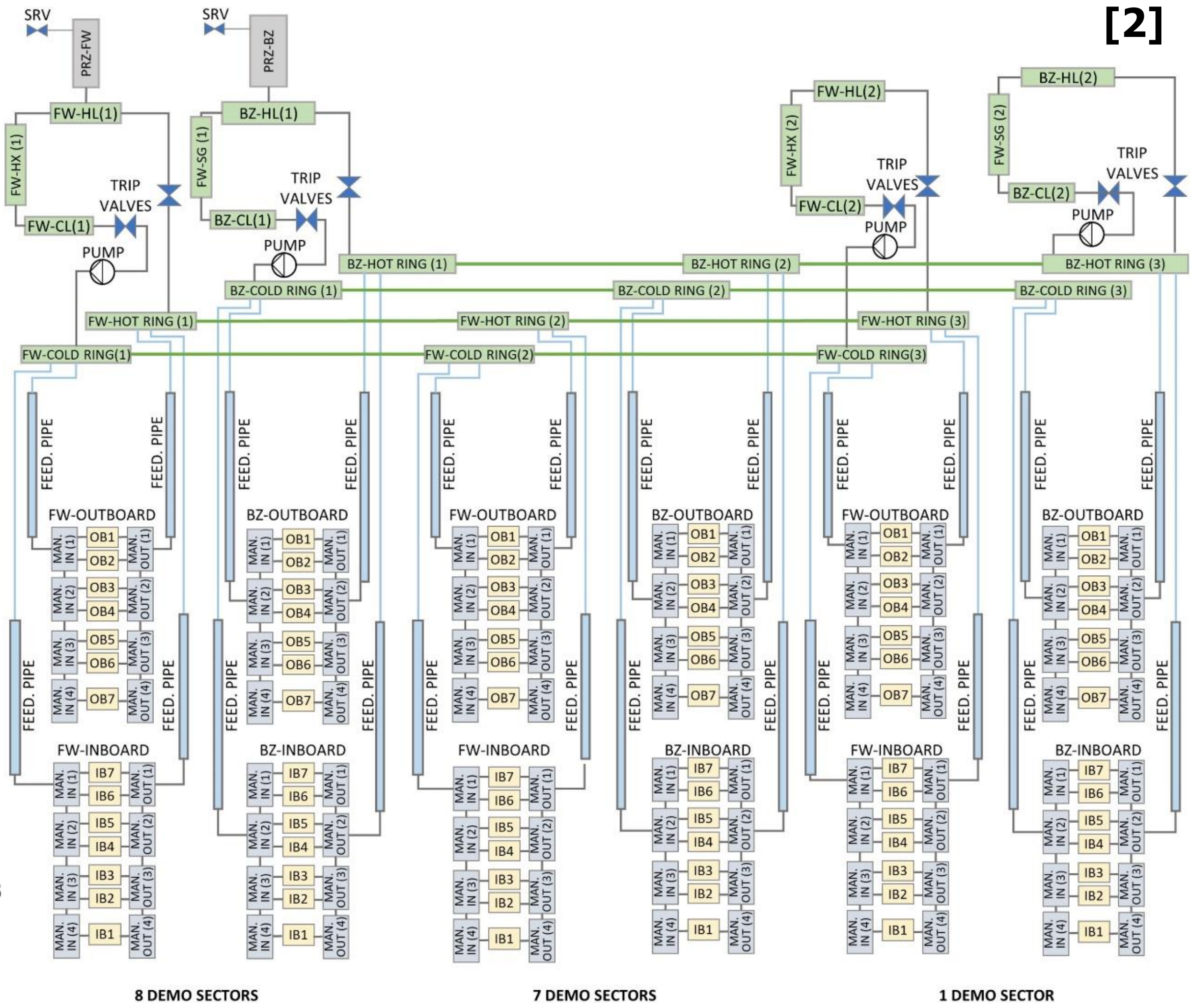
EU-DEMO Water Cooled Lithium Lead Breeding Blanket



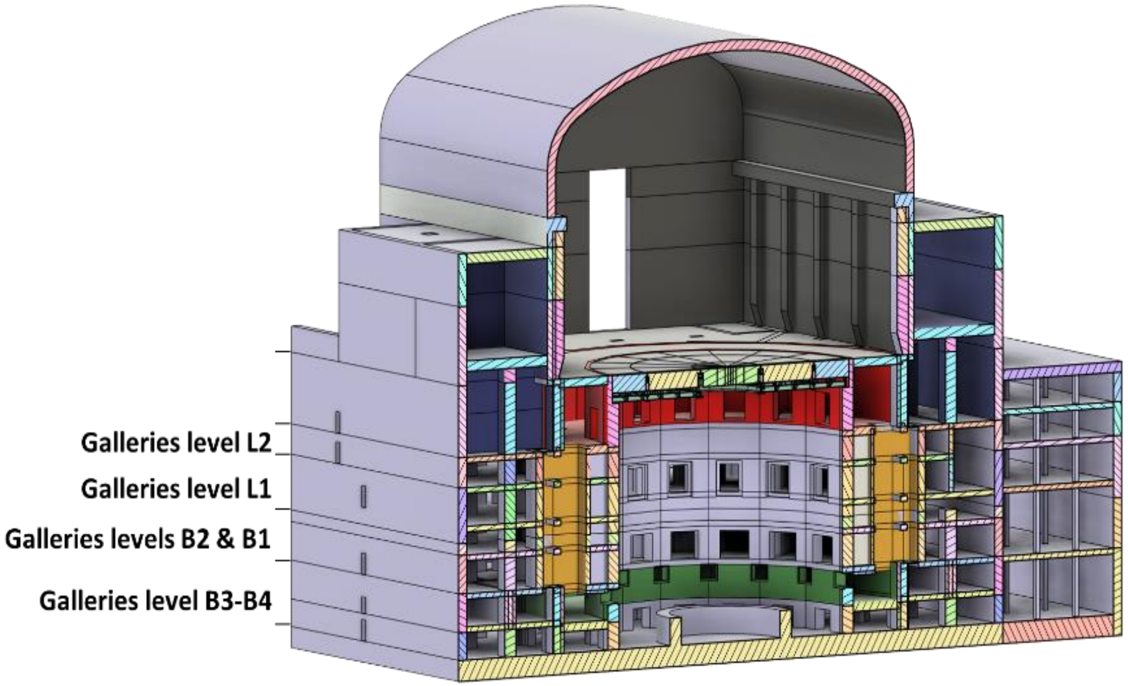
Parameter	Units	Value
Pressure	MPa	15.5
Temperature Range	° C	295-328
Av. Coolant Density	kg/m^3	701.3
FW-PHTS flow rate	kg/s	2273.6
BZ-PHTS	kg/s	7662.4
FW water inventory	m^3	179.2
BZ water inventory	m^3	501.5



[2]

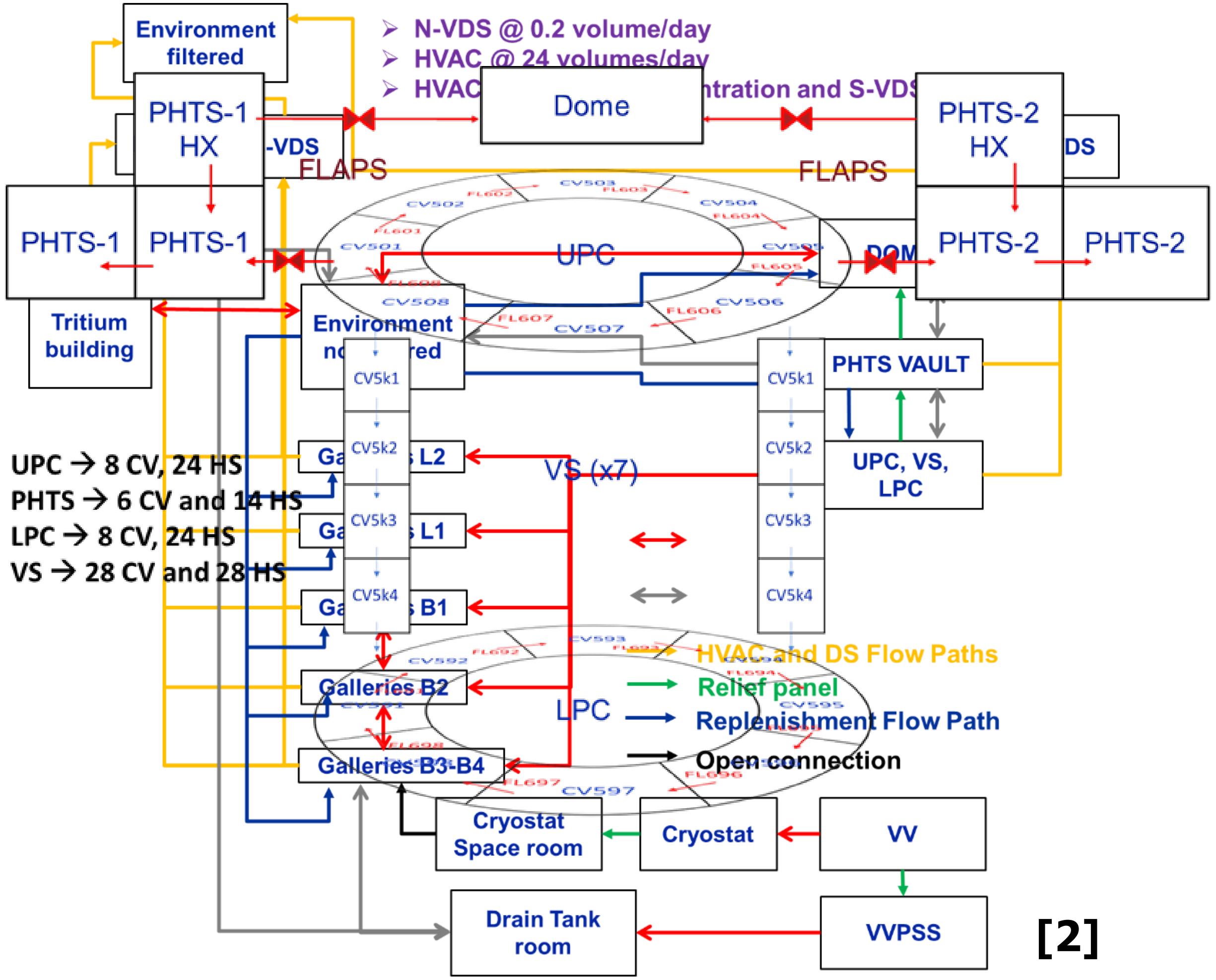


EU-DEMO Tokamak building



- N-VDS @ 0.2 volume/day
- HVAC @ 24 volumes/day
- HVAC ... ntration and S-VDS

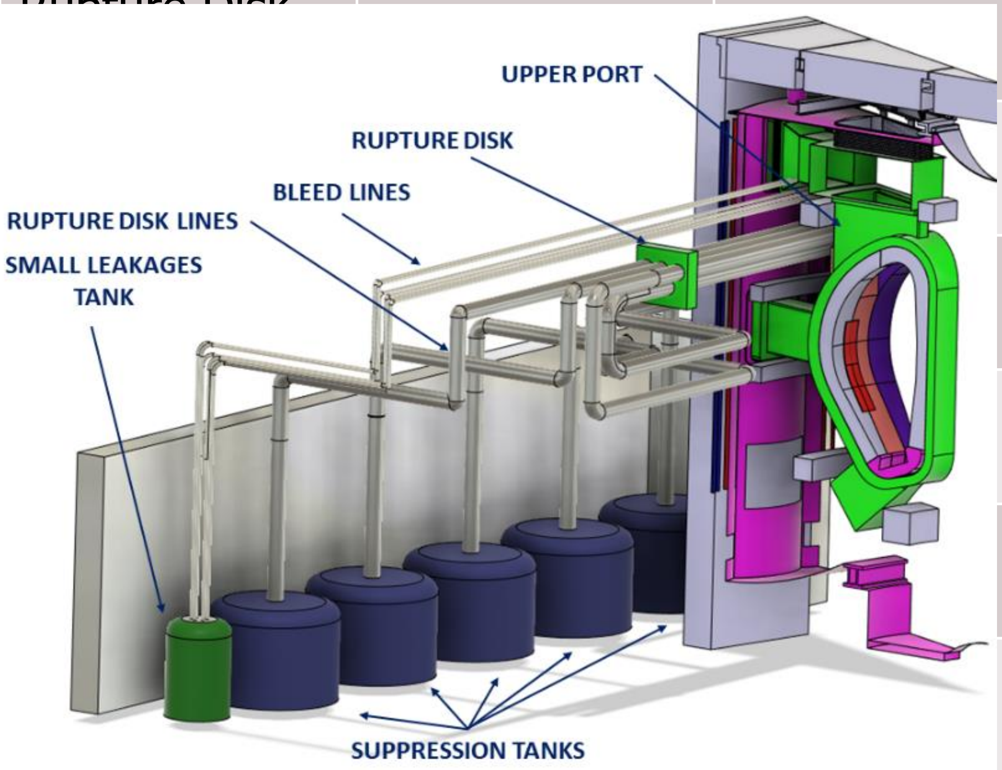
- UPC → 8 CV, 24 HS
- PHTS → 6 CV and 14 HS
- LPC → 8 CV, 24 HS
- VS → 28 CV and 28 HS

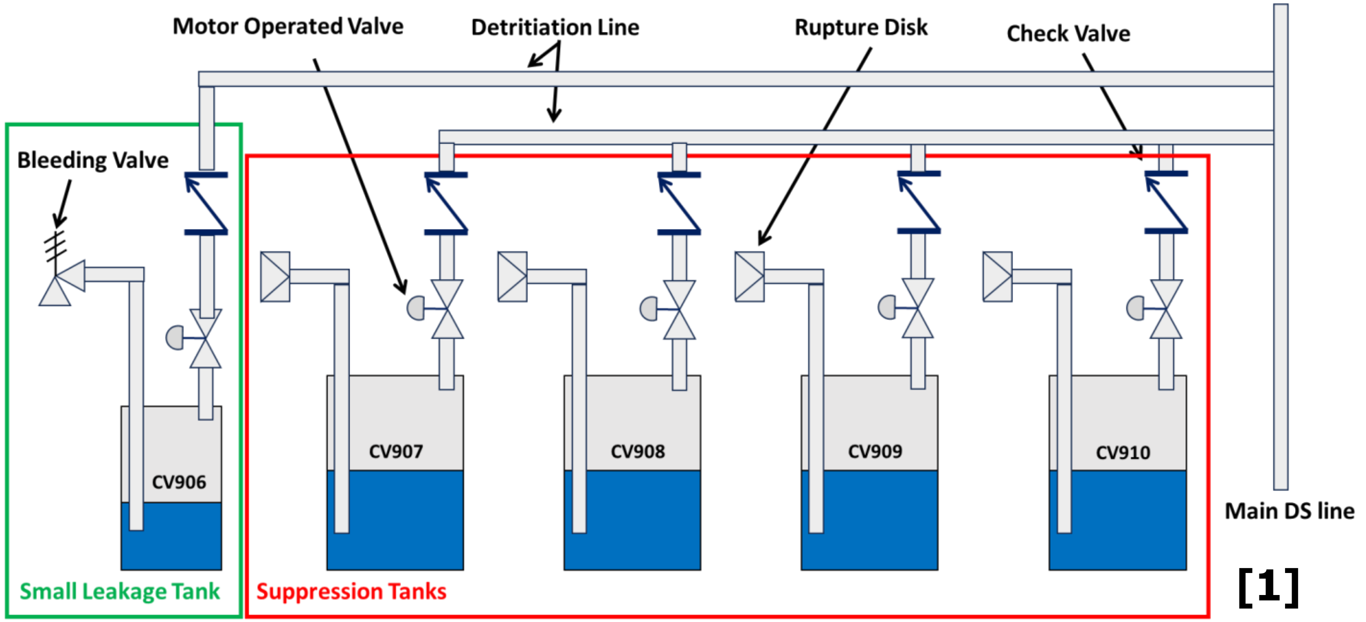


[2]

EU-DEMO Vacuum Vessel Pressure Suppression System

Parameter	Units	Value
Rupture Disk		





[1]

Source Term in Tokamak Reactor

- **Tritium**: b-emitter.
- **Materials activated** under nuclear loads (neutrons, g):
  - ❑ In structures (e.g., stainless steel: ^{56}Mn, ^{55}Fe, ^{52}V, ^{51}Cr, ^{60}Co, ^{57}Ni)
  - ❑ In gas (e.g., air activation is possibly occurring ^{41}Ar or Nitrogen reactions)
  - ❑ In liquids
    - Cooling water gets activated by means of the following reactions: $^{16}O\,(n,\,p)\,^{16}N$, $^{17}O\,(n,\,p)\,^{17}N$)
    - **Activated Corrosion Products**
  - ❑ **Dust** (i.e. Be, W, etc)

Parameter	Unit	Value	where
Tritium	kg	2.6	VV inventory across all components, including PFCs, dust, pumps, and atmosphere.
HTO	g	67.8	Water cooled system of the breeding blanket
Tungsten dust	kg	1034	deposited on VV surfaces
ACP	g	20	ACP mass present in the coolant, including ions and cruds

2. MELCOR 1.8.6 for fusion applications

What MELCOR has and what MELCOR is missing

Fusion Specific applications	MELCOR modifications	
Breeder technology based on WCLL blanket involves a multifluid system	FUN1 CF to model Heat conduction and radiation. Water cooled system as CVH and PbLi as HS coupled with FUN1	✓
Tritium	HTO transport is modeled but Tritium diffusion, permeation not yet included	…
Be, C, W materials in case of in-VV LOCA can be exposed to steam	Oxidation of PFC with steam for hydrogen generation if metal modeled as material of HS	✓
	Oxidation of Tungsten or Berillium dust of eroded PFC surfaces	✗

3. EU-DEMO Safety Analysis

- H-O explosion risk assessment

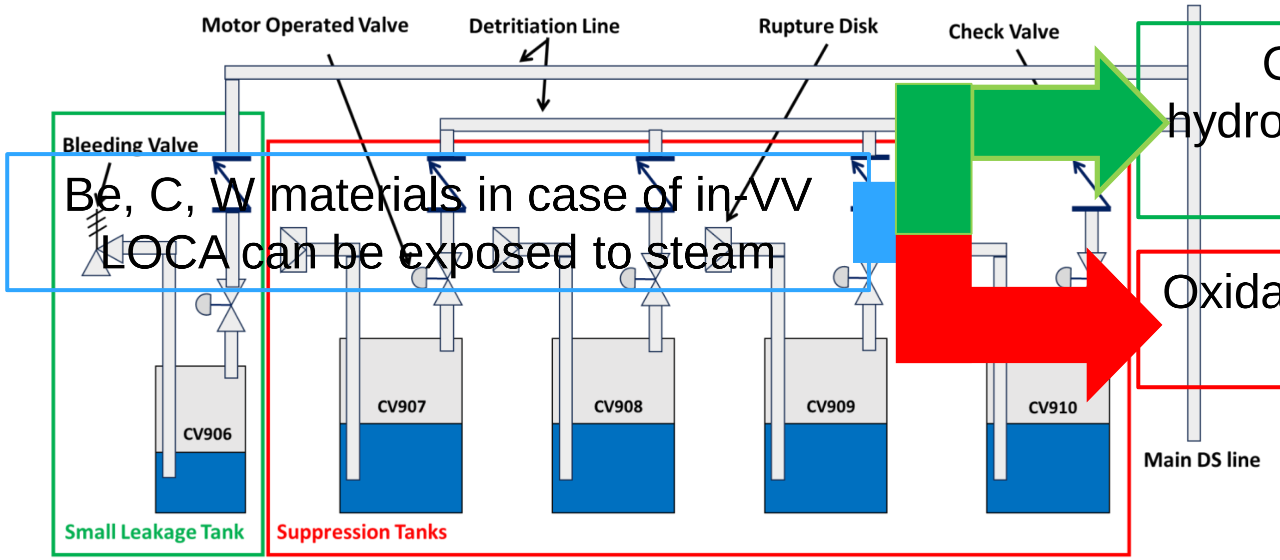
H-O explosion risk assessment

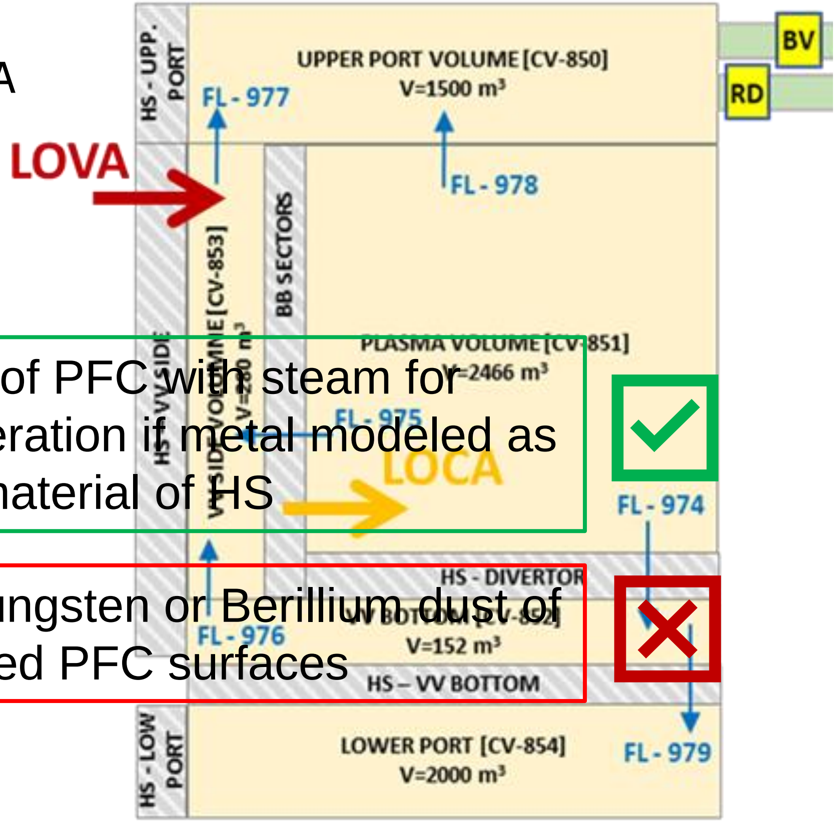
Context: combination of Loss Of Vacuum Accident and small in-vessel Loss Of Coolant Accident

Postulated Initiating Event: break of the Vacuum Vessel side with consequent pressurization of VV and mobilization of air

- ❑ Unmitigated plasma disruption
- ❑ Aggravating failure of OB-FW cooling channels with resulting in-vessel LOCA

Objective: H-O explosion risk assessment in VV, VVPSS and DS (<u>BUR active</u>)





Be, C, W materials in case of in-VV LOCA can be exposed to steam

Oxidation of PFC with steam for hydrogen generation if metal modeled as material of HS ✔

Oxidation of Tungsten or Berillium dust of eroded PFC surfaces ✘

MELCOR DLL user functions

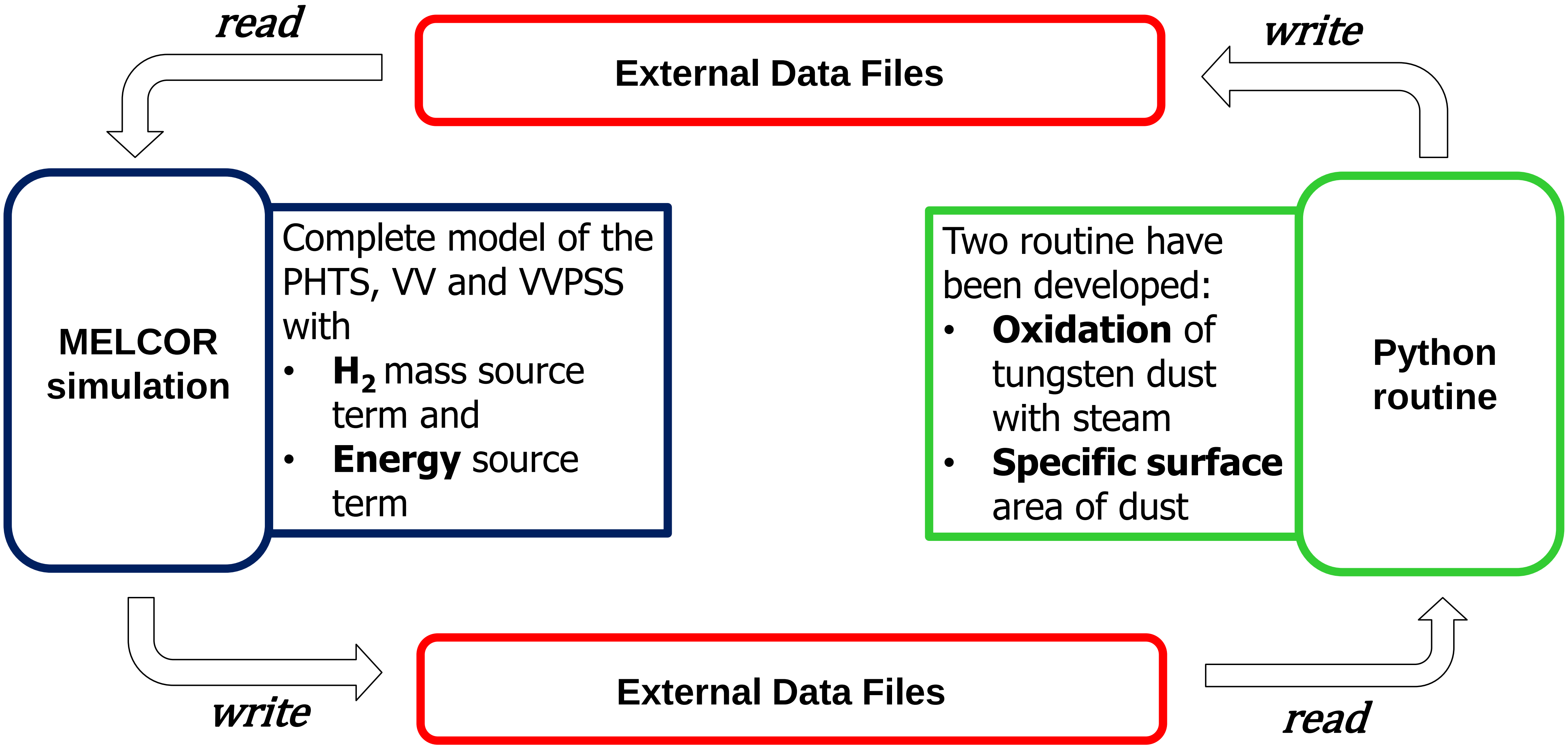
- Found some example of dll usage in the MELCOR **2.2.18019** installation folder under "tools"
- We are attempting to recompile a working MELCOR DLL (melcor_user_extension.so) using Visual Studio + Intel Fortran on Windows (Compiler ifort or ifx), but several issues are blocking the build:
  - Module structure compatibility is fragile, especially between TArgUDF_compatible_structure and TUDFArguments.
  - Common sources of errors:
    - USE ... ONLY: statements referencing non-existent or inaccessible symbols.
    - Variables passed to C_LOC() without the POINTER or TARGET attribute.
    - The Makefile is originally tailored for Linux builds, not for Windows.
    - Conflicting procedure names, e.g., multiple definitions of fun1, fun2, etc.
- How to proceed?
  - Try to debug this reporting to melcorbugs@sandia.gov
  - Wait for the new External MELCOR Plug-In interface?

Program Files (x86) › MELCOR-2.2.18019 › tools › dynamic_link ›   Cerca in dynamic_link

Nome	Ultima modifica	Tipo	Dimensione
Debug	15/02/2021 16:07	Cartella di file	
c_string_copying.f90	23/12/2020 15:49	Fortran Source	7 KB
CopySourceFiles.py	10/09/2020 16:56	Python File	2 KB
entry.f90	19/08/2020 15:06	Fortran Source	8 KB
funbox.f90	23/12/2020 15:49	Fortran Source	12 KB
m_af_argPassing_structures.f90	23/12/2020 15:49	Fortran Source	4 KB
m_Af_user_library_functions.f90	23/12/2020 15:49	Fortran Source	10 KB
m_analytical_function.f90	04/11/2020 18:39	Fortran Source	5 KB
M_ArgCF.f90	23/12/2020 15:49	Fortran Source	1 KB
m_getcstring.f90	23/12/2020 15:49	Fortran Source	1 KB
M_kind.f90	23/12/2020 15:49	Fortran Source	1 KB
m_shared_constant_definitions.f90	23/12/2020 15:49	Fortran Source	2 KB
Makefile	23/12/2020 15:51	File	4 KB
melcor_user_extension.sln	19/08/2020 15:06	Visual Studio Solut...	1 KB
melcor_user_extension.so	19/08/2020 15:06	File SO	647 KB
melcor_user_extension.vfproj	23/12/2020 15:49	Intel Fortran Proje...	4 KB
PrepareForDistribution.py	19/08/2020 15:06	Python File	2 KB
ptr_addressing.f90	23/12/2020 15:49	Fortran Source	2 KB
raw_copying.f90	23/12/2020 15:49	Fortran Source	6 KB
uccf_externals.f90	23/12/2020 15:49	Fortran Source	1 KB
UserCodedCF.f90	23/12/2020 15:49	Fortran Source	8 KB

4. Python external model coupled with MELCOR

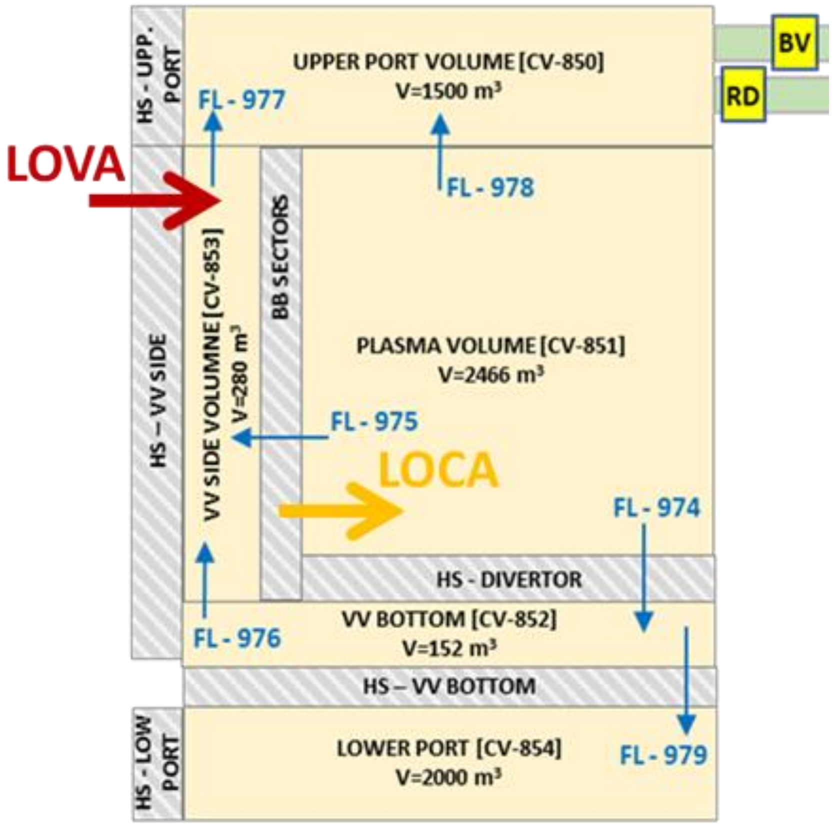
MELCOR simulation coupled with an external Python script



[3][4]

MELCOR side of coupling

Combination of type WRITE and READ EDF files




```
CV85100     'PlasmaVolume'    2  0  3
CV85101     0           0
CV85103     87.0
CV851A0     2
CV851A1     PVOL       100.0
CV851A3     TATM       700.0
CV851A4     PH2O       0.0
CV851A5     MFRC.4     1.0
CV851B0     -11.0996    0.0
CV851B1     -9.32      233.92260
CV851B2     -7.840     544.1425511
CV851B3     -6.361     909.2798113
CV851B4     -4.881     1299.150823
CV851B5     -3.402     1684.829674
CV851B6     -1.923     2047.870852
CV851B7     -0.443     2340.902935
CV851B8     0.6435     2466.0
CV851C0     MASS.5      RATE  CF.8888
CV851C1     ENERGY.A    RATE  EDF.6.2
```

Partial pressure of steam inside the plasma volume

Mass of H_2 produced due to oxidation of tungsten dust used for oxidation

- H_2 as a mass source term for Plasma Volume

Heat generated due to tungsten dust oxidation

- Heat generated from oxidation as energy source

Temperature transient of tungsten dust particles

Tungsten mass reacted

Python External Model for Tungsten Dust Oxidation

Chemical subroutine

$$W + 3H_2O \rightarrow WO_3 + 3H_2 + 156\ [kJ/mol_W]$$

$$RR_w = \left(\frac{P_{H_2O}}{P_o}\right)^{0.78} \times 41.238 \times e^{-\frac{33106.0}{R*T_W}}$$

[5]

RR_w: Reaction rate of Tungsten (kgW/m^2*s)
P_{H_2O}: Partial pressure of steam (Pa)
T_W: Tungsten Temperature (K)
P_0: Standard steam pressure 8.5 × 10^4 (Pa)

Surface Area subroutine

$$f(d_p) = \frac{1}{d_p\sqrt{2\pi}\ ln\sigma_g} \exp\left[\frac{-(lnd_p - lnCMD)^2}{2(ln\sigma_g)^2}\right]$$

$$A_s = \frac{6d_{\bar{s}}^2}{\rho d_{\bar{m}}^3} \qquad d_{\bar{s}} = \sqrt{\frac{A_{tot}}{N\pi}} \qquad d_{\bar{m}} = \left(\frac{6m}{N\rho\pi}\right)^{1/3}$$

[6]

d_p: particle diameter
CMD: Count Mean Diameter (m)
σ_g: Geometric Standard Deviation
A_s: Specific Area of dust (kg/m^2)
$d_{\bar{s}}$:diameter of average mass
$d_{\bar{m}}$diameter of average surface area
***m**:* Total mass of tungsten dust

Input Parameters	
CMD [2]	**0.5 x 10^{-6}**
σ_g [2]	**2.0**
m [3]	**1034.0**

[7] [8]

4. Main Results

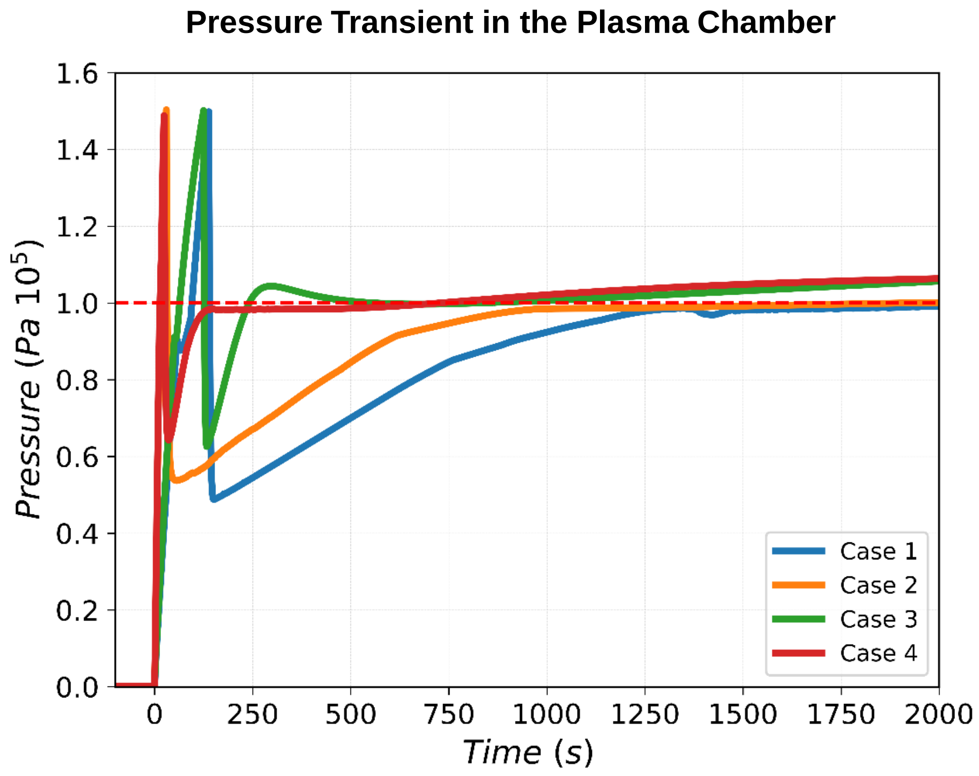
Simulations performed

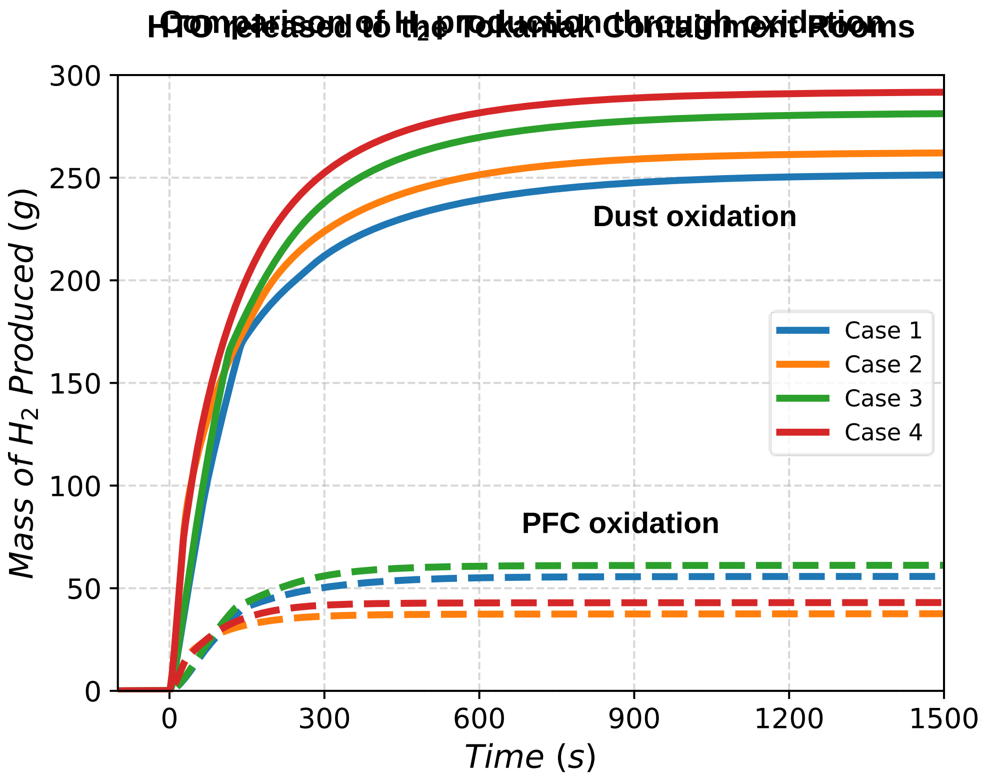
Parametric study based on the size of the LOVA and LOCA to investigate the **worst combination in terms of H_2 explosion risk**.

Scenario ID	LOVA area [m²]	LOCA area [m²]	Notes
Case 1	2.0 E-3	9.8 E-4	(10 FW channels)
Case 2	2.0 E-3	9.8 E-3	(100 FW channels)
Case 3	2.0 E-2	9.8 E-3	(10 FW channels)
Case 4	2.0 E-2	9.8 E-4	(100 FW channels)

First Results show **deflagration** inside VVPSS tanks and inside N-DS lines

Main Results

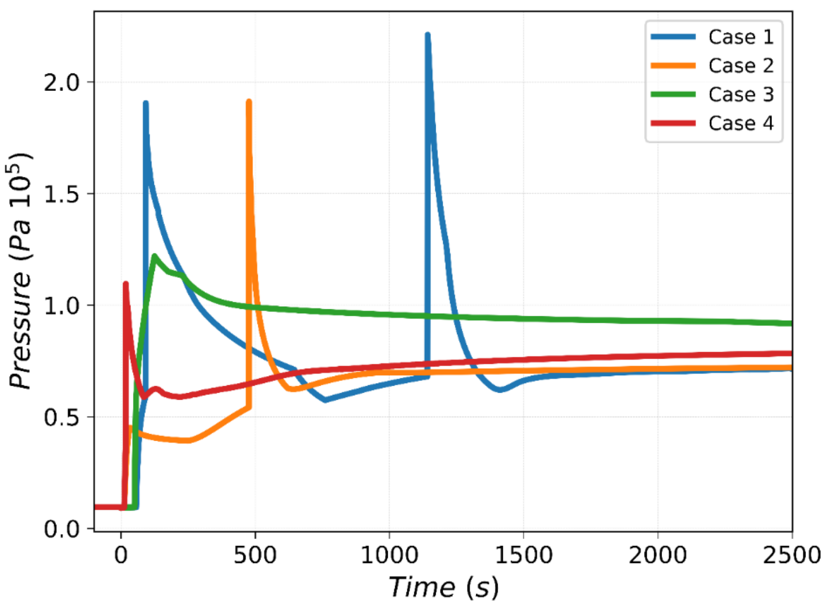




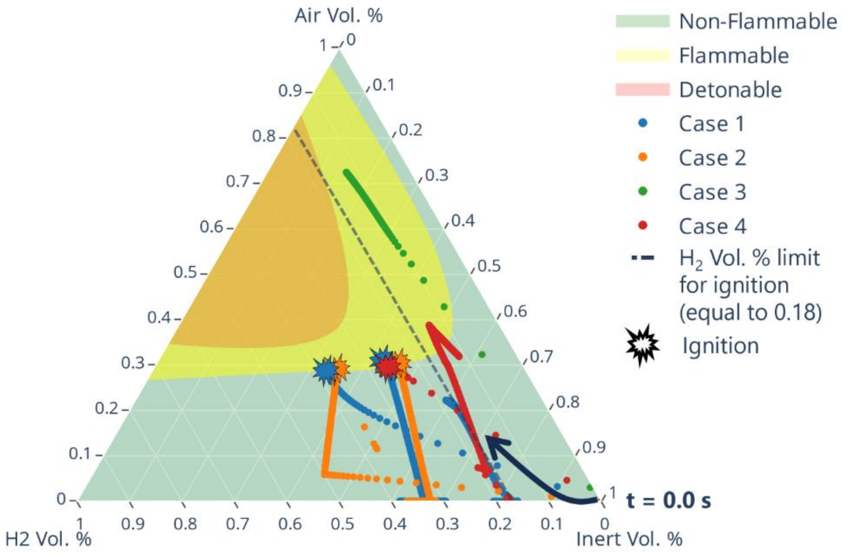
- Pressure transient in the Plasma chamber is safely mitigated due to intervention of VVPSS
- HTO releases outside of the primary confinement barrier due to LOVA breach. Main releases of HTO are to the VVPSS reaching 40% of the initial inventory

Main Results

Pressure Transient in the small leakage tank



Shapiro Diagram for the small leakage tank



Scenario ID	Pressure peak in 10^5 Pa of	
	SL tank	E-DS
Case 1	2.21	1.92
Case 2	1.91	2.62
Case 3	1.22	1.12
Case 4	1.09	0.99

- Deflagration occurs in the small leakage tanks of the VVPSS and flame propagation reaches the E-DS. Ignition of mixtures might damage the connection to the tank with consequent release of HTO condensed in the pool
- Results show that combustion model of MELCOR has some drawbacks. Ignition is highly conservative and in case 1 a highly unrealistic burn is simulated

Conclusion and next steps

Conclusion and Next Steps...

Conclusions:

- Main process of hydrogen production comes from tungsten dust due to the high specific surface (**189 m^2/kg**)
- **Hydrogen in vessel inventory is one order of magnitude higher than the hydrogen produced in vessel**
- For the baseline model of the VVPSS a concurrent **LOVA and LOCA generates explosive mixtures in the SL tank**
- Releases of HTO to Vertical Shaft are in the order of **0.15-0.25 %i.i.** Most of **HTO (~40 %i.i.)** is released towards the **VVPSS**
- Hydrogen Mitigation strategies have been studied and involve the use of **PAR**. Results show that **deflagration of H-O mixtures can be avoided**

Limitation

- MELCOR BUR model approximates ignition

References

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[2] D'Onorio M., Glingler T., Porfiri M.T., Dongiovanni D.N., Ciattaglia S., Gliss C., Elbez-Uzan J., Cortes P., Caruso G., **Development of a Thermal-Hydraulic Model for the EU-DEMO Tokamak Building and LOCA Simulation**. Energies 2023, 16, 1149. https://doi.org/10.3390/en16031149.

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Thanks for the attention!

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