# Enhance MELCOR safety analysis by adopting RAVEN as a multi-purpose framework for UQ, data analysis, model optimization, and DET analysis.

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SAPIENZA
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# Outline

- RAVEN tool
- MELCOR coupling with RAVEN
- UQ application: SFP in the MUSA project
- Design optimization: Hydrogen recombination system
- Conclusions & Future Developments

# RAVEN TOOL

- RAVEN (Risk Analysis Virtual Environment) development has begun in early 2012.
- RAVEN is open-source and can be downloaded from GITHUB:
  - https://github.com/idaholab/raven
- The overall goal was to conceive a tool to enable Risk Informed Safety Margin Characterization (RISMC)
  - Evaluating risk (uncertainty propagation)
  - Understanding risk (limit surface, ranking, sensitivity, data mining)
  - Mitigating risk (optimization)
- Multiple operative systems are supported (Windows, Linux and Mac)
- RAVEN development is performed under a strict Software Quality Assurance process:
  - NQ1 – Lvl. 2
  - User manuals and guides, theory manuals, tests documentation
  - Multiple level of peer-review process
  - Automatic verification (testing) (~650 regression tests)

RAVEN

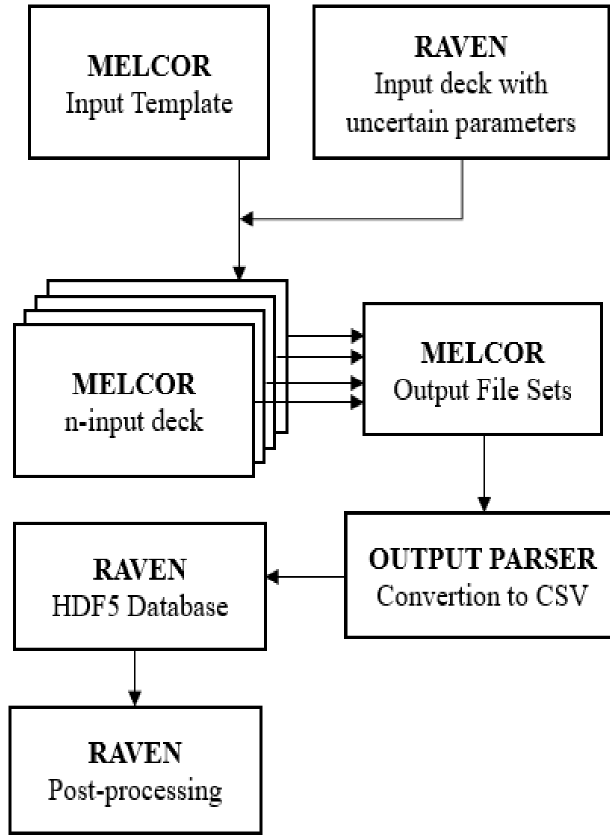
# MELCOR-RAVEN COUPLING FOR UQ

- The coupling has been realized through a `Python` Interface integrated into the source code
- The Interface is capable to:
  1. Generate a run command for MELGEN and MELCOR executable
  2. Convert binary plot file of MELCOR 2.2

Python module used: struct.

- This module performs conversions between Python values and C structs represented as Python strings. This can be used in handling binary data stored in files.

```
In [222]: unpack('I', b'lB\x02\x00')[0]
Out[222]: 148076
In [224]: str(unpack('4s', b'TITL')[0], 'utf-8')
Out[224]: 'TITL'
```




Initial Sampling of:
•Physical parameters
•Initial Conditions
•Transition Conditions, i.e., time of a transition event

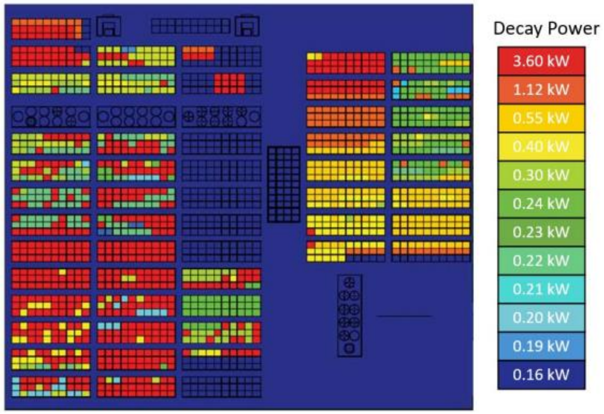
Runs the system simulator using the values previously sampled and eventually applying a random noise to some parameters

Converts each .PTF. To overcome the handling of large datafiles the interface allows to create a file with only variables required by the users. So is possible to obtain an HDF5 database which comprises variables from all MELCOR packages (CVH, FL, COR, RN etc.)

# MELCOR-RAVEN COUPLING

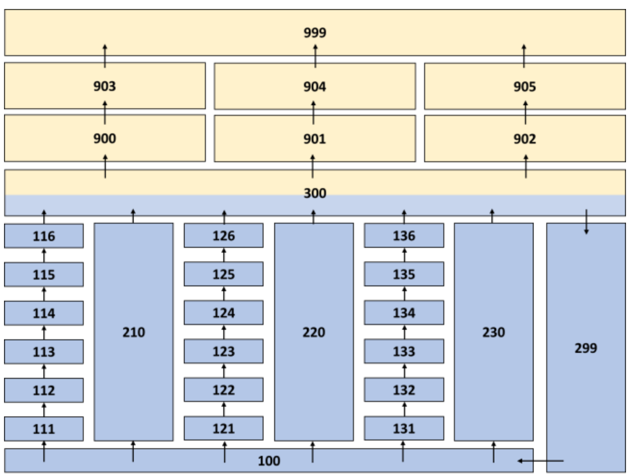
- Open Source: https://github.com/idaholab/raven/pull/1997
- Direct access to all PTF variables
- Not needed to use an EDF
- Possibility to change output variables also at the end of an UQA
- Optimization problems
- Dynamic Event Tree Analysis
- No GUI
- Need to create a RAVEN input deck

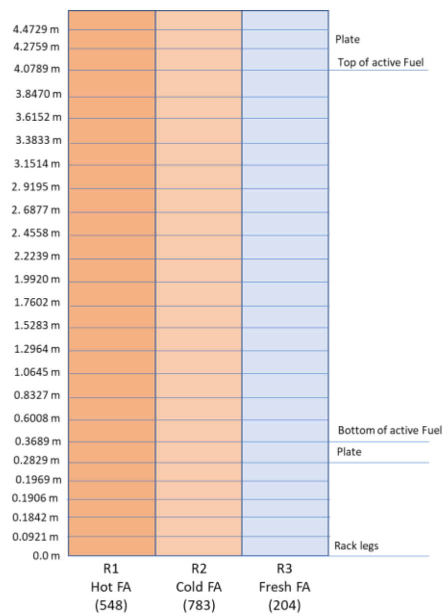
# Uncertainty quantification and sensitivity analysis
# SFP: BASE CASE




- 1535 fuel assemblies. Hot (548 FAs), cold (783 FAs), fresh (204 FAs)
- 33 Control Volumes and 58 flow paths
- 3 radial rings and 26 axial levels

- The total power of Hot FAs is 1.9MW and Cold FAs is 0.5MW according to specification
- A total number of 30 RN classes have been simulated




- Reactor type: SFP-BWR
- Using CN components we experienced code failures as soon as water level reaches the top of the FA.

```
Routine              Line      Source
cor_corvf_           1202      corvf_NSI.f90
cor_corrad_           624      corrad_NSI.f90
cor_corrnl_           802      corrnl_NSI.f90
cor_cordbd_           232      cordbd_NSI.f90
runstep_IP_physic     232      RunStep.f90
runstep_              103      RunStep.f90
m_melcorprog_mp_m     237      m_MelcorProg.f90
MAIN__                 19      Melcor_NSI.f90
Unknown           Unknown      Unknown
Unknown           Unknown      Unknown
```

- Using CB the error is bypassed

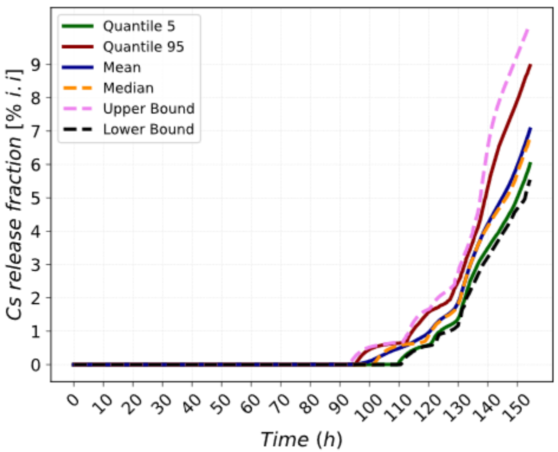
# Uncertainty quantification and sensitivity analysis: SFP

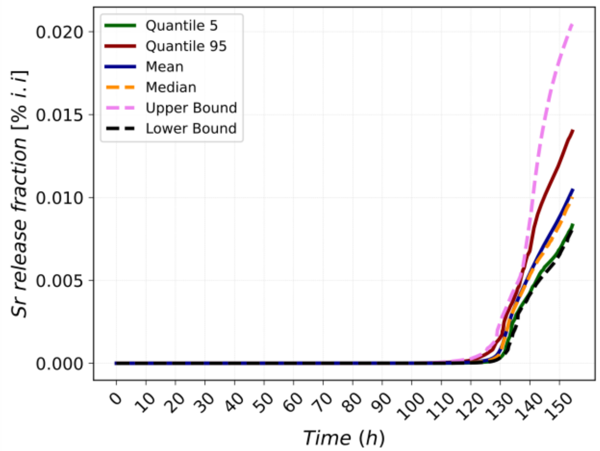
| Name | Short description | Reference value | Range of Variation | PDF Type |
|---|---|---|---|---|
| **SC1214** | Heat transfer to gas/steam mixture by Turbulent Forced Convective Flow in Tubes | | LB: 0.0184<br>UB: 0.0276 | Uniform |
| **SC1001(1,1)** | Metallic Cladding Oxidation Rate Constant Coefficient | | LB: 23.68<br>UB: 35.52 | Uniform |
| **SC1001(1,2)** | Metallic Cladding Oxidation Rate Constant Coefficient | | LB: 21.36<br>UB: 32.04 | Uniform |
| **SC1001(3,1)** | Metallic Cladding Oxidation Rate Constant Coefficient | | LB: 70.32<br>UB:105.48 | Uniform |
| **SC1001(3,2)** | Metallic Cladding Oxidation Rate Constant Coefficient | | LB: 21.36<br>UB: 32.04 | Uniform |
| **SC1001(5,1)** | Upper temperature boundary for low temperature range (H2O oxidation) | 1850.16 [K] | $\mu$ =1850.16<br>$\sigma$ =25. | Normal |
| **SC1001(6,1)** | Lower temperature boundary for high temperature range (H2O oxidation) | 1870.16 [K] | $\mu$ =1870.16<br>$\sigma$ =25. | Normal |
| **SC1004(1)** | Minimum oxidation temperature | 1260.66 [K] | $\mu$ =1260.66<br>$\sigma$ = 87.5 | Normal |
| **SC1131(2)** | Cladding collapse, Maximum ZrO2 temperature permitted to hold up molten Zr in CL | | LB: 2300.<br>UB: 2500. | Uniform |
| **SC1132(1)** | Temperature to which oxidized fuel rods can stand in the absence of unoxidized Zr in the cladding | | LB: 2250.<br>UB: 2750. | Uniform |
| **tssfai** | Supporting structure failure temperature | 1673.15 [K] | LB: 1473.<br>UB: 1789 | Triangular |
| **tnsmax** | Non-Supporting Structure failure temperature | 1520.0 [K] | LB: 1473.<br>UB: 1789. | Triangular |
| **GAP00_CLFAIL** | Gap release temperature | | LB: 1073.<br>UB: 1273. | Uniform |
| **chi** | Aerosol dynamic shape factor | | LB: 1.0<br>UB: 2.0 | Uniform |
| **dmax** | Particle diameter, Upper bound | | LB: 5.0E-6<br>UB: 2.5E-5 | Uniform |
| **rhonom** | Aerosol density | | LB: 1000.<br>UB: 4120. | Uniform |
| **fslip** | Slip factor | | LB: 1.01<br>UB: 1.51 | Uniform |
| **stick** | Sticking coefficient | | LB: 0.5<br>UB: 1.0 | Uniform |
| **ftherm** | Thermal accomodation coefficient | | LB: 1.80<br>UB: 2.70 | Uniform |
| **turbds** | Turbulent dissipation | | LB: 0.001<br>UB: 0.03 | Uniform |
| **tkgop** | Gas thermal conductivity / Particle thermal conductivity | | LB: 0.05<br>UB: 1.0 | Uniform |
| **deldif** | Diffusion boundary layer thickness | | LB: 1.0E-5<br>UB: 8.0E-3 | Uniform |
| **FCNCL** | Radiative exchange factor for radiation from the canister wall to the fuel rod cladding. | | LB: 0.1<br>UB: 0.2 | Uniform |
| **FSSCN** | Radiative exchange factor for radiation | | LB: 0.1 | Uniform |

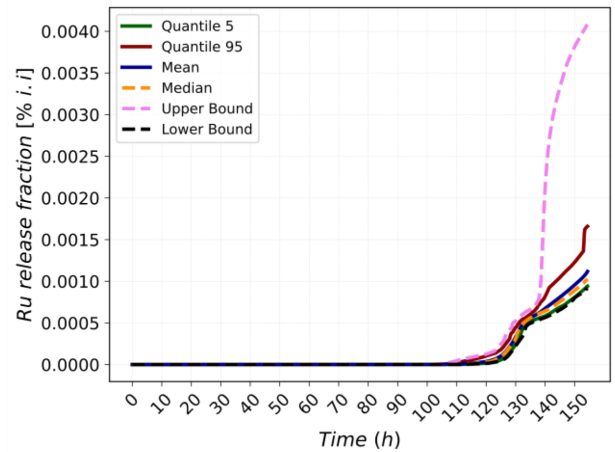
| Name | Short description | Reference value | Range of Variation | PDF Type |
|---|---|---|---|---|
| **FSSCN** | Radiative exchange factor for radiation from NS to the adjacent canister walls or to fuel rods and debris if canister is not present. | | LB: 0.1<br>UB: 1.0 | Uniform |
| **FCELR** | Radiative exchange factor for radiation radially outward from the cell boundary to the next adjacent cell. | | LB: 0.1<br>UB: 1.0 | Uniform |
| **FCELA** | Radiative exchange factor for radiation axially upward from the cell boundary to the next adjacent cell. | | LB: 0.1<br>UB: 1.0 | Uniform |
| **FLPUP** | Radiative exchange factor for radiation from the liquid pool to the core components. | | LB: 0.1<br>UB: 1.0 | Uniform |
| **cl_to_comp** | Radiative exchange factor for radiation from clad of a ring to other components ring | | LB: 0.1<br>UB: 0.3 | Uniform |
| **rk_to_hs** | Radiative exchange factor for radiation from rack of a ring to surrounding HS | | LB: 0.5<br>UB: 1.0 | Uniform |

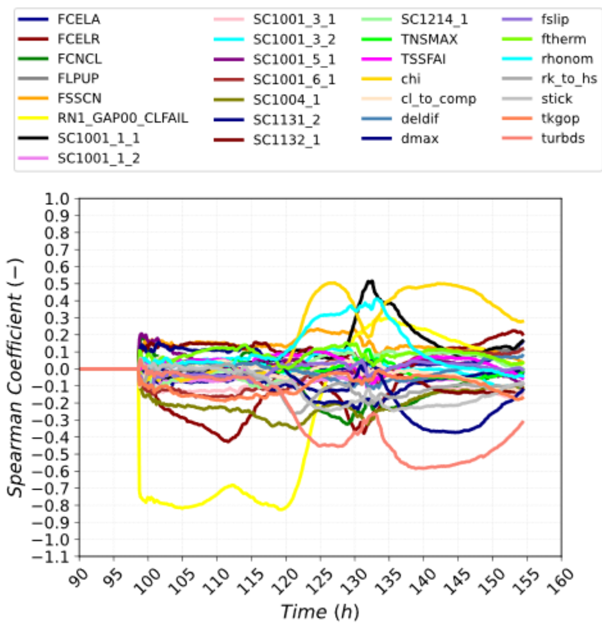
| | |
|---|---|
| **Uncertainty Methodology used** | Probabilistic method to propagate input uncertainty and model uncertainty |
| **Minimum number of Runs** | 93 - Wilks confidence formula (two-sided) |
| **Performed Runs** | 121 |
| **Sampling methods** | Random Monte Carlo |
| **Requested probability content (β)** | 0.95 |
| **Confidence level (γ)** | 0.95 |
| **Input uncertain parameters** | 29 parameters |
| **Uncertainty analyses of the FOMs** | Min value, max value, mean, median, quantile 5, quantile 95, standard deviation, coefficient of variation, Variance, Skewness, Kurtosis, cumulative distribution function -CDF |
| **Sensitivity analyses used to characterize the relation between the input uncertainty parameters and the FOMs** | Spearman and Pearson correlation coefficients for both simple correlation and partial correlation, linear regression parameters, and scatter plots of FOMs vs. uncertain parameters (at the end of the simulation and for Pearson higher than 0.5). |

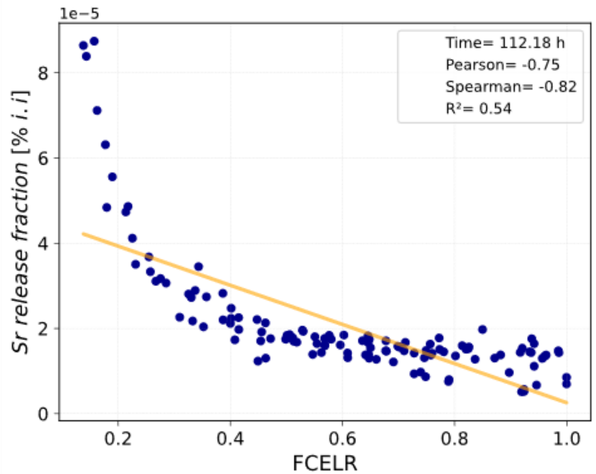
# Uncertainty quantification and sensitivity analysis: SFP

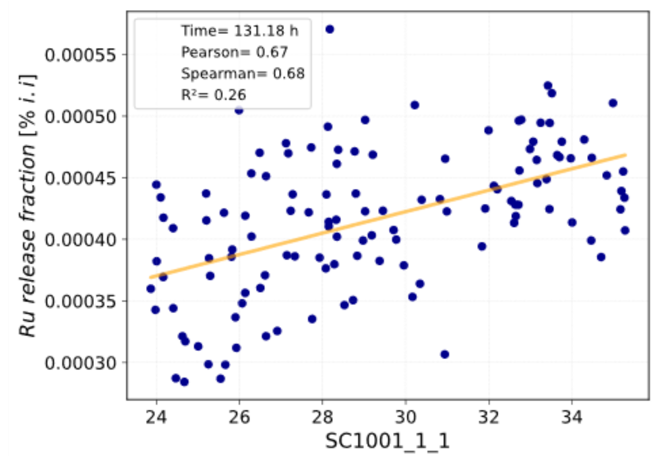


# Optimization algorithms coupled with system codes

- Optimization methodologies are used to find the optimal value of a goal function. The process consists of searching for the best-fitted combination of the variables that affect the goal function within a specified set of boundary conditions.

- One of the optimization algorithms embedded in the RAVEN tool is based on the Gradient Descent method
- It is a deterministic approach based on various gradient estimation techniques, stepping strategies, and acceptance criteria
- The algorithm works by estimating locally the gradient of the objective function
- Each new consequent search tends to decrease the gradient value, changing a set of predefined parameters of the objective function. Once all the acceptance criteria are reached, then the algorithm is considered converged
- Multiple initial parallel trajectories are needed to obtain a global solution that overcomes entrapment in local minima

**Gradient approximation adopted - Central Difference**

For the input space **i = (x; y; z)** and objective function **f(i)**, then 6 perturbations are chosen, and the following perturbation points are evaluated:

- $f(x \pm \alpha, y, z)$,
- $f(x, y \pm \beta, z)$,
- $f(x, y, z \pm \gamma)$

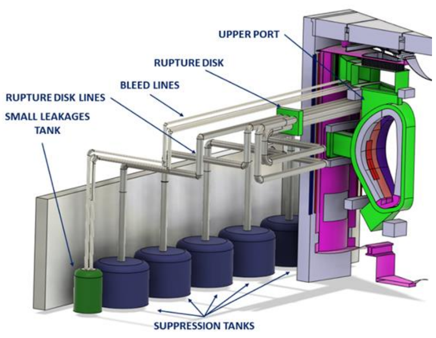
The local gradient is evaluated: $\nabla f = (\nabla^{(x)} f, \nabla^{(y)} f, \nabla^{(z)} f)$

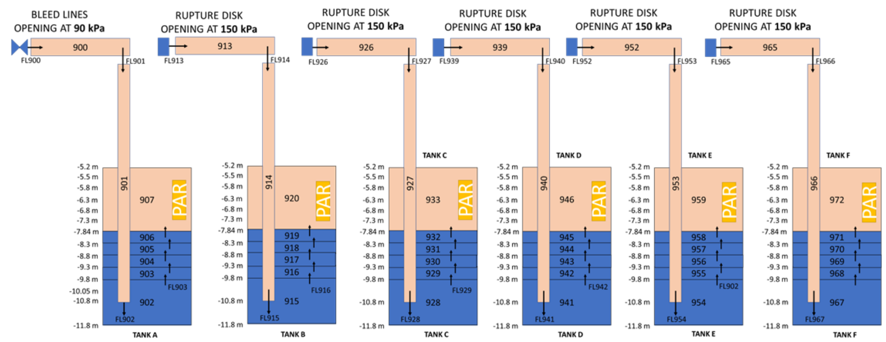
$$\nabla^{(x)} f \approx \frac{f(x+\alpha, y, z) - f(x-\alpha, y, z)}{2\alpha}$$

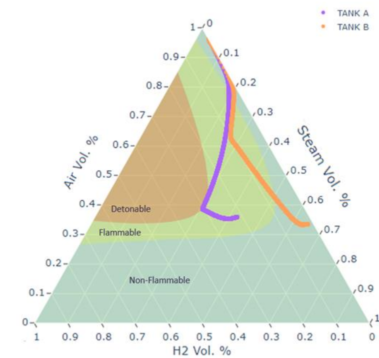
# Optimization algorithms coupled with system codes: H2 rec.

$$m_{H2} = N \cdot \eta \cdot (K_1 \cdot P + K_2) \cdot \nu \cdot \tanh(\upsilon - \min(\nu H_2))$$

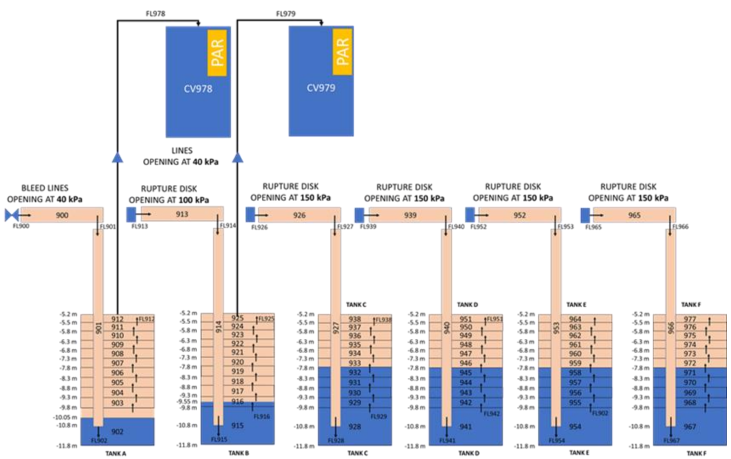
Preliminary simulations have been performed installing PAR in each ST assuming 150 kPa as setpoint for trigger of VVPSS-RDs and 90 kPa for the opening of bleed lines, and that each ST is filled with 60% of water.

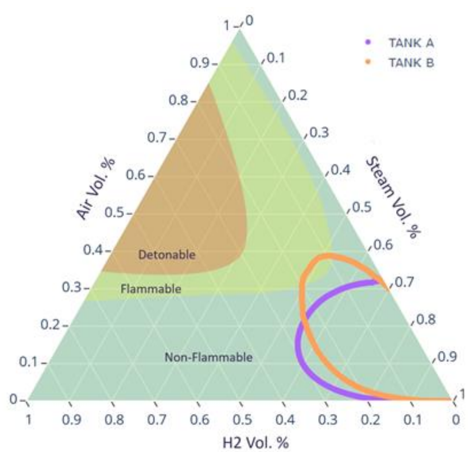


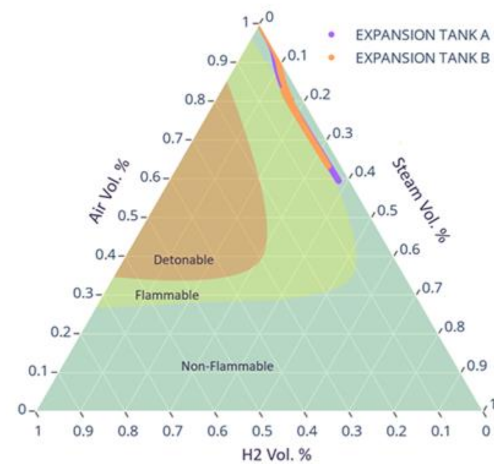




New design proposal



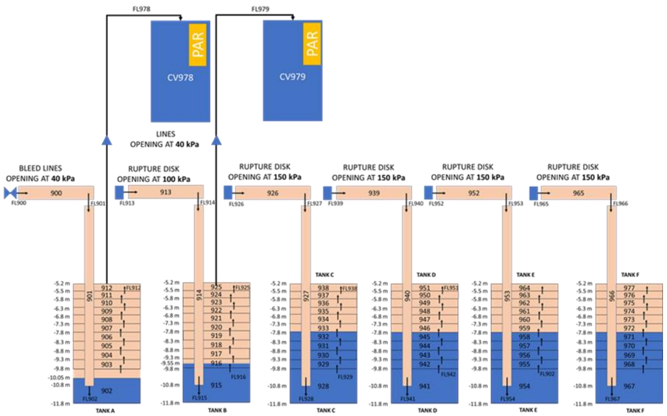



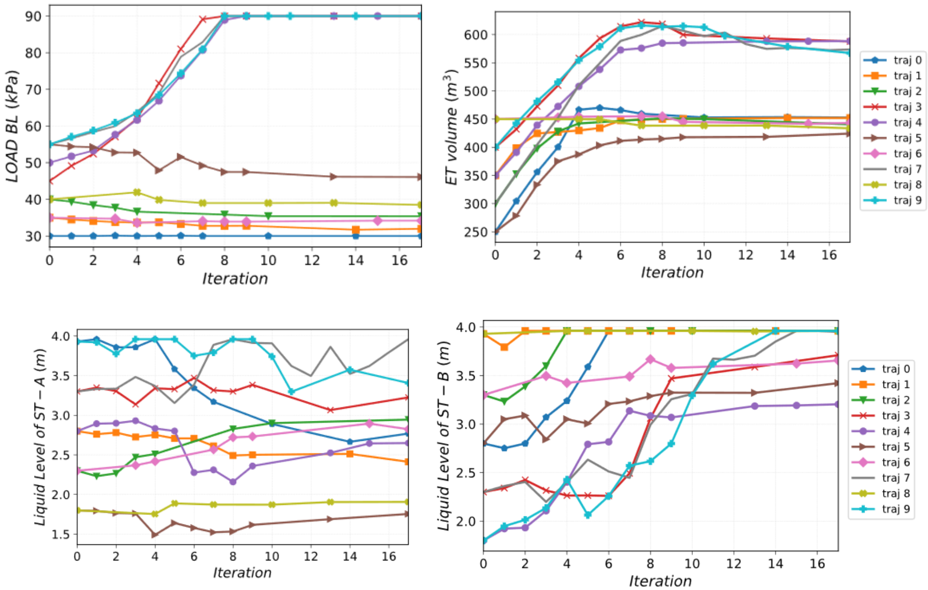

[ref.] M. D'Onorio et al., "Passive Hydrogen Recombination during a Beyond Design Basis Accident in a Fusion DEMO Plant", Energies 2023, 16(6), 2569; https://doi.org/10.3390/en16062569

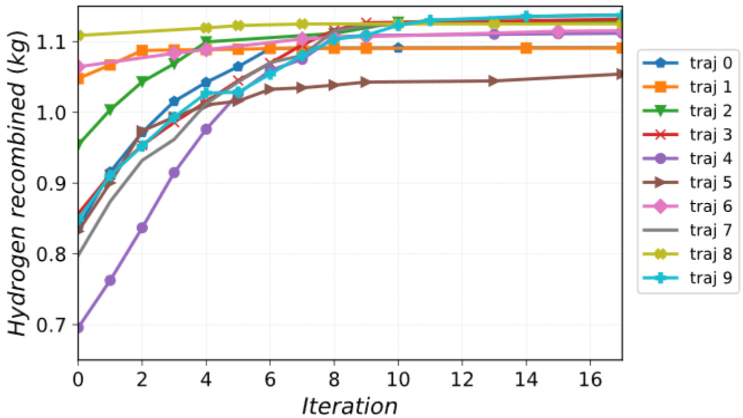
# Optimization algorithms coupled with system codes

- Objective function: Total mass of H2 recombined by both recombiners
- The selected thermal-hydraulic and geometrical parameters to be optimized are:
    - Rupture Disk pressure set point (Pa)
    - Bleeding Line pressure set point (Pa)
    - Liquid Level of Suppression Tank A (m)
    - Liquid Level of Suppression Tank B (m)
    - Expansion Tanks volume ($m^3$)

$$m_{H2} = N \cdot \ \eta \cdot (k_1 \cdot p + k_2) \cdot v \cdot \tanh\left(v - min\left(v_{H_2}\right)\right)$$




[ref.] T. Glingler, G. Caruso, M. D'Onorio "Thermal-hydraulic optimization of a proposed EU-DEMO hydrogen passive removal system", Fusion Eng. Des.,2023, https://doi.org/10.1016/j.fusengdes.2023.113729

# Conclusions & Future Developments

- MELCOR coupling with RAVEN has been completed and used for different applications
- UQ: SFP in the MUSA project
- Optimizer: Hydrogen recombination system
- DET analysis have been perfomed (next presentation)

- Explore/implement MELCOR-RAVEN machine learning algorithms to support safety assessment of nuclear power plants
- Hybrid optimization algorithms
- MELCOR DET analysis + MACCS for risk quantification

# Reference

[1] D'Onorio, M., Giampaolo, A., Caruso, G., Giannetti, F., et. al “Preliminary uncertainty quantification of the core degradation models in predicting the Fukushima Daiichi unit 3 severe accident”, (2021) Nuclear Engineering and Design, 382, art. no. 111383, doi: 10.1016/j.nucengdes.2021.111383
[2] D'Onorio, M., Giannetti, F., Porfiri, M.T., Caruso, G., “Preliminary sensitivity analysis for an ex-vessel LOCA without plasma shutdown for the EU DEMO WCLL blanket concept”, (2020) Fusion Engineering and Design, 158, art. no. 111745, doi: https://doi.org/10.1016/j.fusengdes.2020.111745
[3] D'Onorio, M., Glingler, T., Giannetti, F., Caruso, G., “Dynamic Event Tree Analysis as a Tool for Risk Assessment in Nuclear Fusion Plants Using RAVEN and MELCOR”, (2022) IEEE Transactions on Plasma Science, 2022, doi: 10.1109/TPS.2022.3165170
[4] D'Onorio, M., et. al "Severe accident sensitivity and uncertainty estimation using MELCOR and RAVEN", (2022) Journal of Physics: Conference Series, 2177 (1), art. no. 012021, 2022, doi: 10.1088/1742-6596/2177/1/012021
[5] T. Glingler, G. Caruso, M. D'Onorio ”Thermal-hydraulic optimization of a proposed EU-DEMO hydrogen passive removal system”, Fusion Eng. Des.,2023, https://doi.org/10.1016/j.fusengdes.2023.113729
[6] Glingler T., et al., Dynamic Event Tree Analysis of a Severe Accident Sequence in a Boiling Water Reactor Experiencing a Cyberattack Scenario. Available at SSRN in preprint, (2023) http://dx.doi.org/10.2139/ssrn.4376822

Thank you!