

PHEBUS FPT-1 UNCERTAINTY QUANTIFICATION USING THE MELCOR/DAKOTA COUPLING IN A PYTHON ENVIRONMENT/ARCHITECTURE

G. Agnello^{1,2}, M. Massone¹, F. Mascari¹,

1 FSN-SICNUC, ENEA, C.R. Bologna, Italy2 Department of Engineering, University of Palermo, Italy

13th Meeting of the European MELCOR and MACCS User Group, 27-29 April 2022

CONTENTS

✤ INTRODUCTION

- PHEBUS FPT-1 MELCOR INPUT-DECK AND REFERENCE CASE DESCRIPTION
- UNCERTAINTY QUANTIFICATION METHODOLOGY DESCRIPTION
- UNCERTAINTY QUANTIFICATION HYPOTHESES
- THE MELCOR/DAKOTA COUPLING IN A PYTHON ENVIRONMENT/ARCHITECTURE
- ✤ RESULTS OF THE UNCERTAINTY ANALYSIS

CONCLUSIONS



INTRODUCTION

- Since the last years, the interest of International Nuclear Scientific Community has been focused on the development and application of methodology to carry out Uncertainty Quantification (UQ) in Severe Accident (SA) domain.
- In this framework, the H2020 "Management and Uncertainty Of Severe Accident" (MUSA) project, aims to establish a harmonized approach, among both EU and non-EU entities, for the analysis of uncertainties and sensitivities associated with SAs [1].
- The MUSA WP4, coordinated by ENEA (Italy), named Application of UQ Methods against Integral Experiments (AUQMIE) [2], aims to getting experience and insights into the application of the UQ methodologies against the internationally recognized PHEBUS FPT-1 experiment [3-6].
- □ In this activity, developed along the MUSA WP4, to develop the Uncertainty Analysis (UA) using the probabilistic method to propagate input uncertainty, the MELCOR/DAKOTA coupling in a Python environment/architecture has been developed.



PHEBUS FPT-1 MELCOR INPUT-DECK AND REFERENCE CASE DESCRIPTION

- Since Italy is a member of USNRC's Cooperative Severe Accident Research Program (CSARP) [7], ENEA has requested a PHEBUS FPT-1 input-deck to USNRC. USNRC disclosed it and granted permission to ENEA to use it as a part of international collaboration on the MUSA project.
- □ The nodalization of the PHEBUS FPT-1 used for this study is composed by 31 Control Volumes (CVs), 29 Flow Path (FLs) and 68 Heat Structures (HSs).
- ❑ The bundle hydraulic region is axially subdivided into 11 CVs, modelled with the MELCOR CVH package. The fuel bundle is modelled, in the MELCOR COR package, simulating the core behavior and degradation phenomena, by 31 axial regions and 2 radial regions.
- ❑ Release of iodine from the test fuel bundle, release of caesium from the test fuel bundle, caesium retention in the circuit, aerosol suspended mass in the containment's atmosphere, amount of suspended iodine in the containment's atmosphere and the total deposited iodine in the containment have been analysed in the reference case before the UA.



PHEBUS FPT-1 MELCOR INPUT-DECK AND REFERENCE CASE DESCRIPTION



PHEBUS FPT-1 MELCOR INPUT-DECK AND REFERENCE CASE DESCRIPTION





UNCERTAINTY QUANTIFICATION METHODOLOGY DESCRIPTION



The probabilistic method to propagate input uncertainty

- The probabilistic method to propagate input uncertainty has been chosen to conduct the UA [14].
- In general, this method is based on a preliminary random sampling of selected uncertain input parameters in order to define N sets of the sampled values of the input parameters and N code runs. To determine the minimum number of N, the Wilks method can be used [15,16].
- After the resolution of the N code runs, the statistical analysis of the FOMs is performed.
- To evaluate the statistical correlation between the FOMs and the selected input parameters, correlation coefficients can be computed (e.g. Pearson and Spearman coefficients).



UNCERTAINY QUANTIFICATION HYPOTHESES

Uncertainty input parameters selected for the present UQ analysis [17]

Name	Distribution Type	Mean	Parameters	
Aerosol dynamic shape factor (CHI) [-]	Beta	1	α	1
			β	1.5
			min	1
			max	5
Aerosol agglomeration shape factor (GAMMA) [-]	Beta	1	α	1
			β	1.5
			min	1
			max	5
Particle slip coefficient (FSLIP) [-]	Beta	1.257	α	4
			β	4
			min	1.2
			max	1.3
Particle sticking coefficient (STICK) [-]	Beta	1	α	2.5
			β	1
			mın	0.5
			max	1
Turbulence dissipation rate (TURBDS) [m²/s³]	Uniform	0.001	min	0.00075
			max	0.00125
Ratio of the thermal conductivity of the gas over that for the particle (TKGOP) [-]	Log-Uniform	0.05	min	0.006
			max	0.06
Thermal accommodation coefficient (FTHERM) [-]	Uniform	2.25	min	2
	Unitorni		max	2.5
Diffusion boundary layer thickness (DELDIF) [m]	Uniform	1.00E-05	min	0.000005
			max	0.0002

- □ In this present UQ application, the aerosol suspended mass in the containment atmosphere has been selected as FOMs and the aerosol miscellaneous constants have been selected as uncertainty input parameters. These uncertain input parameters distribution and ranges have been taken from MUSA WP2.
- Based on Wilks, in case only one FOM is investigated and for the twosided tolerance interval, a minimum of 93 code runs is required for a probability and confidence level of 95%

To consider potential code runs failures, a total of 130 code runs have been performed.



MELCOR/DAKOTA COUPLING IN A PYTHON ENVIRONMENT ARCHITECTURE

- DAKOTA (Design Analysis Kit for Optimization and Terascale Application) is an open-source software developed in C++ by Sandia National Laboratories (SNL) to perform sensitivity analysis, optimization, parameter estimation, parametric and UA.
- The MELCOR/DAKOTA coupling in a Python environment/architecture permits to set the UA in terms of uncertainty input parameters Probabilistic Density Functions (PDFs), sampling methods (e.g. Random Sampling, Latin Hypercube, etc.) and response data.
- □ Through Python scripts, DAKOTA substitute the sampled uncertain input parameters in the sets of MELGEN/MELCOR inputs, run MELCOR simulations and extract the desired FOMs channels through the AptBatch executable.
- □ The FOMs values return to DAKOTA which performs the UA and writes the output file with the UQ results.
- In the present activity, Python performs also, through in-house scripts, the entire statistical analyses and the computation of the Pearson and Spearman correlation coefficients.



MELCOR/DAKOTA COUPLING IN A PYTHON ENVIRONMENT ARCHITECTURE



environment/architecture workflow



RESULTS OF THE UNCERTAINTY ANALYSIS



- The UA has been conducted evaluating the main statistical parameters of the FOM (e.g. mean, median, upper and lower bound, etc.) along the entire transient.
- Furthermore, in order to have an accurate statistical analysis of the maximum value of the FOM, a separate scalar analysis has been performed.
- A total of 10 failed runs have been encountered during the analysis and are not considered for the statistical analysis.
- □ The failed runs seems to not depend on a particular uncertainty input parameter or a combinations of them.



RESULTS OF THE UNCERTAINTY ANALYSIS: TIME DEPENDENT ANALYSIS



RESULTS OF THE UNCERTAINTY ANALYSIS: TIME DEPENDENT ANALYSIS

- □ The reference case and the experimental data appear to be within the uncertainty band along the entire test.
- The uncertainty band width is not significant along the thermal calibration phase. It begin to increase during the pre-oxidation and oxidation period and increase considerably during the heat-up period reaching the maximum width at about 16000 s (124 g). This behavior is also underlined by the standard deviation and coefficient of variation.
- □ The mean and the median value present a general good agreement respect to the experimental data.
- The CHI and GAMMA parameters, representing the aerosol dynamic shape factor and the aerosol agglomeration shape factor, present a significant linear and monotonous correlation along the thermal calibration, oxidation and heat-up periods.



RESULTS OF THE UNCERTAINTY ANALYSIS: SCALAR ANALYSIS ON THE FOM MAXIMUM





Statistical parameters of the maximum FOM value

Statistical parameter	Value	
Mean (g)	67.14	
Median (g)	66.94	
Lower Bound (g)	20.71	
Upper Bound (g)	134.74	
Standard deviation (g)	25.60	
Coefficient of variation (-)	0.38	



Uncertain input parameters

RESULTS OF THE UNCERTAINTY ANALYSIS: SCALAR ANALYSIS ON THE FOM MAXIMUM

- □ The maximum value of the FOM presents an uncertainty band of 114 g.
- The calculated mean and median values are closer to the experimental one (65.65 g) instead of the reference calculation.
- □ A moderate linear positive correlation with CHI and a significant negative linear and monotonous correlation with GAMMA are underlined.



CONCLUSIONS

- □ In the present activity, developed in the framework of MUSA WP4 (AUQMIE), the UA of the PHEBUS FPT-1 has been developed.
- ❑ The reference case, performed with the SA code MELCOR, has been performed studying four parameters related to fission products releases: release of iodine and caesium from the bundle test, caesium retention in the circuit and the aerosol suspended mass in the containment atmosphere.
- ❑ The aerosol suspended mass in the containment has been selected as FOM for the UA and the aerosol miscellaneous constants have been selected as uncertainty input parameters.
- □ To conduct the UA adopting the probabilistic method to propagate input uncertainty, the MELCOR/DAKOTA coupling in a Python environment/architecture has been developed.
- ❑ The statistical analysis of the FOM has been conducted evaluating the uncertainty band of the FOM and the main statistical parameters and the correlation analysis has been underlined a significant correlation of the FOM with the CHI and GAMMA parameters.







This project has received funding from the Euratom research and training programme 2014-2018 under grant agreement No 847441



REFERENCES

- 1. L. E. Herranz, S. Beck, V. H. Sánchez-Espinoza, F. Mascari, S. Brumm, O. Coindreau, S. Paci, "The EC MUSA Project on Management and Uncertainty of Severe Accidents: Main Pillars and Status", *Energies* 14, 4473 (2021). DOI: <u>https://doi.org/10.3390/en14154473</u>
- 2. F. Mascari et al, "First outcomes from the Phebus FPT1 uncertainty application done in the EU-MUSA Project", paper presented at the 19th International Topical Meeting on Nuclear Reactor Thermal Hydraulic (NURETH-19).
- 3. H. Scheurer, B. Clement, "PHEBUS Data Book FPT1", Document PH-PF IS/92/49", Institut de protection et de sureté nucléaire (IPSN), Cadarache, France (1997)
- 4. D. Jacquemain, S. Bourdon, A. de Braemaeker, M. Barrachin, "PHEBUS FTP1 Final Report", Institut de protection et de sureté nucléaire, IPSN/DRS/SEA/PEPF Report SEA1/00,IP/00/479, Cadarache, France (2000).
- 5. B. Clément, R. Zeyen, "The objectives of the Phebus FP experimental programme and main findings", Annals of Nuclear Energy, 61, pp. 4-10 (2013). DOI: https://doi.org/10.1016/j.anucene.2013.03.037
- 6. M. Schwarz, G. Hache, P. Von der Hardt, "PHEBUS FP: a severe accident research programme for current and advanced light water reactors", *Nuclear Engineering and Design*, **187**, pp. 47-69 (1999). DOI: https://doi.org/10.1016/S0029-5493(98)00257-X
- 7. Cooperative Severe Accident Research Program (CSARP), NUREG/BR-0524
- 8. D. Jacquemain, "Nuclear power reactor core melt accidents", EDP sciences, France (2015).
- M. Schwarz, B. Clément, A.V. Jones, "Applicability of Phebus FP results to severe accident safety evaluations and management measures", *Nuclear Engineering and Design* 209, pp. 173-181 (2001). DOI: https://doi.org/10.1016/S0029-5493(01)00400-9
- 10. M. P. Kissane, I. Drosik, "Interpretation of fission-product transport behaviour in the Phebus FPT0 and FPT1 tests, *Nuclear Engineering and Design* 236, pp. 1210-1223 (2006). DOI: https://doi.org/10.1016/j.nucengdes.2005.10.012
- 11. Dubourg, H. Faure-Geors, G. Nicaise, M. Barrachin, "Fission product release in the first two PHEBUS tests FPT0 and FPT1", *Nuclear Engineering and Design* 235, pp. 2183-2208 (2005). DOI: https://doi.org/10.1016/j.nucengdes.2005.03.007
- 12. B. Clément et al., «Thematic network for a Phebus FPT1 international standard problem (THENPHEBISP)», Nuclear Engineering and Design 235, pp. 347-357 (2005).
- 13. Bosland, L., Weber, G., Klein-Hessling, W., Girault, N. & Clement, B., 2012. Modeling and Interpretation of Iodine Behavior in PHEBUS FPT-1 Containment with ASTEC and COCOSYS Codes, Nuclear Technology, 177:1, 36-62.
- 14. H. Glaeser, "GRS Method for Uncertainty and Sensitivity Evaluation of Code Results and Applications", *Science and Technology of Nuclear Installation*, **2008**, 798901 (2008). DOI: https://doi.org/10.1155/2008/798901
- 15. S. S. Wilks, "Determination of sample size for setting tolerance limits", The Annals of Mathematical Statistics 12(1), pp. 91-96 (1941). DOI: https://doi.org/10.1214/aoms/1177731788
- 16. S.S. Wilks, "Statistical prediction with special reference to the problem of tolerance limits", *The Annals of Mathematical Statistics* **13**(4), pp. 400-409 (1942). DOI: https://doi.org/10.1214/aoms/1177731537
- 17. R. O. Gauntt, T. Radel, D. A. Kalinich, M. Salay, "Analysis of Main Steam Isolation Valve Leakage in Design Basis Accidents Using MELCOR 1.8.6 and RADTRAD", SAND2088-6601 (2008).

Giuseppe Agnello Fulvio Mascari

giuseppe.agnello04@unipa.it fulvio.mascari@enea.it

