

MELCOR/DAKOTA COUPLING IN THE SNAP ENVIRONMENT/ARCHITECTURE

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F. Mascari¹, A. Bersano², G. Agnello³, M. Angelucci⁴

1 ENEA, Bologna, Italy.
 2 Politecnico di Torino, Torino, Italy
 3 UNIPA, Palermo, Italy
 4 UNIPI, Pisa, Italy

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INTRODUCTION

- Nowadays, for the evaluation of the safety margins, the use of BEPU approach is of great interest for the International Scientific Nuclear Community.
- □ Considering the key role of Severe Accident (SA) codes for deterministic safety analyses and source term evaluations, several research activities in national and international frameworks are in progress and are planned to reduce and/or estimate the uncertainty in SA phenomena prediction.
- □ In this framework, from an operative point of view, one of the key needs is to have an automatic coupling between the UTs and the SA code.
 - For example, by using the probabilistic method to propagate input uncertainty, the Uncertaity Tool (Uts) will perform several steps and several parameters should be selected by the user when performing an Uncertainty Analyses (UA).
 - The use of a user-friendly environment/architecture, that permits a direct coupling between the SA code and the UTs, for characterizing the UA and to perform all the uncertainty steps, is one of key operative needs.



INTRODUTION

- USNRC codes (e.g. MELCOR, TRACE, etc.) can be used together with a userfriendly front end, Symbolic Nuclear Analysis Package (SNAP), able to:
 - Support the code user in the development and visualization of the nodalization,
 - o Show a direct visualization of selected calculated data, and
 - Accept existing code inputs.
- One of the features of SNAP of current interest for the International Technical Nuclear Community, is the possibility of coupling USNRC codes with the DAKOTA toolkit. Through SNAP it is possible to set up the DAKOTA uncertainty analysis and to perform automatically all the necessary steps.
- The target of this presentations is to briefly show:
 - Main details of the MELCOR/DAKOTA coupling in a SNAP environment/architecture;
 - Different steps necessary to set it up;
 - Some exemplificative applications to show the potentiality of the coupling.



INTRODUCTION

- Several methodologies have been developed in the past to perform UA. In particular these uncertainty methodologies can be grouped in:
 - Methods to propagate input uncertainty, divided in
 - Probabilistic (e.g. CSAU, GRS, IPSN, etc.);
 - Deterministic methods (e.g. AEAW, EDF-Framatome, etc.);
 - Method to extrapolate output uncertainty (e.g. UMAE).
- □ The probabilistic method to propagate input uncertainty can be applied through the DAKOTA toolkit developed by SANDIA.
- DAKOTA can be also coupled with the USNRC codes in the SNAP environment/architecture to automate the uncertainty analysis execution.



PROBABILISTIC METHOD TO PROPAGATE INPUT UNCERTAINTIES IN A CODE

- □ The probabilistic method to propagate input uncertainty is based on the creation of a set code runs.
- Each individual run is obtained by randomly selecting a value from each uncertain parameter Probability Density Function (PDF).
- □ The model input is adjusted, implementing these values, to create a singular instance of the model input of which an analysis is to be performed.
- □ A set of N models and corresponding code analyses are created and solved with a given analysis code.
- □ Then, through correlation analysis, the relationship between the selected uncertain input parameters and the results is characterized for selected FOMs.
- □ Each uncertain input parameter is defined by its range of variation and its PDF.



MELCOR/DAKOTA COUPLING IN A SNAP ENVIRONMENT/ARCHITECTURE-DAKOTA TOOLKIT

- DAKOTA is an open source software written in C++ and developed by Sandia National Laboratories to perform parametric and uncertainty analysis in a fast and automatic way.
- □ The aim of this toolkit is to bridge simulation codes and analysis methods for parametric evaluation, uncertainty quantification and system optimization.
- □ The DAKOTA toolkit is also provided as a plug-in for SNAP, which is a graphical user interface designed to support the use of USNRC nuclear codes (e.g. MELCOR, TRACE, etc.).
- □ Using SNAP, it is possible to build the input model in a graphical environment and to have a direct visualization of the computed data by using animation capability within SNAP.

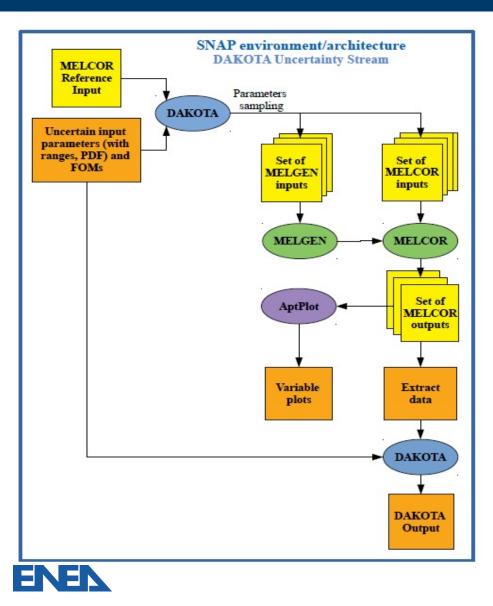
Through SNAP it is possible to set up a DAKOTA UA and to perform all analytical steps automatically.



MELCOR/DAKOTA COUPLING IN A SNAP ENVIRONMENT/ARCHITECTURE - SNAP

- □ USNRC codes (e.g. MELCOR, TRACE) can be used together with a user-friendly front end, SNAP, able to:
 - o Support the user in the development and visualization of the nodalization,
 - Show a direct visualization of selected calculated data,
 - Accept existing code input.
- □ SNAP is a suite of integrated applications including:
 - o "Model Editor",
 - "Job Status",
 - o "Configuration Tool", and
 - "Calculation Server".
- □ In particular, the "Model Editor" is used for the nodalization development and visualization and for the visualization of the selected calculated data by using its graphical and animation model capability.
- □ SNAP allows the:
 - o Development of input-decks from scratch,
 - o Import of existing input-decks developed in native ASCII format,
 - Development of the post processing of the simulations by using:
 - SNAP animation modelling capabilities and
 - AptPlot plot capabilities,
 - Execution of uncertainty analyses that automatically:
 - Run different random sampling tasks,
 - Develop requested dispersion plots, and
 - Generate statistical and response correlation analyses.

DAKOTA UNCERTAINTY ANALYSIS WORKFLOW FOR MELCOR CODE IN A SNAP ENVIRONMENT/ARCHITECTURE



- In particular, the DAKOTA plugin allows the following:
 - Enter the uncertain input parameters with their range and PDF,
 - Select the sampling method (Monte Carlo or Latin Hypercube),
 - Enter the desired FOMs for the analysis, and
 - Set the final report that contains the results of the UA application; this report is automatically generated at the end of the uncertainty quantification analysis.
- DAKOTA is run first to sample the uncertain input parameter values and to generate the set of code inputs.
- After the solution of the set of code inputs and the extraction of the desired data, DAKOTA is run a second time to perform the uncertainty analysis and applies correlation techniques to evaluate the correlation between input and output parameters selected as FOMs.

MELCOR/DAKOTA COUPLING IN A SNAP ENVIRONMENT/ARCHITECTURE

- **□** The minimum number of code runs, N, depends on the requested probability content α , the confidence level β and the number of FOMs.
- In case only one FOM is investigated, for the one-sided tolerance interval, the required number of code runs can be found, based on Wilks, by solving the following equation with respect to N:

$$1-\alpha^N=\beta$$

□ If more than one FOM is investigated, for the one-sided tolerance interval, the required number of code runs can be found by solving the following equation with respect to N

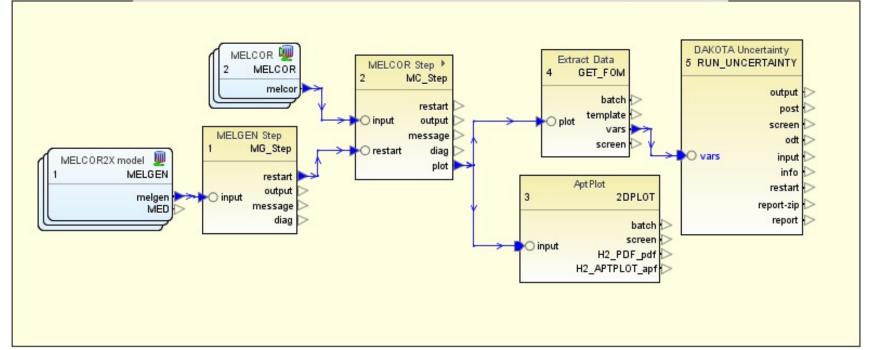
$$\beta = \sum_{j=0}^{N-p} \frac{N!}{(N-j)! j!} \alpha^{j} (1-\alpha)^{N-j}$$

where p is the number of FOMs.



STEPS NECESSARY TO SETUP A MELCOR/DAKOTA COUPLING IN A SNAP NVIRONMENT/ARCHITECTURE

- 1. Creation of the DAKOTA Uncertainty Job Stream for a Two-Step MELGEN/MELCOR Stream and selection of the MELGEN and MELCOR executables,
- 2. Definition of the DAKOTA application properties, characterization of the PDF, setup of the automatically generated report,
- 3. Definition of the Plotting Step properties,
- 4. Creation and set-up of the Data Extraction and DAKOTA Uncertainty Steps,
- 5. Creation and set-up of DAKOTA Uncertainty Steps,
- 6. Execution of the Uncertainty Analysis.



ALL the STEPS are described in detail in the NUREG-IA

DEFINITION OF THE DAKOTA APPLICATION PROPERTIES, CHARACTERIZATION OF THE PDF, SET-UP OF THE AUTOMATICALLY GENERATED REPORT

□ After setting up the MELGEN and MELCOR steps, the characterization of the different uncertain parameters may be defined.

□ From the EDIT UNCERTAINTY CONFIGURATION, various Tabs allow users to:

- Characterize the sampling process:
 - "Number of Samples": In order to select the number of samples a "Calculated Samples Button" is available to the user to evaluate the required number of tasks considering the Order, Probability, and Confidence selected by the user. The calculation is based on Wilks formula.
 - o "Random Seed";
 - "Sampling Method" (Monte-Carlo or Latin Hypercube method);
 - "Input Error Handling" (ignore model check errors; filter out inputs that fail model check; replace input that fail model check),
 - FOMs,
 - Order, probability and confidence level;
 - Replacement factor.
- o Identify uncertain input parameters and their related distribution characteristics;
- Identify the FOMs;
- Specifying the aspects of the automatically generated report.



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"EDIT UNCERTAINTY CONFIGURATION/REPORT" SNAP TAB

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DAKOTA UA REPORT

- ❑ The report is automatically generated by DAKOTA at the end of the UA as characterized in the "Edit Uncertainty Configuration View/Report" Tab along with the input specifications.
- □ The report includes the following sections:
 - o Introduction section,
 - Uncertainty quantification input options section,
 - Variate and response data section,
 - DAKOTA Results:
 - In this section after a summary of the second DAKOTA run, the following information are reported for each FOM:
 - Cumulative distribution function and probability density function,
 - Statistical results, and
 - Response correlation.
 - DAKOTA Input File: The input file used in a -pre_run DAKOTA invocation to generate the random variates.



DAKOTA UA REPORT

□ REPORT: Variate and Response data:

- The Uncertainty quantification input options section includes:
 - A tabulated summary of the main information characterizing the UA application,
 - A tabulated summary of distributions, their characteristic parameters, and the selected model variables,
 - A table listing the application used in the job stream is reported, and
 - User identified FOMs in the analysis.

REPORT: Variate and Response data:

- In the Variate and response data section, after a summary of the first DAKOTA run, the following information are present:
 - Plot requested in the "Edit Uncertainty Configuration/Report"
 - Variate data (input uncertain parameters value for each task) and response data table (FOM value for each task).
- The plots present in the DAKOTA automatically generated report are:
 - Input uncertain parameter against iteration index,
 - FOM VS input uncertain parameter, and
 - Input uncertain parameter VS another input uncertain parameter.
- For each FOM the follow is reported:
 - A table presenting response data for each task and
 - A table presenting the value of each uncertain parameter for each task.

REPORT: DAKOTA results

- In relation to the DAKOTA statistical results of the FOM, the following information can be found in the automatically generated report:
 - Plots: Cumulative distribution function and Probability density function,



• Tabulated Data: Statistical results -Min value, Max value, Mean value, Median value and the related task, Standard deviation, and Coefficient of variance.

MELCOR/DAKOTA COUPLING, IN A SNAP ENVIRONMENT/ARCHITECTURE - ENEA SAMPLES

□ ENEA MELCOR/DAKOTA uncertainty studies are reported here:

- SAMPLE 1: MELCOR/DAKOTA COUPLING AGAINST CSTF-AB1 test
- SAMPLE 2: MELCOR/DAKOTA COUPLING FOR A PWR
- These represent only the first ENEA exercises showing complete application of the coupling procedure of MELCOR and DAKOTA within the SNAP environment/architecture.
- □ The purpose of these exercises is not to be a complete and representative analysis of the MELCOR code nor the most relevant input parameters or their associated PDFs but instead is only intended to demonstrate the methodology.
- □ Therefore, the main purpose of these applications is to:
 - Show the feasibility of the MELCOR/DAKOTA coupling,
 - o Provide detailed on the capabilities provided by this methodology, and
 - Show the great advantage of using SNAP:



SAMPLE 1 - MELCOR/DAKOTA COUPLING AGAINST CSTF-AB1 TEST: FOMS

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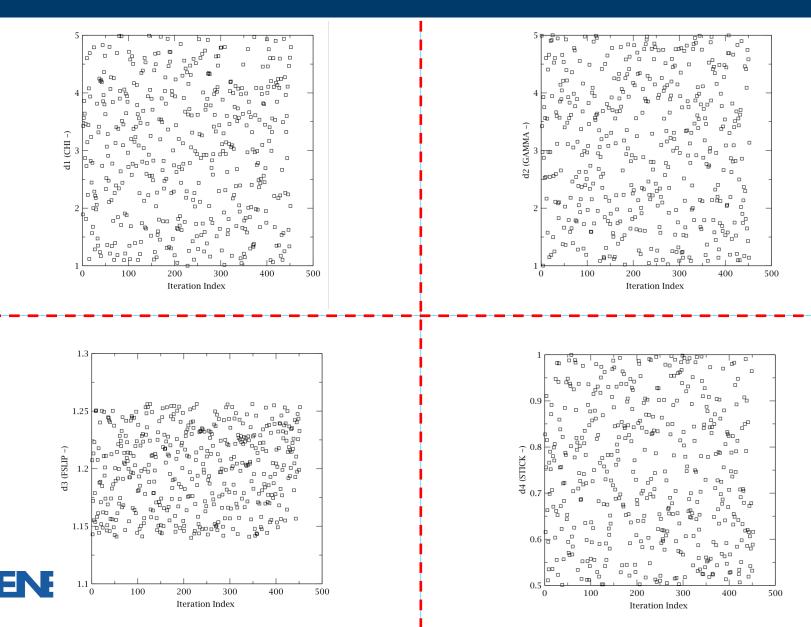
The following four figures of merit are defined for this uncertainty analysis:

- SUSP: Suspended airborne concentration
- MMD: Aerosol mass median diameter
 - SSD: Geometric standard deviation of the aerosol distribution
- TOT_DEP: Tot mass deposited



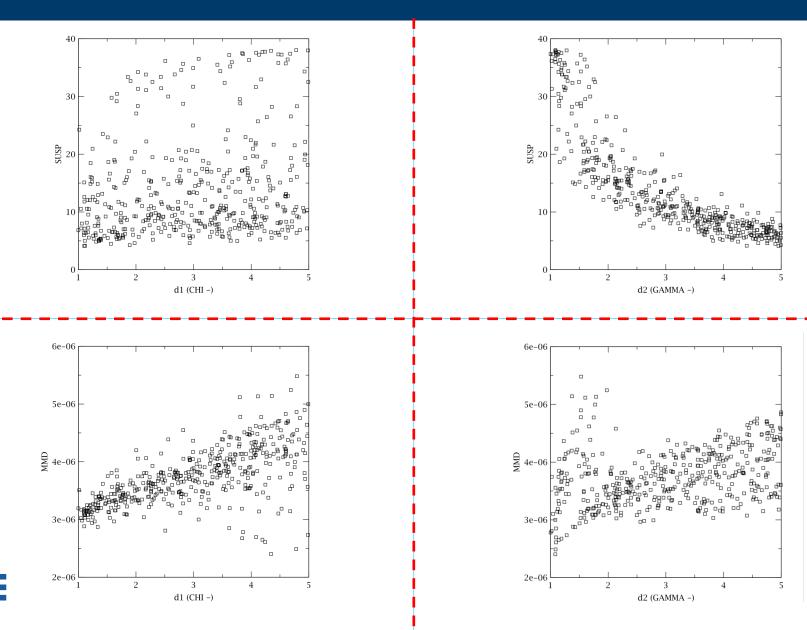
An model input set of 452 runs is computed such that the four specified FOMs with a 98.0% probability and a 98.0% confidence level are satisfied.

SAMPLE 1 - VARIATE AND RESPONSE DATA: INPUT UNCERTAIN PARAMETER VS ITERATION INDEX FOR THE CASE1



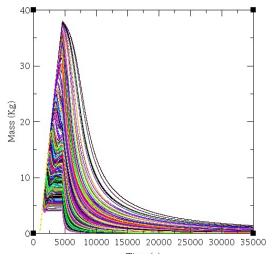
21

SAMPLE 1: VARIATE AND RESPONSE DATA: FOM VS INPUT UNCERTAIN PARAMETERS

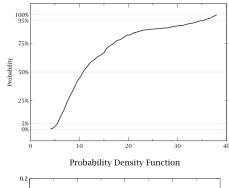


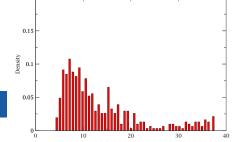
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SAMPLE 1 - MELCOR/DAKOTA COUPLING AGAINST CSTF-AB1 TEST : SUSPENDED MASS AT THE END OF THE POOL FIRE



Cumulative Distribution Function





Statistical results

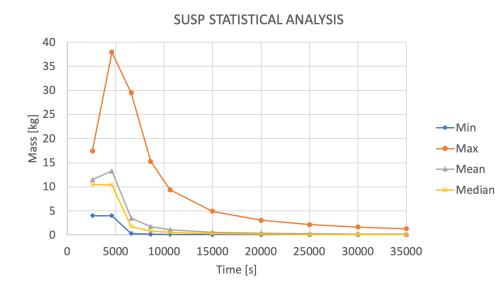
Summary	Value	Task#
Min Value	4.10529	121
Max Value	38.00867	300
Mean	13.88923	-
Median	10.69479	average of 419 and 436
Standard Deviation	8.68916	
Coefficient of Variance	1.38387	-

Response correlation reported in the automatically generated DAKOTA report based on the 59 samples

	Simple	Partial	Simple Rank	Partial Rank
dl	0.212682	0.45182	0.22458	0.809953
d2	-0.839444	-0.891894	-0.920448	-0.984271
d3	-0.00536477	-0.052228	0.00593418	-0.0868283
d4	-0.166987	-0.376395	-0.151035	-0.685502
d5	-0.160288	-0.37879	-0.201699	-0.793493
d6	0.0381186	0.0479846	0.0215019	-0.00823322
d7	0.00950152	-0.0383844	0.0139928	-0.0606922
d8	0.019709	0.0737938	-0.0320248	-0.134612
MMD	-0.107979	-	-0.138996	-
SSD	-0.797382	-	-0.716527	-
TOT_DEP	-1.0	2	-1.0	-

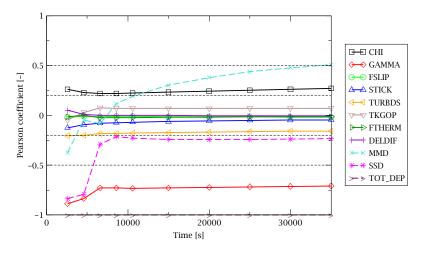
Note: NaN values typically indicate an insufficient number of tasks were supplied to perform the analysis.

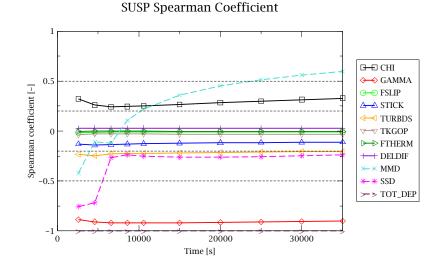
SAMPLE 1 - MELCOR/DAKOTA COUPLING AGAINST CSTF-AB1 TEST: SUSPENDED MASS – TIME DEPENDENT ANALYSES





SUSP Pearson Coefficient





SAMPLE 1 - TIME DEPENDENT ANALYSIS, APTPLOT SCRIPT FOR THE DATA EXTRACTION

```
C Edit AptPlot Script
                                                                   ×
Enter AptPlot commands to extract data into the indicated variables:
MELCOR PTF "${PlotFile}"
 CALC "SUSP = 0.0"
 CALC "MMD = 0.0"
 CALC "SSD = 0.0"
 CALC "TOT DEP = 0.0"
 CALC "SUSP = getYval( ${TIME}, M0 (RN1-ATMG 1))"
 CALC "MMD = getYval( ${TIME}, M0_(RN1-MMDD_1))"
 CALC "SSD = getYval( ${TIME}, M0_(RN1-GSDD_1))"
 CALC "TOT DEP = getYval( ${TIME}, M0 (RN1-TMDTT))"
 SAVEVAR "<SUSP VEC>"
 SAVEVAR "<MMD VEC>"
 SAVEVAR "<SSD VEC>"
 SAVEVAR "<TOT DEP VEC>"
 WRITEVARS ASCII "${VariableFile}"
 EXIT
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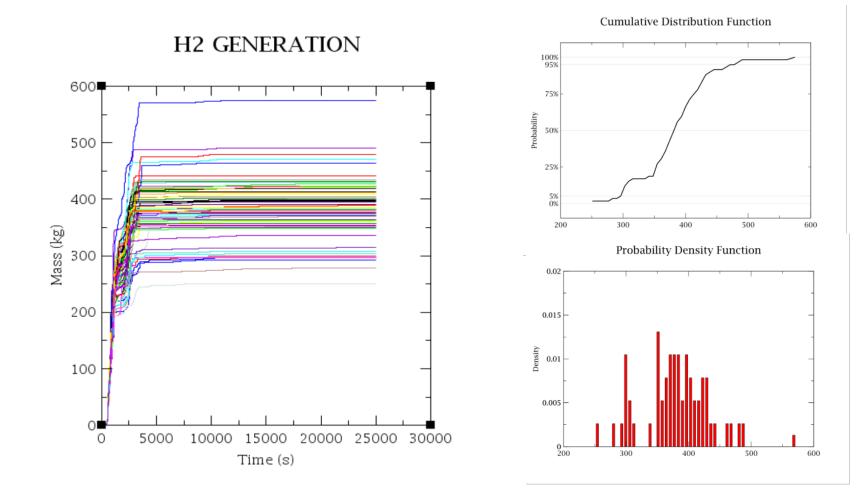
SAMPLE 2: MELCOR/DAKOTA COUPLING FOR A PWR

- In the CSARP framework, a MELCOR/DAKOTA sample input model has been developed by ENEA using the _PWR_v2-0.inp input available for MELCOR users.
- Since the file was available in ASCII format, the steps that have been performed with SNAP are:
 - Import the _PWR_v2-0.inp into SNAP and create a .med file,
 - Create the Job Stream for the MELCOR and DAKOTA analysis,
 - Identify uncertain input parameters and their related distribution characteristics;
 - Run the analyses with SNAP.
- The total cumulative hydrogen production in the core from all the oxidation processes (COR-DMH2-TOT) at the end the transient has been selected as the only FOM for this analysis.

An model input set of 59 runs is computed such that the 1 specified FOM with a 95.0% probability and a 95.0% confidence level are satisfied.



SAMPLE-2: TOT HYDROGEN MASS GENERATED DISPERSION, CUMULATIVE DISTRIBUTION FUNCTION, AND PROBABILITY DENSITY FUNCTION





SAMPLE 2 - STATISTICAL AND RESPONSE CORRELATION RESULTS

Statistical results based on the 59 samples

Summary	Value	Task #
Min Value	250.87505	54
Max Value	574.76666	51
Mean	381.43805	-
Median	382.44507	40
Standard Deviation	56.8461	-
Coefficient of Variance	0.38578	-

Response correlation reported in the automatically generated DAKOTA report based on the 59 samples

	Simple	Partial	Simple Rank	Partial Rank
d5	0.0979063	0.102384	0.135067	0.268539
d6	0.110172	0.146704	0.0338983	0.0599765
d7	0.098521	0.123725	0.126768	0.209831
d1	0.737284	0.791904	0.765926	0.855157
d2	-0.495872	-0.627241	-0.379486	-0.653184
d3	0.03035	0.00594472	0.0189947	0.0516358
d4	-0.0188159	0.0125986	-0.0151373	0.0108442



SAMPLE 2- DAKOTA INPUT REPORTED IN THE AUTOMATICALLY GENERATED REPORT

REPORT

Update for Chapter Headers

3.2 DAKOTA Input File

The input file used in a -pre_run DAKOTA invocation to generate the random variates.

```
method,
   nond sampling,
       samples = 59
       # stub response levels
       response levels = 0.0 1.0
       sample type random
       distribution cumulative
variables,
   normal uncertain = 3
     descriptors = 'd5' 'd6' 'd7'
means = 2700.0 5.0 2800.0
     std deviations = 120.0 1.0 150.0
      lower bounds = -1.7976931348623157E308 -1.7976931348623157E308 -
1.7976931348623157E308
       upper bounds = 1.7976931348623157E308 1.7976931348623157E308
1.7976931348623157E308
   triangular uncertain = 4
     descriptors = 'd1' 'd2' 'd3' 'd4'
lower_bounds = 2098.0 0.01 0.05 50.0
      upper_bounds = 2550.0 1.0 1.2 1100.0
modes = 2400.0 0.083 0.1 1000.0
interface.
   system
       analysis driver = '<not used>'
responses,
   num response functions = 1
   no gradients
  no hessians
```



SAMPLE 2- NOT TIME DEPENDENT ANALYSIS, APTPLOT SCRIPT FOR THE DATA EXTRACTION

2 Edit AptPlot Script	>
Enter AptPlot commands to extract data into the indicated variables:	
MELCOR PIF "4{PlotFile}" CALC "H2_GEN = 0.0"	
CALC "H_GEN = getYval(24000.0, M0_(COR-DMH2-TOT))"	
SAVEVAR "H2_GEN" WRITEVARS ASCII "\${VariableFile}" EXII	
ОК	Cancel



SAMPLE 2- SNAP JOB-STATUS DURING THE DAKOTA UNCERTAINTY APPLICATION

– 🗗 🗙

😐 💿 🎓 🖬 🖬 🏦 🛄

calcserv://Local/UNCERTAINTY/MELCOR/PWR_UQ/

Job	Priority	Job Type	Status 🔻	Submitted	Started	Completed	Calc Time	Loaded	Evaluation
PWR_UQ	4	Stream	Complete	Aug 05 12:21	Aug 05 12:21	Aug 05 12:33	No Data	No	
2DPLOT	5	AptPlot	Complete	Aug 05 12:30	Aug 05 12:32	Aug 05 12:32	No Data	No	
GET_FOM_T01	5	AptPlotExtract	Complete	Aug 05 12:24	Aug 05 12:30	Aug 05 12:30	No Data	No	
GET_FOM_T02	5	AptPlotExtract	Complete	Aug 05 12:24	Aug 05 12:30	Aug 05 12:30	No Data	No	
GET_FOM_T03	5	AptPlotExtract	Complete	Aug 05 12:24	Aug 05 12:30	Aug 05 12:30	No Data	No	
GET_FOM_T04	5	AptPlotExtract	Complete	Aug 05 12:24	Aug 05 12:30	Aug 05 12:30	No Data	No	
GET_FOM_T05	5	AptPlotExtract	Complete	Aug 05 12:25	Aug 05 12:30	Aug 05 12:31	No Data	No	
GET_FOM_T06	5	AptPlotExtract	Complete	Aug 05 12:25	Aug 05 12:30	Aug 05 12:31	No Data	No	
GET_FOM_T07	5	AptPlotExtract	Complete	Aug 05 12:24	Aug 05 12:30	Aug 05 12:31	No Data	No	
GET_FOM_T08	5	AptPlotExtract	Complete	Aug 05 12:25	Aug 05 12:31	Aug 05 12:31	No Data	No	
GET_FOM_T09	5	AptPlotExtract	Complete	Aug 05 12:25	Aug 05 12:30	Aug 05 12:31	No Data	No	
GET_FOM_T10	5	AptPlotExtract	Complete	Aug 05 12:25	Aug 05 12:30	Aug 05 12:31	No Data	No	
GET_FOM_T11	5	AptPlotExtract	Complete	Aug 05 12:25	Aug 05 12:31	Aug 05 12:31	No Data	No	
GET_FOM_T12	5	AptPlotExtract	Complete	Aug 05 12:25	Aug 05 12:31	Aug 05 12:31	No Data	No	
GET_FOM_T13	5	AptPlotExtract	Complete	Aug 05 12:25	Aug 05 12:31	Aug 05 12:31	No Data	No	
GET_FOM_T14	5	AptPlotExtract	Complete	Aug 05 12:25	Aug 05 12:31	Aug 05 12:31	No Data	No	
GET_FOM_T15	5	AptPlotExtract	Complete	Aug 05 12:26	Aug 05 12:31	Aug 05 12:31	No Data	No	
GET_FOM_T16	5	AptPlotExtract	Complete	Aug 05 12:26	Aug 05 12:31	Aug 05 12:31	No Data	No	
GET_FOM_T17	5	AptPlotExtract	Complete	Aug 05 12:26	Aug 05 12:31	Aug 05 12:31	No Data	No	
GET_FOM_T18	5	AptPlotExtract	Complete	Aug 05 12:26	Aug 05 12:31	Aug 05 12:31	No Data	No	
GET_FOM_T19	5	AptPlotExtract	Complete	Aug 05 12:26	Aug 05 12:31	Aug 05 12:31	No Data	No	
GET_FOM_T20	5	AptPlotExtract	Complete	Aug 05 12:26	Aug 05 12:31	Aug 05 12:31	No Data	No	
GET_FOM_T21	5	AptPlotExtract	Complete	Aug 05 12:26	Aug 05 12:31	Aug 05 12:31	No Data	No	
GET FOM T22	5	AptPlotExtract	Complete	Aug 05 12:26	Aug 05 12:31	Aug 05 12:31	No Data	No	
GET_FOM_T23	5	AptPlotExtract	Complete	Aug 05 12:27	Aug 05 12:31	Aug 05 12:31	No Data	No	
GET_FOM_T24	5	AptPlotExtract	Complete	Aug 05 12:27	Aug 05 12:31	Aug 05 12:31	No Data	No	
GET FOM T25	5	AptPlotExtract	Complete	Aug 05 12:27	Aug 05 12:31	Aug 05 12:31	No Data	No	
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GET_FOM_T29	5	AptPlotExtract	Complete	Aug 05 12:27				No	
GET_FOM_T30	5	AptPlotExtract	Complete	Aug 05 12:27	-	-			
GET_FOM_T31	5	AptPlotExtract	Complete	Aug 05 12:28	-	-			
GET FOM T32	5	AptPlotExtract	Complete	Aug 05 12:27					
GET FOM T33	5	AptPlotExtract	Complete	Aug 05 12:27	-	-			
DET FOR THE	r		Onenalata	Aur 05 40:00					



IN PROGRESS NUREG-IA

- Considering the interest of the International Community (e.g. EU-MUSA, IAEA-CRP(I31033), etc.) on the MELCOR/DAKOTA coupling a NUREG–IA, developed together with SANDIA and POLITO, is in review phase and has the main target of:
 - Showing the main details of the MELCOR/DAKOTA coupling in a SNAP environment/architecture;
 - Showing the different steps necessary to set it up;
 - Describing two sample applications to show the feasibility and to analyze the capabilities of this coupling (these first excercises aim to show only the complete application of the coupling procedure of MELCOR and DAKOTA in a SNAP environment/architecture; they do not want to represent a complete and representative analyses of the MELCOR code uncertainty).
 - Supporting MECOR users.



A NUREG-IA, in SANDIA REVIEW process, has been prepared to investigate the MELCOR/DAKOTA coupling in a SNAP environment/architecture and to be an endorsed user-guide

NUREG/IA-



International Agreement Report

MELCOR – DAKOTA Coupling for Uncertainty Analyses, in a SNAP Environment/Architecture

Prepared by: Fulvio Mascari*, Andrea Bersano**, Jesse Phillips***

*ENEA, Nuclear Safety, Security and Sustainability Division (FSN-SICNUC), Via Martiri di Monte Sole 4, Bologna, 40129, Italy

**Politecnico di Torino, Energy Department (DENERG), Corso Duca degli Abruzzi 24, Turin, 10129, Italy

***Sandia National Laboratories, 1515 Eubank SE Albuquerque, New Mexico 87123

H. Hossein, NRC Project Manager

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A NUREG-IA, in SANDIA REVIEW process, has been prepared to investigate the MELCOR/DAKOTA coupling in a SNAP environment/architecture and to be an endorsed user-guide

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R	efere	CONCLUSION	

The activity is done in collaboration with POLITO, SANDIA.

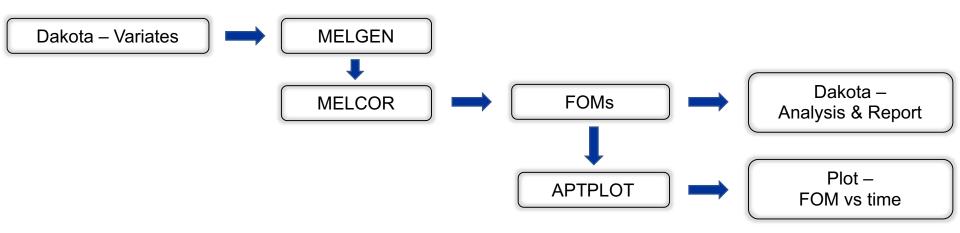
CONCLUSIONS- ON MELCOR/DAKOTA COUPLING THROUGH SNAP GUI

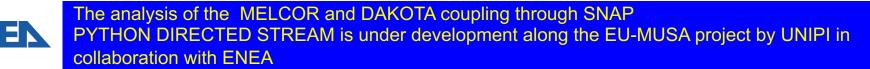
- □ MELCOR can be coupled with DAKOTA to perform Uncertainty Analysis.
- □ The coupling can be done in SNAP or "stand alone" with scripts.
- □ Using SNAP, it is possible to build the input model in a graphical environment and to have a direct visualization of the computed data by using animation capability within SNAP.
- □ Two sample applications about the MELCOR/DAKOTA coupling in a SNAP environment/architecture have been carried out by ENEA.
- A NUREG-IA is in progress to support the MELCOR users in the development of the MELCOR/DAKOTA coupling in SNAP.
- Currently if one calculation fails it prevents finalizing the UA application in SNAP:
 - New Python directed job-stream capability in SNAP have been added;
 - In the version 1.7 of the SNAP uncertainty plugin "the uncertainty quantification support in Python Directed streams was updated to support a specified number of "Replacement Samples" that are used to run additional tasks to replace those that fail to execute" (https://www.aptplot.com/snap/plugins/uncertainty/changes.jsp).

DEVELOPMENT OF MELCOR AND DAKOTA THROUGH THE NEW PYTHON DIRECTED JOB-STREAM CAPABILITY IN SNAP

- Currently the "replacement samples" option is not available when using the SNAP/GUI. Therefore, if one calculation fails, it prevents Uncertainty Analysis finalization:
- □ New Python Directed job-stream feature has been added in SNAP.

MELCOR and DAKOTA coupling through SNAP PYTHON DIRECTED STREAM



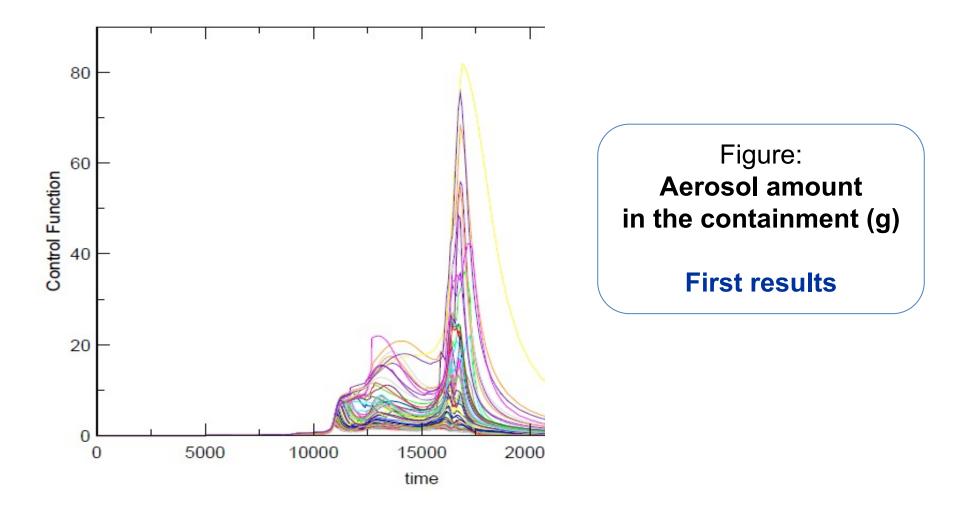


DEVELOPMENT OF MELCOR AND DAKOTA THROUGH THE NEW PYTHON DIRECTED JOB-STREAM CAPABILITY IN SNAP

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 Sodium Chemistry III Transfer Process Eases [1] 		1}	<pre>stream = streams.get_stream()</pre>	
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 	1_Uncertainty_Analys	sis_v3_5 _≡	<pre>actors=[] for row in parametric.get_table(): row.apply_values(phebus)</pre>	
 Connections [398] Numerics [8] Views [4] 		•	actor_name = row.new_task_name("Melgen_Job")	
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Name	Ру		actors.append(melgen_run)	
Description	-	2 2 2	<pre>actor_name2 = row.new_task_name("Melcor_Job")</pre>	
Stream Type Platform	Python Dire	• • •	<pre>melcor_run = MelcorActor(actor_name2, input=phebus.case('MELCOR'), restart_in=melgen_run.restart_out)</pre>	
Root Folder	Py_Dir_T V		actors.append(melcor_run) <pre>#stream.add([melgen_run, melcor_run])</pre>	
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DEVELOPMENT OF MELCOR AND DAKOTA THROUGH THE NEW PYTHON DIRECTED JOB-STREAM CAPABILITY IN SNAP





DEVELOPMENT OF MELCOR AND DAKOTA THROUGH THE NEW PYTHON DIRECTED JOB-STREAM CAPABILITY IN SNAP

SNAP (Dakota Uncertainty Plugin - GUI):

Problems in handling failed MELCOR calculations \rightarrow

→ ExtractionData & Uncertainty steps fail

SNAP (Python Directed Stream):

- Script phase seems not user friendly;
- "Replacement samples" option: additional samplings created, but currently failed calculations not re-run;
- Stream manager current failures when adding jobs to the stream;
- "generate_report" currently fails.

Considering the current commitments in the EU-MUSA project and IAEA CRP (I31033) and the current close deadlines for developing the planned research activity, the direct support of SNAP developers could be necessary to develop uncertainty estimation that handle the failed calculations (through GUI or Python direct stream).



MELCOR/DAKOTA COUPLING GROUP

- The quantification of the uncertainty in a SA transient calculation is a currently relevant topic in the BEPU framework.
- Among the available methodologies, the probabilistic method to propagate input uncertainties is widely adopted in deterministic safety analyses.
- Several MELCOR users are currently applying this method with the DAKOTA Uncertainty Tool (UT), developed by SNL.
- The goal of this group is to create a platform for MELCOR users for sharing experience and discussing the coupling with DAKOTA, both through the Symbolic Nuclear Analysis Package (SNAP) and with other coupling methods (e.g. Python scripts).
- □ The activity is performed in the framework of the USNRC Cooperative Severe Accident Research Program (CSARP).
- A «MELCOR/DAKOTA coupling» Project has been set in ResearchGate for sharing public material.
- □ Meetings:
 - Two meetings have been already carried out;
 - A third meeting will be planned in the next months for discussing and consolidate the current approaches for coupling MELCOR and UT tools
- □ The group is open to all MELCOR users and it is currently done in collaboration with:
 - CIEMAT, ENEA, JACOBS, KIT, POLITO, PSI, SANDIA, UNIPA, UNIPI, UNIROMA1, USNRC



NEXT MELCOR/DAKOTA COUPLING GROUP MEETING

- Considering the feedback from the previous meetings we propose to have a further dedicated meeting open to:
 - MELCOR user community,
 - MELCOR developer,
 - o DAKOTA developer,
 - o SNAP developer

to discuss in detail the MELCOR/DAKOTA coupling aspects.

- At the end of this meeting will be useful to prepare a document that could be a consolidate and endorsed reference to perform uncertainty analyses with MELCOR.
- Eventually this document could be a NUREG-IA that could be an endorsed reference that summarize the use of MELCOR with uncertainty tools as DAKOTA or RAVEN.
- The possible date could be in May but the date is open to discussion to optimize the interaction and effectiveness with EU-MUSA and IAEA-CRP(I31033) activities where a lot of use of MELCOR/DAKOTA activity is in progress.



ACKNOWLEDGEMENTS

Special thanks to USNRC and Sandia National Laboratories for their comments during the preparation of the activities

Part of the activity has been done through the MUSA project:



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







Fulvio Mascari: fulvio.mascari@enea.it







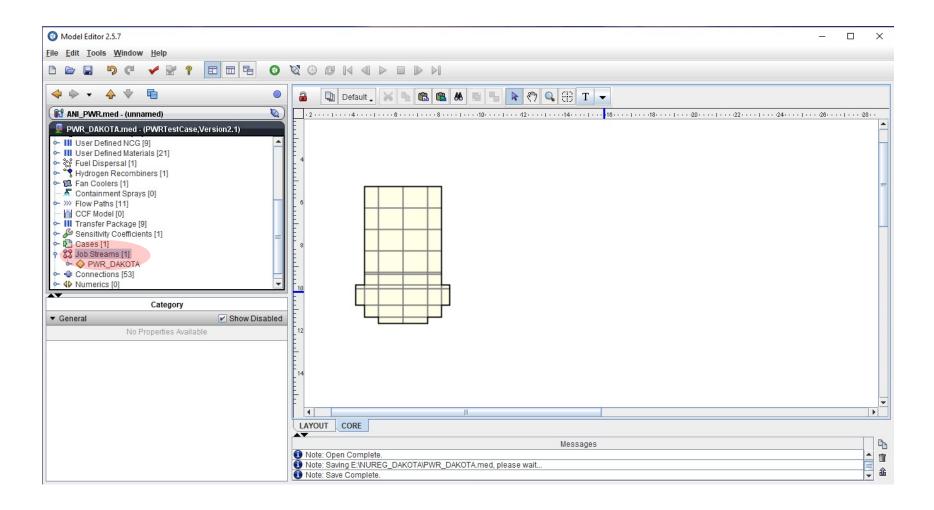






STEPS NECESSARY TO SET-UP A MELCOR/DAKOTA COUPLING IN A SNAP ENVRONMENT/ARCHITECTURE THROUGH THE GUI

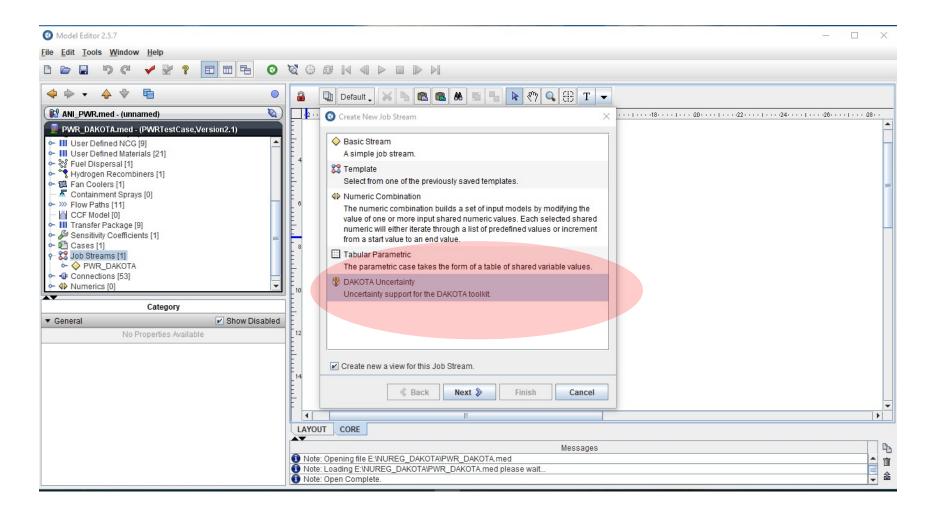




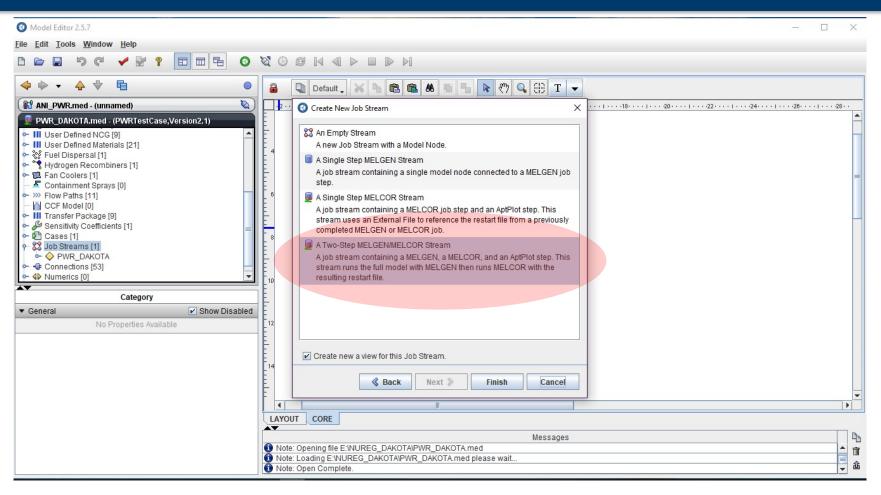


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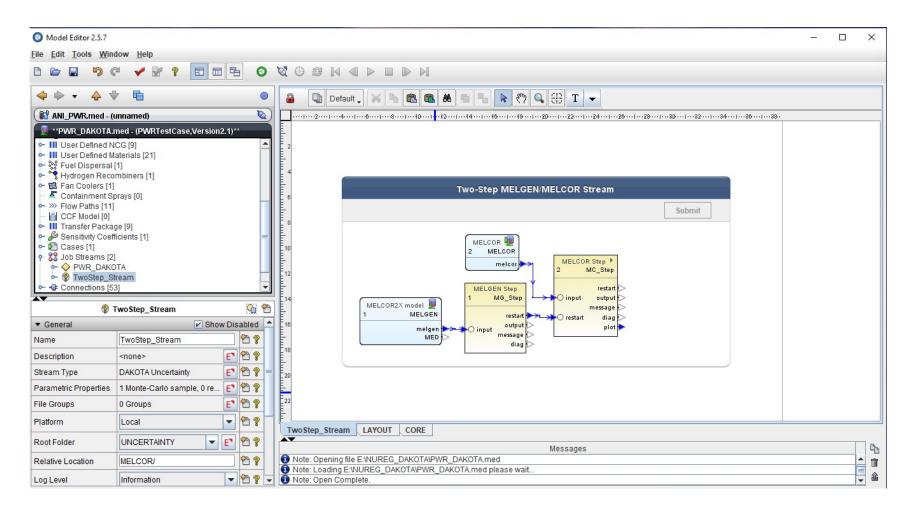




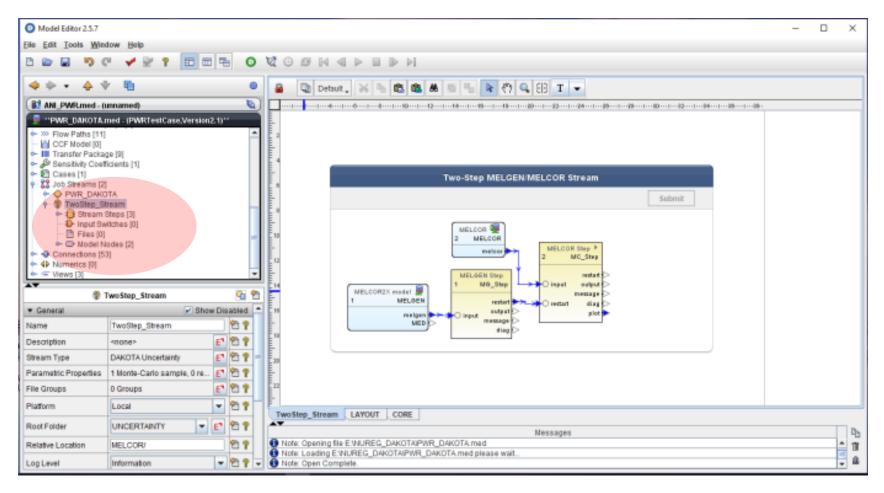


In a more recent version of SNAP (e.g. Model Editor 3.1.3) a Two-Step MELGEN/MELCOR stream, and a Three-Step MELGEN/MELCOR/APTPLOT Stream are available. In the case of the Three-Step MELGEN/MELCOR/APTPLOT Stream, the AptPlot stream step is automatically generated. In a more recent Model Editor version (e.g. 3.1.3) in the Two-Step MELGEN/MELCOR job stream, the AptPlot stream step should be added by the code user. To be consistent with the description of this report, based on the Model Editor 2.5.7. the reader should select the Three-Step MELGEN/MELCOR/APTPLOT Stream, if available in the version that he is using.

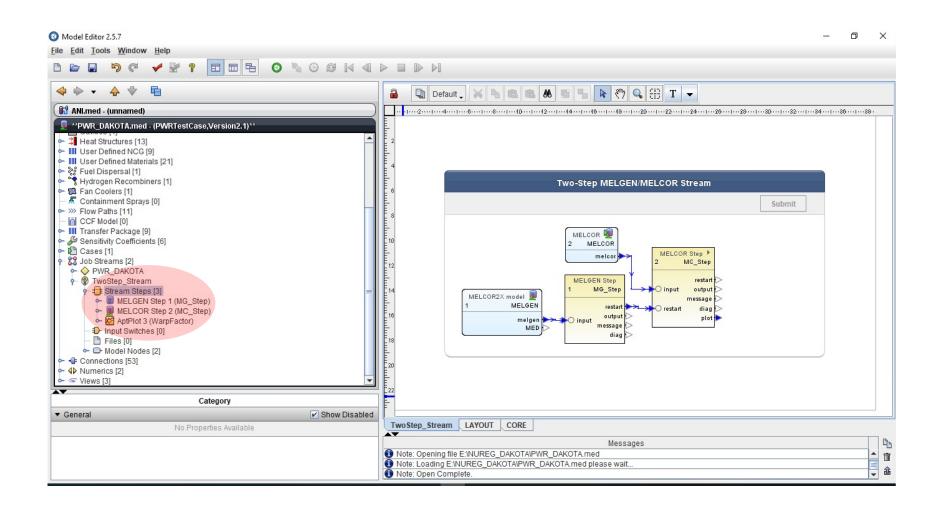














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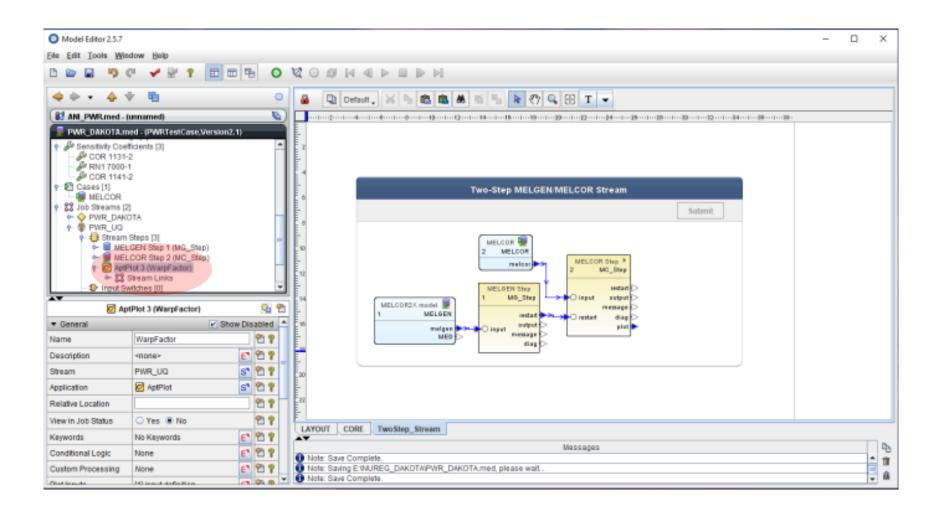


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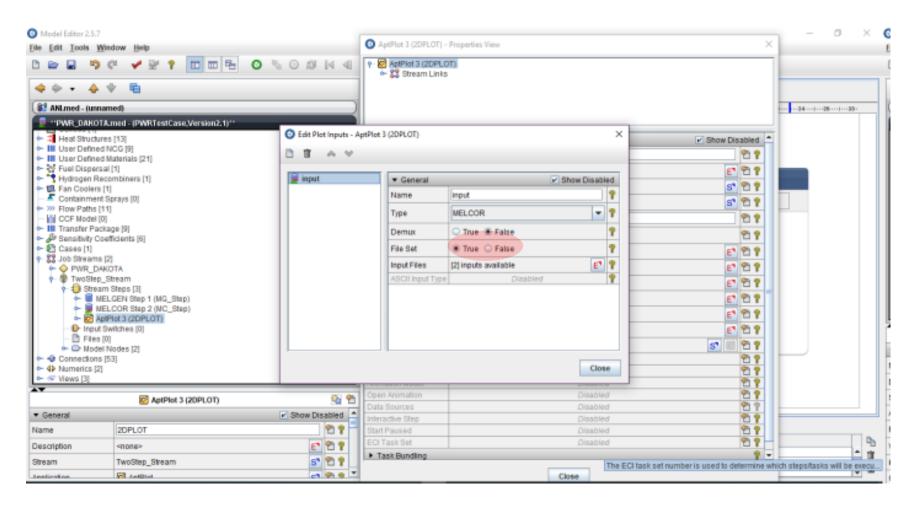


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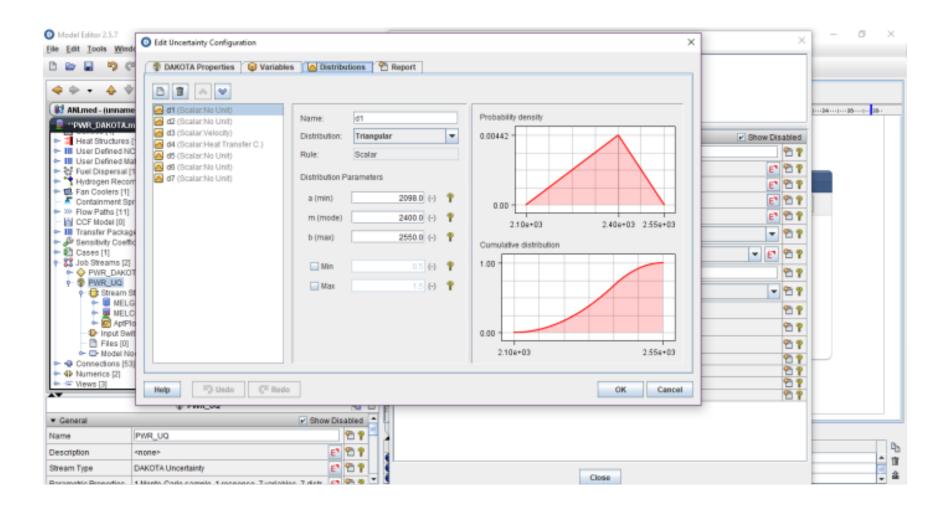


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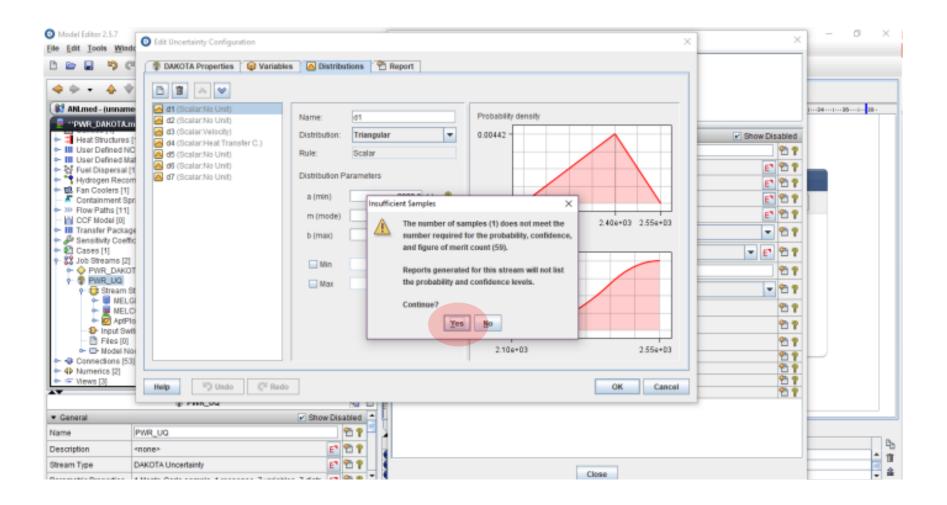


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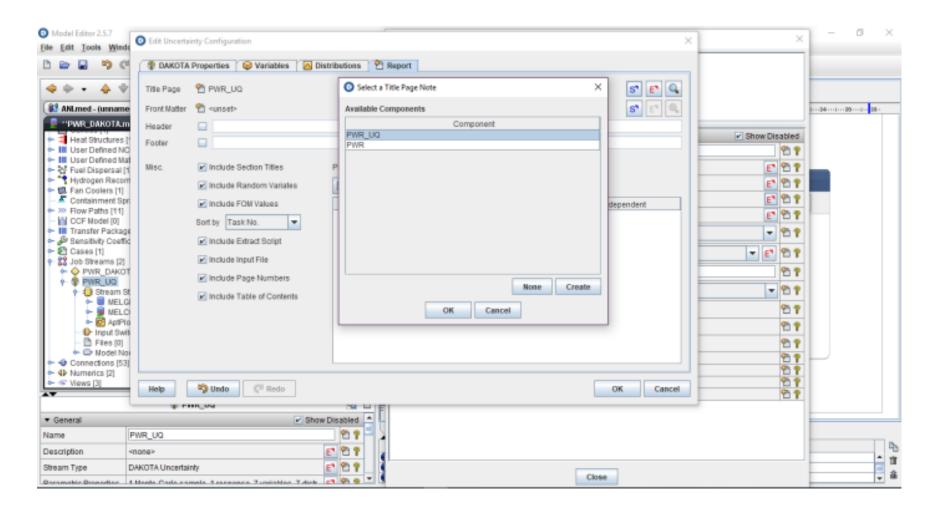


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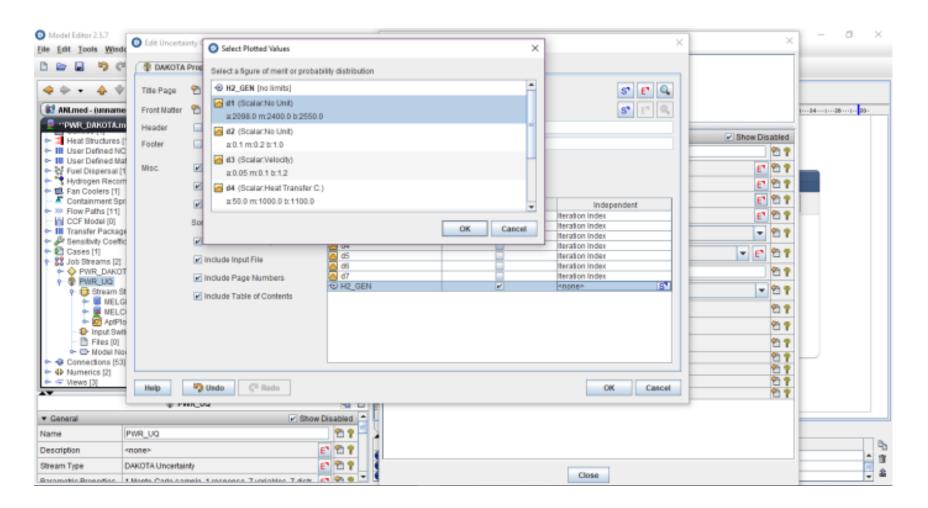


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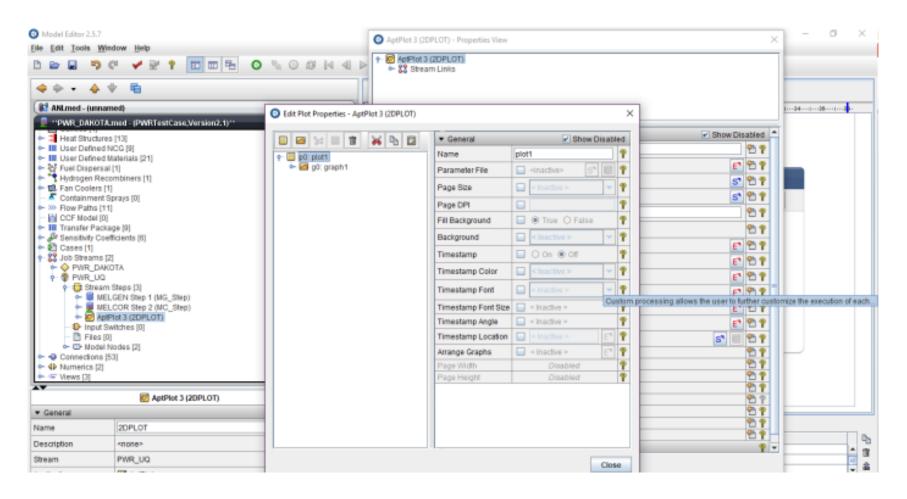
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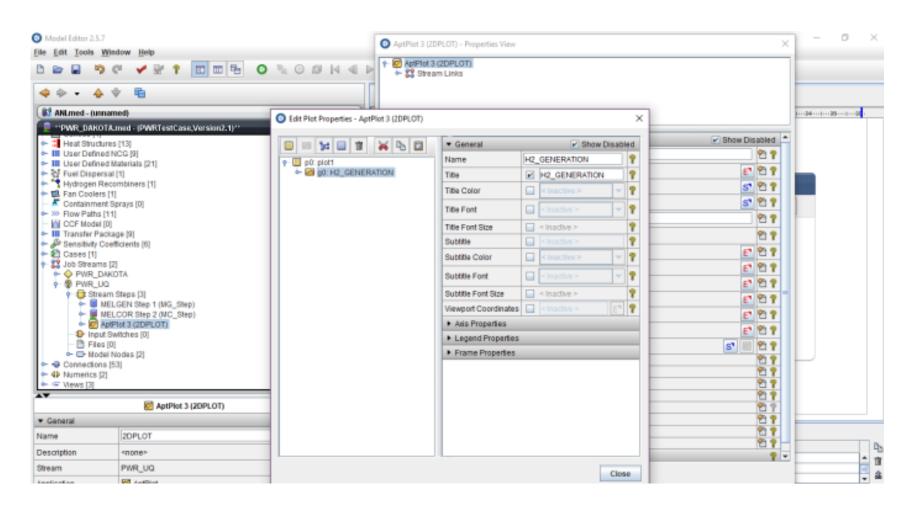
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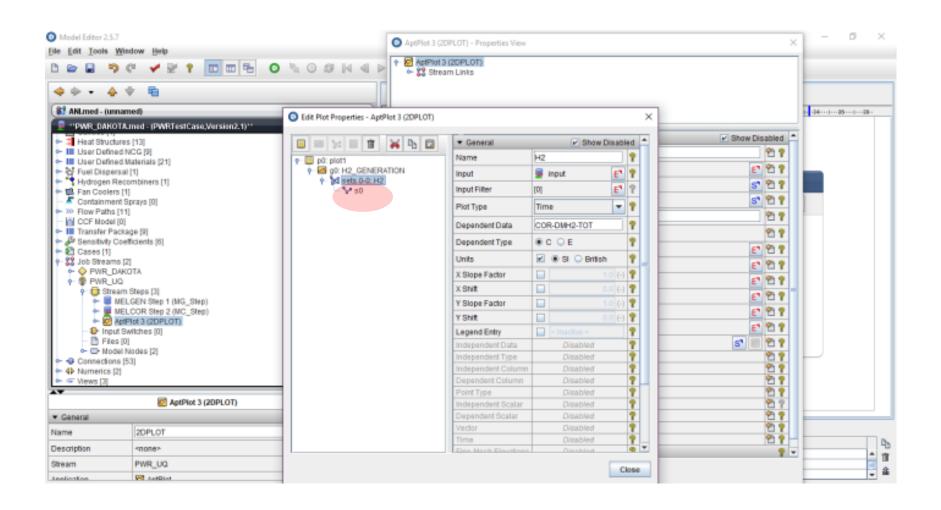
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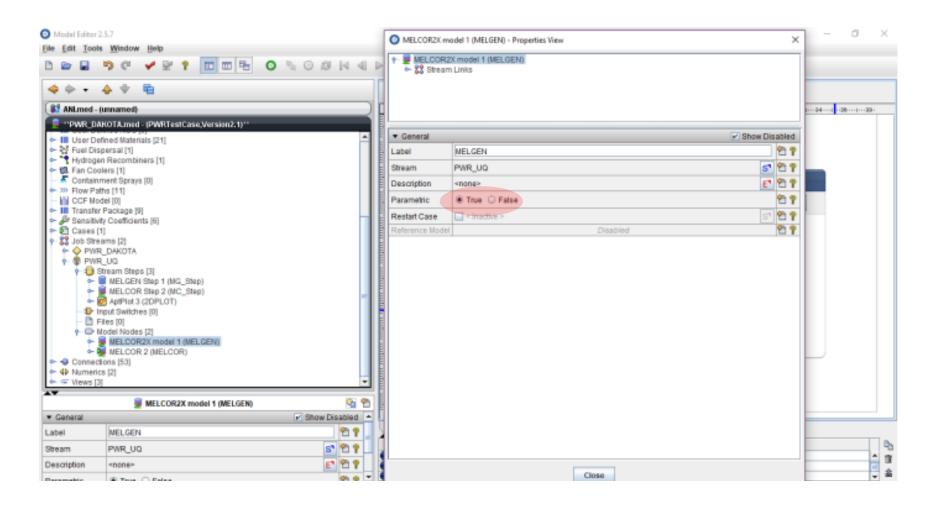




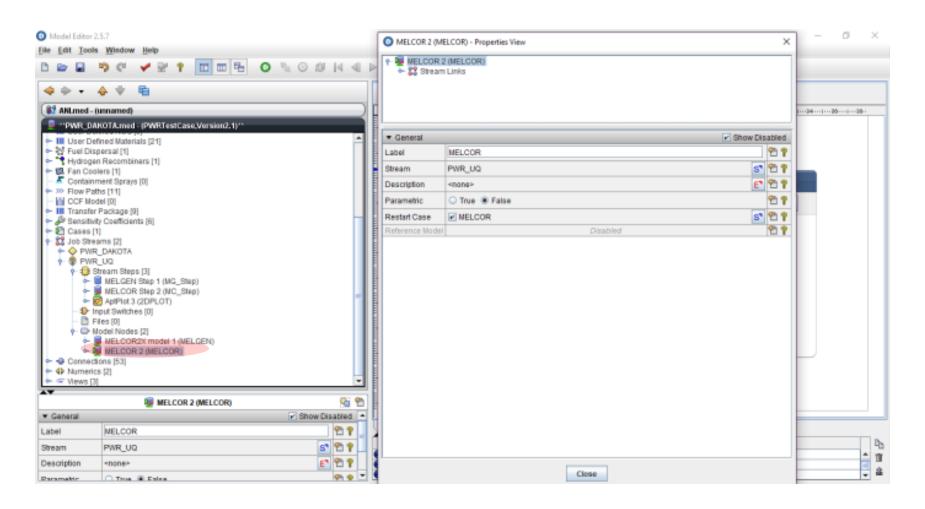


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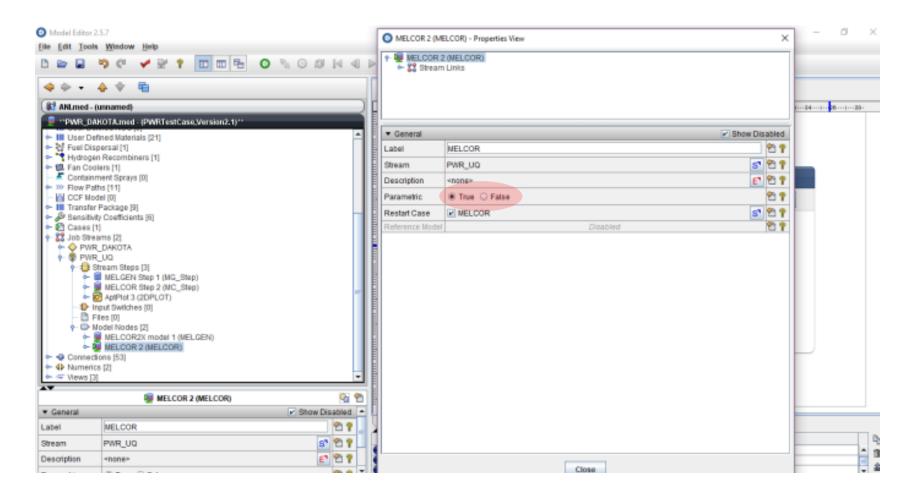




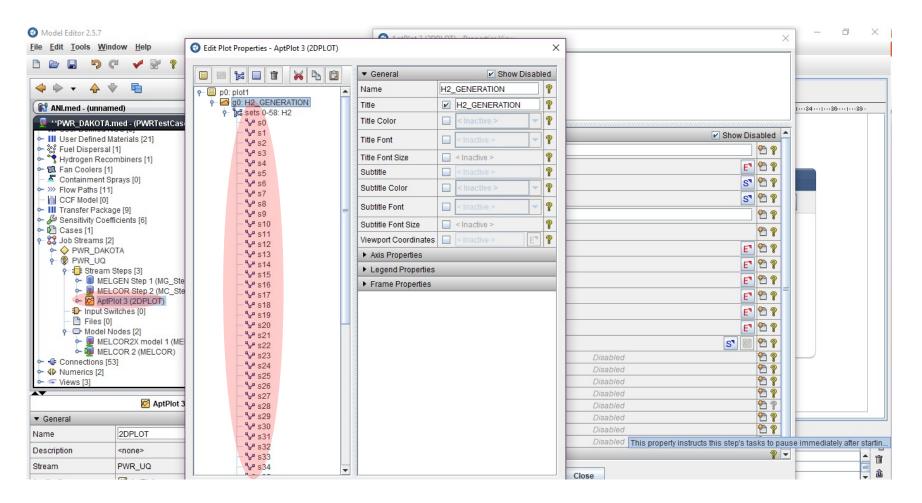








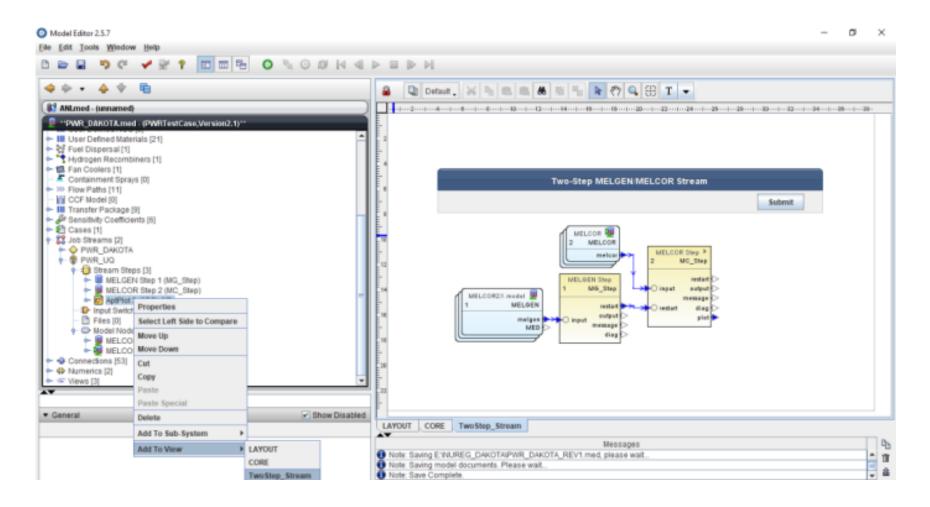




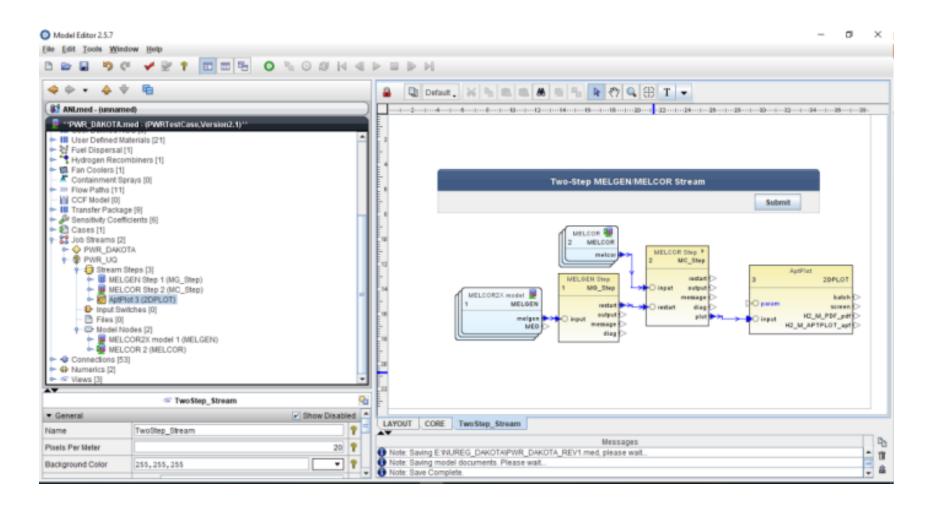


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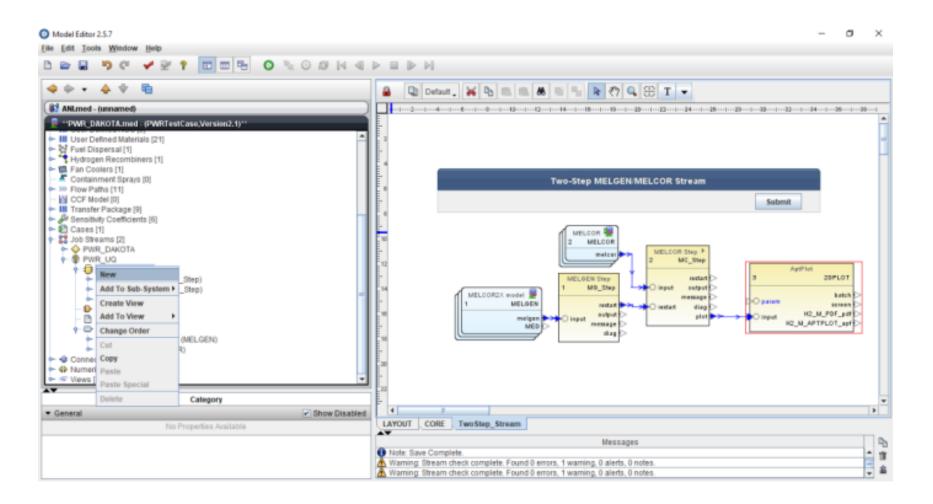




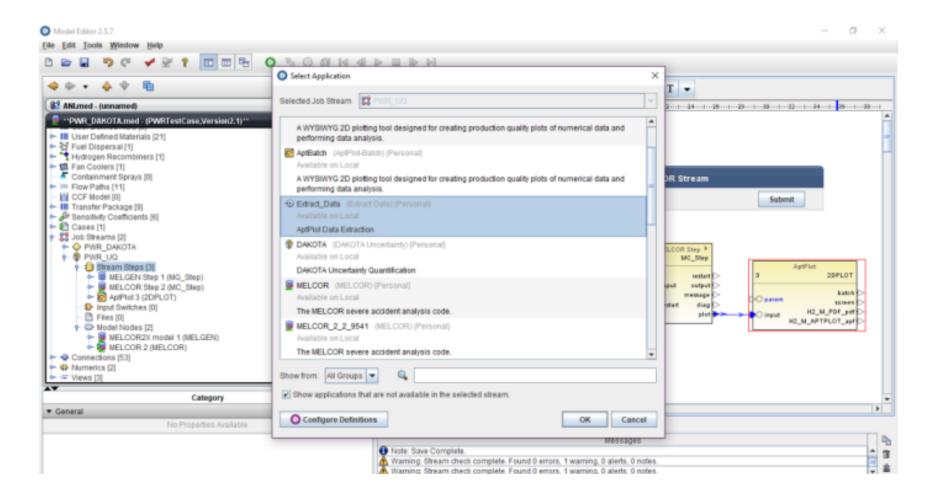












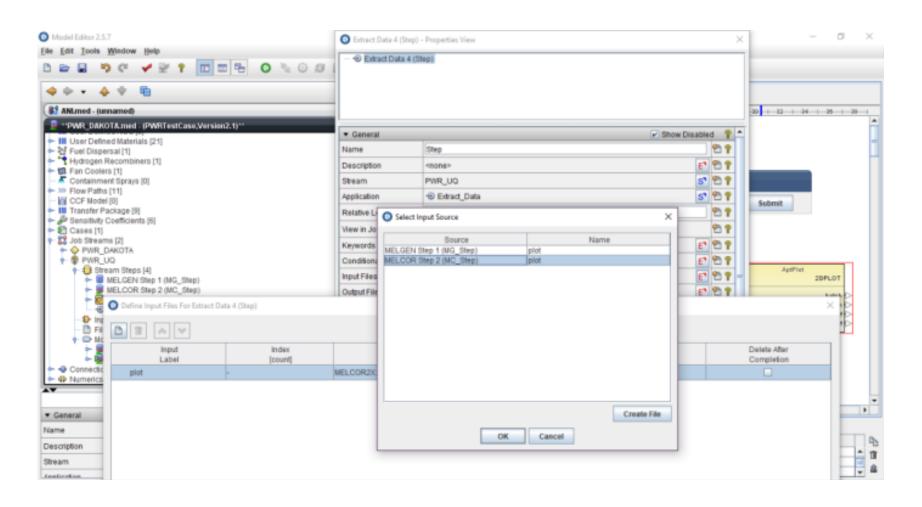


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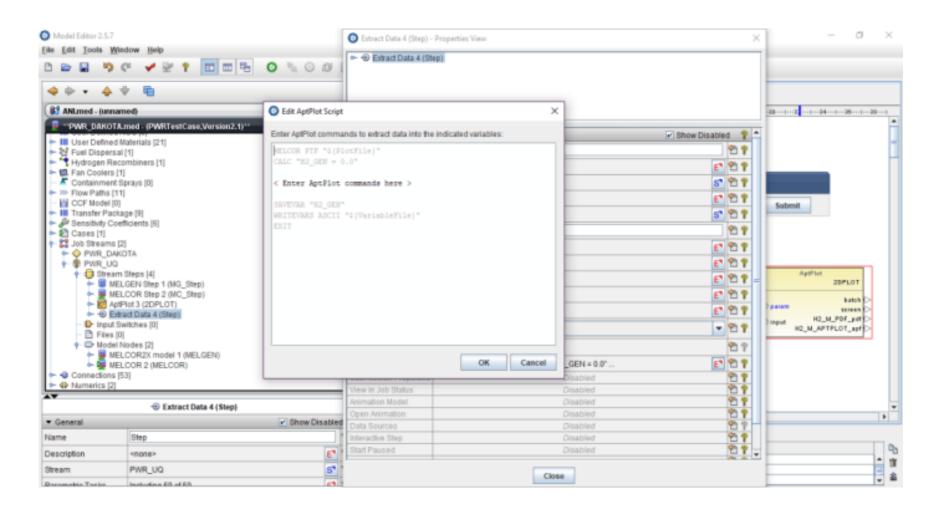


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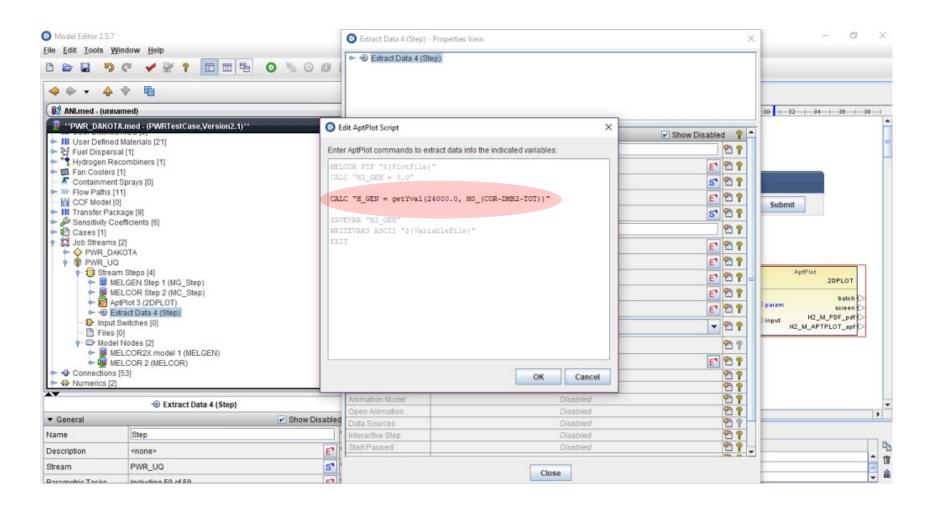


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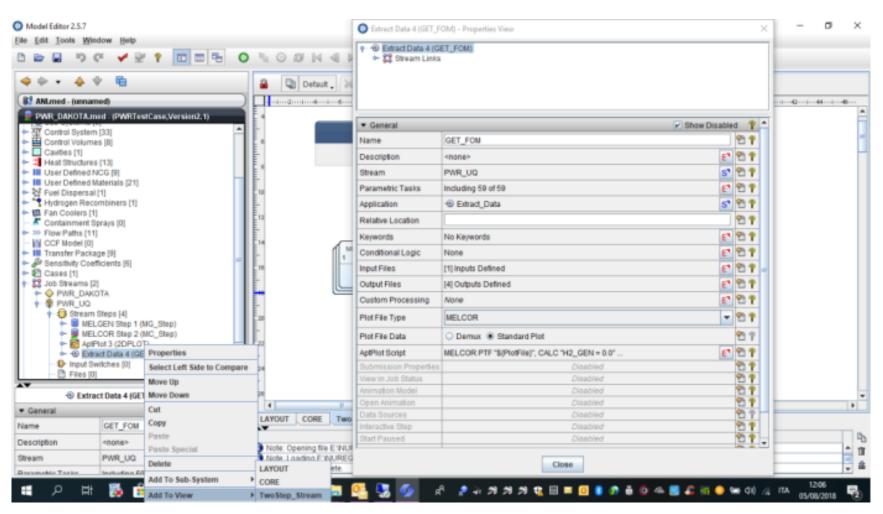




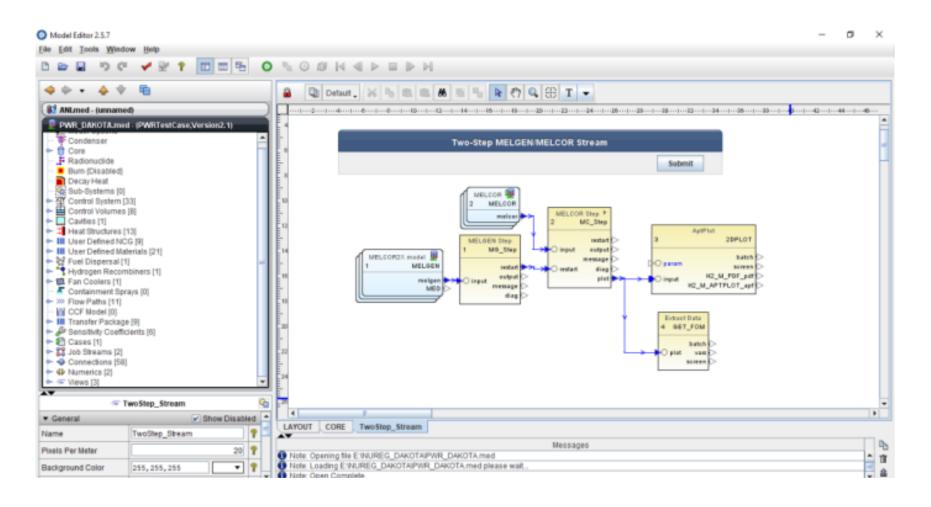








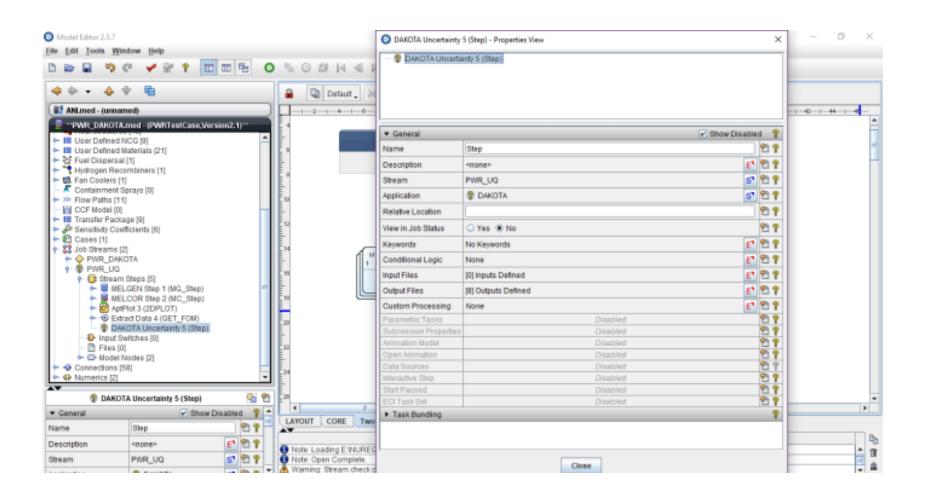




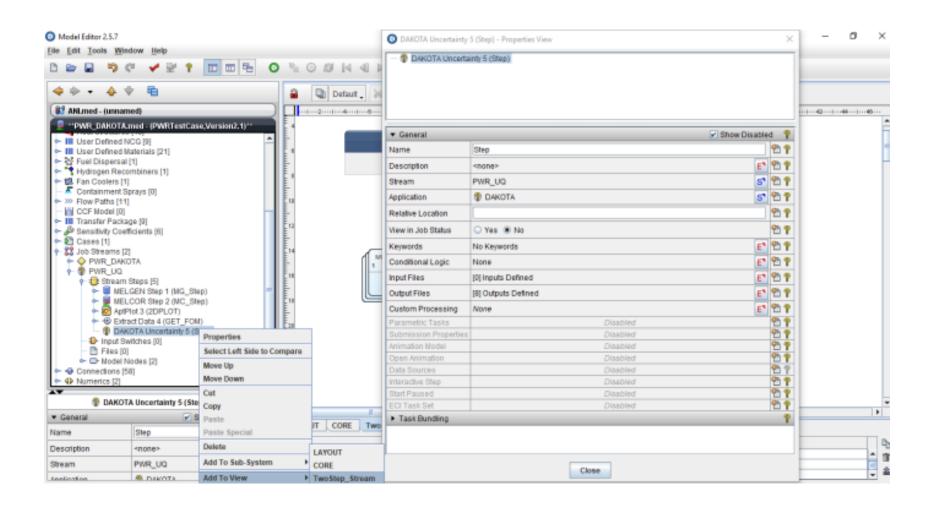


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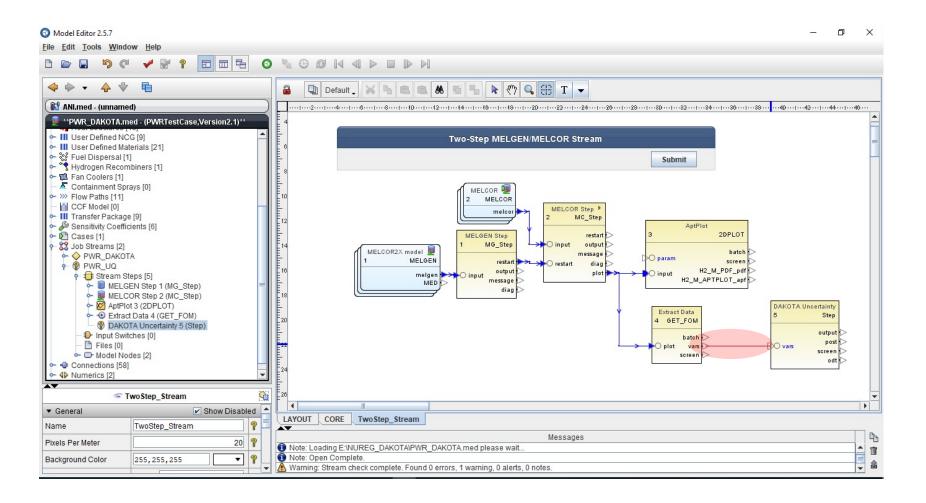




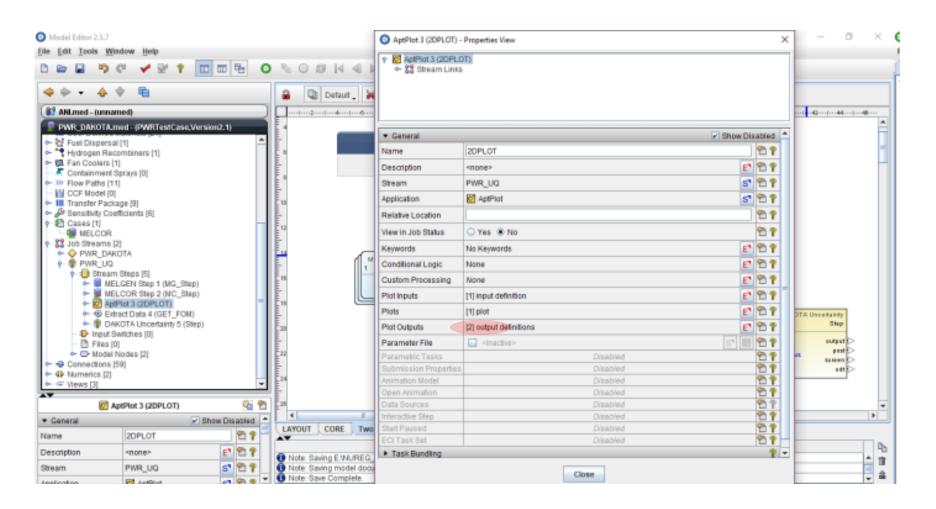


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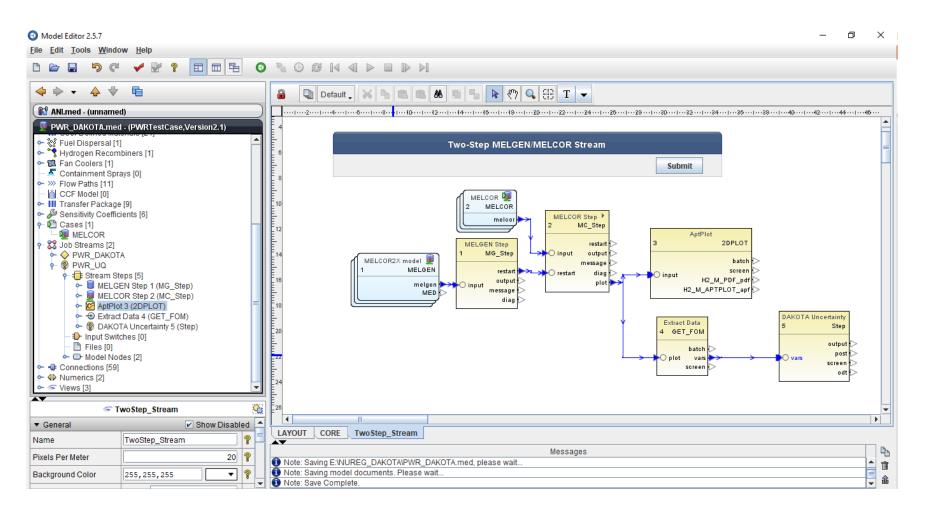




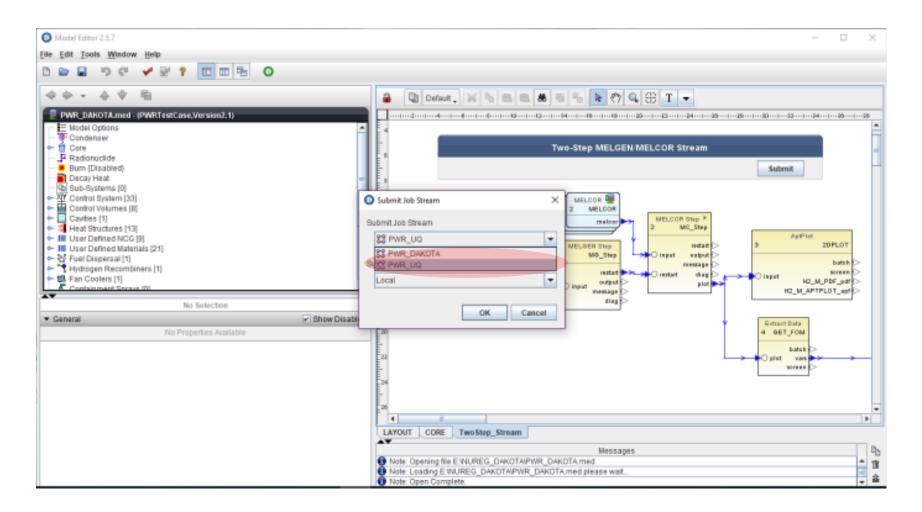




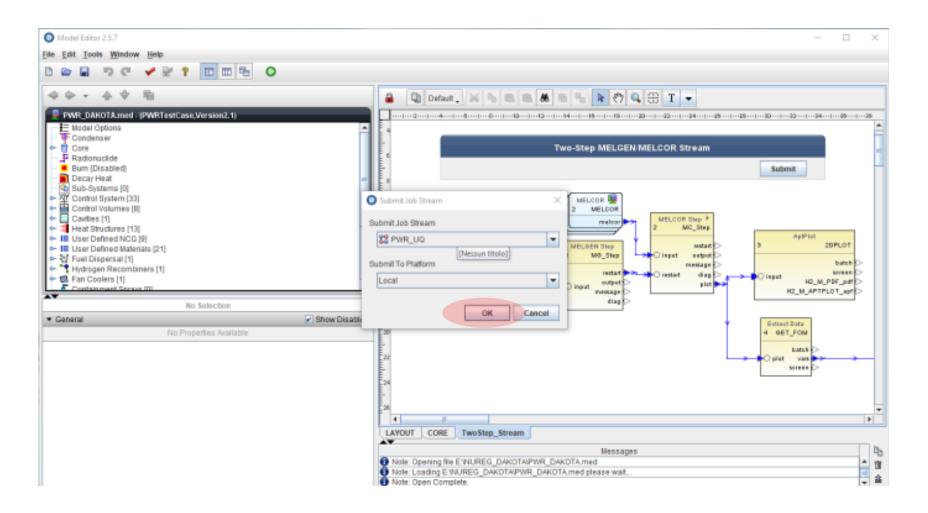










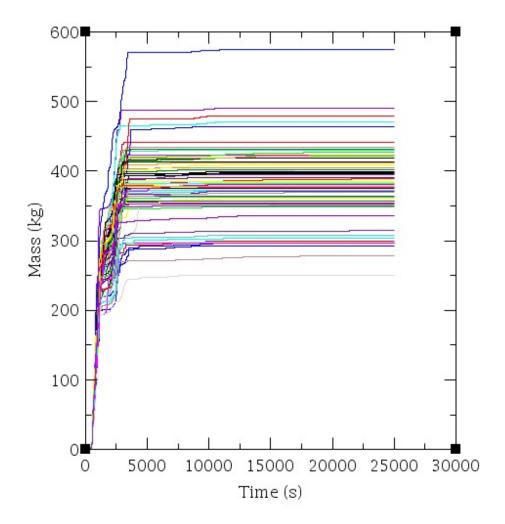




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H2 GENERATION





Statistical Analyses:

Statistical results based on 59 samples:

Summary	Value	Task #
Min Value	250.87505	54
Max Value	574.76666	51
Mean	381.43805	2
Median	382.44507	40
Standard Deviation	56.8461	-
Coefficient of Variance	0.38578	-

Response Correlations

	Simple	Partial	Simple Rank	Partial Rank
d5	0.0979063	0.102384	0.135067	0.268539
d6	0.110172	0.146704	0.0338983	0.0599765
d7	0.098521	0.123725	0.126768	0.209831
d1	0.737284	0.791904	0.765926	0.855157
d2	-0.495872	-0.627241	-0.379486	-0.653184
d3	0.03035	0.00594472	0.0189947	0.0516358
d4	-0.0188159	0.0125986	-0.0151373	0.0108442



Probability Density Function

