NUREG/IA-0532

International Agreement Report

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

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Manuscript Completed: March 2022
Date Published: April 2023

Prepared as part of
The Agreement on Research Participation and Technical Exchange
Under the Cooperative Severe Accident Research Program (CSARP)

Published by
U.S. Nuclear Regulatory Commission

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ABSTRACT

Uncertainty estimation to assess figure-of-merits characterizing evolution of a severe accident transient is a topic of current investigation in development of best-estimate plus uncertainty methodology. The probabilistic method to propagate input uncertainty is one of the methodologies used to develop Uncertainty Analyses (UAs). Using this methodology, UAs are performed by sampling probability distributions that describe the range of possible values that computer simulation model inputs can have. For each sample (or realization) of a set of uncertain input parameters, a computer simulation is performed. From the range of code simulation results obtained for each input realization, a distribution of code results is obtained. In this process, the distribution of input uncertainties is *propagated* to obtain a distribution of possible code results (i.e., the code output uncertainty). This probabilistic methodology is facilitated using Uncertainty Tools (UTs), which can be coupled with the accident analysis computer code to perform an UA. One of the UTs currently available is DAKOTA, developed by Sandia National Laboratories. DAKOTA is also provided as a SNAP plug-in. SNAP is a graphical user interface designed to support the use of USNRC codes. This report demonstrates the workflow within SNAP to assist other interested analysts with their applications given they are members of the USNRC Cooperative Severe Accident Research Program (CSARP). Two sample applications are shown.

FOREWORD

The Best-Estimate Plus Uncertainty (BEPU) approach has become an internationally accepted method for assessing safety margins for a range of high-consequence systems. This approach has increasingly been adopted by the international nuclear energy safety community to characterize the true safety margin and remove analysis conservatisms. Considering the key role of Severe Accidents (SA) codes for deterministic safety analyses and source term evaluations, several research activities in national and international frameworks are currently underway or being planned. These efforts are actively investigating the role that parametric modeling uncertainties play with respect to the evaluation of SA safety issues. In many cases, these SA uncertainty assessments enable more realistic characterization of safety margin. Recent efforts, such as the State-of-the-Art Reactor Consequence Analyses (SOARCA) uncertainty assessments, have identified an overall lower level of risk posed to public health and safety from nuclear power than previously estimated by methods accounting for uncertainties in a bounding manner. In other cases, uncertainty assessments have enabled an integrated perspective on overall importance of uncertainty in various SA models, clarifying where effort to reduce uncertainties will have the greatest impact on estimates of public health and safety risk. To achieve the significant benefits to decision-making through deployment of this SA uncertainty assessment framework, a key need is establishing an analytical platform that automatically couples the Uncertainty Tool (UT) and the SA code. For example, by using the probabilistic sampling method to propagate input uncertainty, UTs require the user to characterize the probability distributions for a set of model input parameters prior to performing any random sampling. This is then followed by a number of steps to prepare the set of input files to the SA code given the sampled input parameters. Finally, the execution of the SA code for each of these inputs file sets is performed. Given the large number of operations required at each step, a user-friendly environment/architecture that permits a direct coupling between the SA code and the UTs is critical. The Symbolic Nuclear Analysis Package (SNAP) provides a very attractive option to achieve a user-friendly and automated coupling of UTs and an SA code. SNAP has been developed to interface with USNRC codes (e.g. MELCOR, TRACE, etc.). It has a user-friendly front end and is thus able to support the code user in the development and visualization of nodalization, as well as direct visualization of selected calculated data. Another feature of SNAP quite helpful for users is its ability to process existing code inputs not prepared using SNAP. Since SNAP is able to couple US Nuclear Regulatory Commission (USNRC) computer codes with the DAKOTA toolkit, it provides a very powerful, and user-friendly platform capable of coupling an SA code such as MELCOR with a UT such as DAKOTA. Through SNAP, it is possible to set up the DAKOTA uncertainty analysis and to automatically perform all the steps required to complete a code uncertainty assessment. The target of this report is to show the main details of the MELCOR/DAKOTA coupling in a SNAP environment/architecture, and the different steps necessary to set it up. In addition, some example applications are presented to illustrate the benefits of process involved in this coupling. The current study is performed under the USNRC Cooperative Severe Accident Research Program (CSARP) framework; it also includes one of the output of the activities done in the framework of the Work Package 4 (Application of Uncertainty Quantification Methods against Integral Experiments – AUQMIE -) of the MUSA H2020 EURATOM project. It will be generally beneficial to MELCOR users as well as current and future international initiatives.

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EXECUTIVE SUMMARY

This report describes an approach, and the use of associated tools, to efficiently conduct SA uncertainty analyses. Such analyses are increasingly supporting a range of safety cases and regulatory assessments for current and next generation Nuclear Power Plants (NPP). An impediment to a broader application of UA remains knowledge of the application of methods and available tools. This report fills a critical gap in the body-of-knowledge related to the practical application of methods and use of available tools by a broader community of analysts. The focus of this report is on establishing an approach that is accessible to the broadest range of analysts, reducing significantly existing barriers facing analysts required to conduct a SA uncertainty study.

Nuclear regulatory authorities ensure that the operation of a range of nuclear facilities does not introduce an unacceptable additional level of risk to public health and safety relative to other societal activities. The United States Nuclear Regulatory Commission (USNRC) regulates nuclear power facilities according to a set of two qualitative safety goals and two supporting quantitative safety objectives. These supporting objectives were developed to ensure that nuclear risks are not a significant addition to other societal risks. The qualitative safety goals against which the USNRC evaluates a range of activities in the United States are [51 FR 28044].[1]

- *Individual members of the public should be provided a level of protection from the consequences of nuclear power plant operation such that individuals bear no significant additional risk to life and health*
- *Societal risks of life and health from nuclear power plant operation should be comparable to or less than the risks of generating electricity by viable competing technologies and should not be a significant addition to other societal risks*

Derived from these qualitative safety goals are the following quantitative safety objectives intended to measure achievement of these safety goals [51 FR 28044]

- *The risk to an average individual in the vicinity of a nuclear power plant of prompt fatalities that might result from reactor accidents should not exceed on-tenth of one percent (0.1 percent) of the sum of prompt fatality risks resulting from other accidents to which members of the U.S. population are generally exposed*
- *The risk to the population in the area near a nuclear power plant of cancer fatalities that might result from nuclear power plant operation should not exeed one-tenth of one percent (0.1 percent) of the sum of cancer fatality risks results from all other causes*

NPP design follows a defense-in-depth strategy to ensure that a number of layers of protection exist, providing natural and engineered measures to limit escalation of consequences to a level severe enough to challenge life and health. This approach ensures that overall NPP risk is low, with derived performance criteria for engineering systems intended to provide robust margin to reaching a level of consequence (i.e., radiological release to the environment) that could lead to either prompt or cancer fatalities.

Traditional safety analysis methods for evaluation of plant performance under normal and off-normal conditions, up to and including Design Basis Accidents (DBAs), are intended to demonstrate achievement of these derived performance criteria. In the original licensing of many Light Water Reactor (LWR) power plants operating in the United States and internationally, conservatisms were incorporated in these analysis methods. These

[1] 51 FR 28044, Safety Goals for the Operation of Nuclear Power Plants (1986).

conservatisms ensured that, despite prevailing *uncertainties* in analytical characterization of plant performance under off-normal and accident conditions, sufficient safety margin would be incorporated into the design and robust plant performance could be achieved, even under the most severe conditions within the plant's design envelope.

With advances in a) knowledge of phenomena and processes governing plant behavior under off-normal and accident conditions, and b) computational and safety analysis methods, it is now possible to more completely characterize the impact of uncertainties on safety margin. This has led to the development of a new class of safety analysis methods that are commonly referred to as Best Estimate Plus Uncertainty (BEPU). These methods all generally focus on establishing best estimate conditions associated with

- Initial plant conditions;
- Boundary conditions not explicitly modeled by the analysis, but necessary to define any coupling of assessed systems to the environment external to the analyzed system;
- Parameters governing models of physical processes or phenomena necessary to describe performance of systems under off-normal conditions;
- Performance limits for engineered systems, structures or components necessary to maintain overall plant response under off-normal conditions.

With respect to each of these classes of conditions or parameters, BEPU methods then establish a range of variability introduced by uncertainty in the *true* values. Such variability is typically characterized as a probability distribution such that the best estimate condition or parameter represents the distribution's 50^{th} percentile. BEPU methods all are intended to propagate these uncertainties through an analysis to establish an estimate for the best estimate (50^{th} percentile) safety margin and the probability that given uncertainty safety margin could be lost.

BEPU methods are examples of uncertainty quantification intended to characterize overall performance margins for an engineered system. Since these methods are focused on evaluating performance of an engineered system to prevent undesirable conditions, the overall system remains in a *controlled* condition (i.e., within its design envelope). In this manner, performance of the engineered system ensures that a NPP will not enter into a state where there is a potential for harm to life and health.

A robust design basis, however, only ensures that the potential for more severe consequences to arise is low (i.e., the probability of the design basis being exceeded is low). There still exists a very low probability that a beyond design basis accident with more severe consequences could evolve. This *residual* risk must be established to comply with the supporting quantitative safety objectives introduced above. The estimation of the level of residual risk requires assessment of accidents that lead to more severe consequences due to exceeding the design basis for the power plant. In most cases, severe NPP accidents involve significant disruption to the structural integrity of nuclear fuel in a reactor, or other on-site sources of radiological material such as spent nuclear fuel.

The knowledge-base of nuclear power plant accident and SA phenomena has developed significantly since the early Probabilistic Risk Assessments (PRAs), such as WASH-1400[2], and the Three Mile Island-Unit 2 (TMI-2) accident. This knowledge-base has been incorporated into a number of integral plant response accident analysis computer codes developed globally (e.g.,

[2] WASH-1400, 'The Reactor Safety Study' (1975).

ASTEC, MAAP, MELCOR). These codes couple thermal-hydraulics and the SA phenomena into an integral computer code capable of performing the transient analysis of postulated accidents. These codes compute relevant Figures-Of-Merit (FOMs) utilized in safety and risk-informed decision-making processes regarding Beyond Design Basis Accidents (BDBA). Examples of such FOMs include key event timings and the timing, magnitude, and duration of radiological releases to the environment.

Over the past 20 years, the SA knowledge-base and integral plant response computer codes have achieved a significant level of maturity. While substantial uncertainties still remain in some areas, the understanding of and ability to quantitatively model the broad spectrum of SA phenomena has enabled the application of SA computer code analysis to resolution of a broad range of BDBA safety issues. This has been exemplified most recently by the application of codes such as MELCOR and MAAP to resolution of post-Fukushima safety issues. An important element of these issue resolutions was consideration of the impact of uncertainties on quantitative estimates (e.g., FOMs) utilized as part of the overall decision-making process. While still under active development, significant interest has developed in the area of characterizing uncertainties in SA analyses.

This report demonstrates a methodology for performing analyses commonly needed to support a parametric studies or UAs by applying codes developed by the USNRC. The method described in this report is based on standard BEPU methods developed for design basis safety margin assessments. The overall method integrates the following components:

- A systems analysis, or integral plant response, computer code performing transient accident analysis. TRACE is an example of a computer code utilized for systems thermal-hydraulic analysis. MELCOR by contrast is an integral plant response analysis code that integrates the broad spectrum of phenomena and processes that are relevant to assessment of plant behavior under BDBA conditions. In this report, MELCOR is used to perform SA analyses. It is available through the USNRC Cooperative Severe Accident Research Program (CSARP)[3].

- An Uncertainty Tool (UT) that facilitates the propagation of uncertainties in the inputs defining a transient accident analysis to characterize uncertainty in code-calculated FOMs. The optimization and uncertainty quantification toolkit called DAKOTA, developed by Sandia National Laboratories (SNL), is an example of a commonly used UT that is adopted in this report. It is used in this report to create a pre-determined number of MELCOR accident analysis code calculations (i.e., the MELCOR input-decks with different realizations of uncertain input parameters). Each accident analysis code calculation input-deck is generated through a random sampling of input parameter probability distributions, which is performed by DAKOTA. Finally, statistical analysis methods available in DAKOTA are utilized to perform a number of statistical and correlation analyses of selected FOMs.

- A front-end application that couples the transient accident analysis code with the UT to orchestrate the overall uncertainty study. The Symbolic Nuclear Analysis Package (SNAP), developed by the USNRC for use with its nuclear analysis codes, is adopted in this report to perform the coupling between the MELCOR SA analysis code and DAKOTA. SNAP makes the appropriate calls to DAKOTA to perform the generation of

[3] Cooperative Severe Accident Research Program (CSARP)(NUREG/BR-0524) (2015). https://www.nrc.gov/reading-rm/doc-collections/nuregs/brochures/br0524/index.html.

MELCOR inputs for each accident case realization, then executes MELCOR for each of the realized input cases, and finally calls DAKOTA to perform the necessary post-processing to generate a range of statistical and correlation analyses of FOMs.

The report is organized as follows:

- Section 2 of this report describes the DAKOTA uncertainty analysis workflow in the SNAP environment/architecture for MELCOR applications. Firstly, DAKOTA is used to sample the uncertain input parameter values and to generate the set of model inputs. Then, after the solution of the set of code inputs and the extraction of the desired data, DAKOTA performs the UA and computes correlation coefficients to characterize the relation between the selected uncertain input parameters and the output selected as a FOMs. This is performed through a second application of DAKOTA.

- In Section 3 of this report, the different steps necessary to create the MELCOR/DAKOTA analyses within the SNAP environment/architecture are described. In particular the creation of DAKOTA Uncertainty Job Stream for a Two-Step MELGEN/MELCOR Stream, the definition of the DAKOTA application properties, the characterization of the Probability Density Function (PDF), the set-up of the automatically generated report, the definition of the Plotting Step properties, the creation and set-up of the Data Extraction and of a further DAKOTA Uncertainty Step, and the execution of the UA is described in detail.

- In section 4, the report automatically generated by DAKOTA is described. In particular the uncertainty quantification input options, the variate and response data section, DAKOTA Results, and the response correlation are described in detail.

- In section 5 of this report, two MELCOR/DAKOTA uncertainty studies are reported. In particular these studies represent only the first exercises intending to show the complete application of the coupling procedure of MELCOR and DAKOTA in the SNAP environment/architecture. These studies show the feasibility of the MELCOR/DAKOTA coupling, the support capabilities such as automated report generation, and the advantage of a streamline application through the SNAP platform for performing UAs. It should be noted that the purpose of this work is not to represent a complete or representative analysis of the MELCOR code uncertainty. Also, the selected uncertain input parameters and related PDFs are only chosen for methodology demonstration purposes. In order to have indication about the range and PDF of selected uncertainty input parameters the SOARCA studies can be considered by the reader[4].

- In section 6 the conclusions are summarized.

- In Appendix A the new Python directed job-stream capability in SNAP is presented. This approach can be used to overcome the current limitations of the SNAP/GUI in the case of failed calculations.

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[4] State-of-the-Art Reactor Consequence Analyses Project, Uncertainty Analysis of the Unmitigated Short-Term Station, Blackout of the Surry Power Station, Draft Report, https://www.nrc.gov/docs/ML1522/ML15224A001.pdf.

State-of-the-Art Reactor Consequence Analyses Project Uncertainty Analysis of the Unmitigated Long-Term Station Blackout of the Peach Bottom Atomic Power Station, NUREG/CR-7155 SAND2012-10702P, Draft Report, https://www.nrc.gov/docs/ML1318/ML13189A145.pdf.

ACKNOWLEDGMENTS

Special thanks to USNRC for their comments during the preparation of this document.

Part of the activity has been conducted in the framework of the MUSA project.
This project has received funding from the Euratom research and training programme 2014-2018 under grant agreement No 847441.

ABBREVIATIONS AND ACRONYMS

ASTEC	Accident Source Term Evaluation Code
BDBA	Beyond Design Basis Accident
BE	Best Estimate
BEPU	Best Estimate Plus Uncertainty
CDF	Cumulative Distribution Function
CRP	Coordinate Research Project
CSARP	Cooperative Severe Accident Research Program
DAKOTA	Design Analysis Kit for Optimization and Terascale Application
DBA	Design Basis Accident
EMUG	European MELCOR User Group
ENEA	Agenzia nazionale per le nuove tecnologie, l'energia e lo sviluppo economico sostenibile
FOM	Figure of Merit
IAEA	International Atomic Energy Agency
LWR	Light Water Reactor
MAAP	Modular Accident Analysis Program
MELCOR	Methods of Estimation of Leakages and Consequences of Releases
MUSA	Management And Uncertainties Of Severe Accidents
NPP	Nuclear Power Plant
PDF	Probability Density Function
PRA	Probabilistic Risk Assessment
PWR	Pressurized Water Reactor
RELAP	Reactor Excursion and Leak Analysis Program
SA	Severe Accident
SAMG	Severe Accident Management Guidelines
SNAP	Symbolic Nuclear Analysis Package
SNL	Sandia National Laboratories
SOARCA	State-of-the-Art Reactor Consequence Analyses
TRACE	TRAC/RELAP Advanced Computational Engine
UA	Uncertainty Analysis
USNRC	U. S. Nuclear Regulatory Commission
UT	Uncertainty Tool

1 INTRODUCTION

Considering the complexity of and the numerous interacting/ interrelated phenomena/processes that occur during the course of SA evolution, state-of-the-art SA integral codes [1,2,3] have come to play an important role in understanding overall plant behavior. Codes such as ASTEC [4], MAAP [5], and MELCOR [6] are relied on in the U.S. and internationally to evaluation accident progression and determine characteristics of radiological release to the environment. These analytical capabilities enable determination of the main FOMs utilized in a range of safety case development and regulatory decision-making applications. These capabilities have also been used to inform and evaluate accident management strategies.

Several models/correlations have been implemented in state-of-the-art SA codes and have to be set by a code user during input deck development. Models/correlations that are implemented in an SA code reflect state-of-the-art knowledge of severe phenomena/processes, even though several experimental campaigns in the field of SA phenomena [7-11] have been performed and provided valuable "assessment database" [12] to assess SA simulation tools, the analyses of the current State-of-the-Art shows that there is need to reduce some uncertainties[5] still present [1,13], and a consequent investigation of phenomena/processes, to date not investigated in detail in geometric prototypical experimental facility with prototypical material, should be addressed. Therefore, discrepancies in some of the core degradation phenomena can be still observed when comparing the results as predicted by different SA simulation tools considering the different core degradation models implemented in the codes [1,14].

Considering the need to reduce and/or evaluate some uncertainties still present and considering the reached level of development and maturity of SA codes and their application in the assessment of SAMG, the discussion and application of SA progression analyses with uncertainty estimation is currently a key topic in the BEPU framework [15,16]. Today, in fact, for the evaluation of the safety margins, the use of BEPU approach by coupling selected calculated parameters with the related uncertainty range is of great interest for the International Scientific Community [15]. Considering the key role of 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 two main activities are currently in progress: the Management and Uncertainties Of Severe Accidents (MUSA) project [17, 46], founded in Horizon 2020 EURATOM NFRP-2018-1- Safety assessments to improve accident management strategies for Generation II & III reactors, and the IAEA CRP on "Advancing the State-of-Practice in Uncertainty and Sensitivity Methodologies for Severe Accident Analysis in Water Cooled Reactors (I31033) [18].

In this framework, as already underlined in [19], from an operative point of view, one of the key needs is to have an automatically coupling between the UT and the SA code. For example, by

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[5] Uncertainty is used as a measure of the error made with the code in predicting the plant behavior [12]. In general, the sources of uncertainty can be grouped in [20]:

- Code uncertainty (e.g. approximations in the conservation equation and in the closure models and correlations);
- Representation uncertainty (nodalization effect);
- Scaling issue (codes validated against scaled-down facilities);
- Plant uncertainty (e.g. initial and boundary conditions);
- User effect.

using the probabilistic method to propagate input uncertainty[6] [20], the UTs will perform several steps (e.g. creation of a certain number of code runs obtained combining the input uncertain parameters selected by the user through a random sampling, statistical and correlation analysis of the selected FOMs, etc.) and several parameters should be selected by the user (selection of PDF type and parameters, selection of the random sampling methods, selection of correlation coefficients for the analyses, etc.) for setting the UA. Therefore, the use of a user-friendly environment/architecture, which permits a direct coupling between the SA code and the UT, for characterizing the UA and to perform all the uncertainty steps, is one of key operative needs.

Within this regard, USNRC codes (e.g. MELCOR [6], TRACE [21]) can be used together with a user-friendly front end, SNAP [22], able to support the user in the development and visualization of the nodalization, to show a direct visualization of selected calculated data, and to accept existing code input. SNAP is a suite of integrated applications including the Model Editor, the Job Status, the Configuration Tool client applications and the 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 [23,24].

One of the features of SNAP, of current interest for the International Technical Community, is to give the possibility of coupling USNRC codes with the DAKOTA toolkit [22,25]. DAKOTA, in fact, is provided as a plug-in [25] in SNAP, and through SNAP it is possible to set up the DAKOTA uncertainty analysis [25,26,27] and to perform automatically all the steps of the UA.

Considering that currently the International Nuclear Technical Community is exploring the possibility of using SA codes in a BEPU framework, the target of this report is to show the main details of the MELCOR/DAKOTA coupling in a SNAP environment/architecture, and the different steps necessary to set it up. Two sample applications have been presented to show the feasibility of the MELCOR/DAKOTA coupling, to analyze the capabilities of this coupling, and the great advantage to use SNAP to perform the UA.

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[6] Several methodologies have been developed in the past to perform UA, and they can be grouped in:

- Methods to propagate input uncertainty:
    - Probabilistic (e.g. CSAU, GRS, IPSN, etc.);
    - Deterministic (e.g. AEAW, EDF-Framatome, etc.);
- Method to extrapolate output uncertainty (e.g. UMAE) [20].

2 MELCOR/DAKOTA COUPLING IN A SNAP ENVIRONMENT/ARCHITECTURE

2.1 Propagation of Computer Code Model Input Parameter Uncertainties

The probabilistic method to propagate input uncertainty [28], through the random sampling, is a common approach to propagating computer code model input parameter uncertainties. In this approach, the following steps are involved:

- Identify the uncertain input parameters necessary to characterize the model used by the computer code for transient analysis;
- Define the plausible random variability of each input parameter by defining a Probability Density Function (PDF);
- Generate N random realizations (i.e., input for code runs) by randomly generating an input value for each input parameter by sampling from its PDF;
- Create code inputs for each realization of input parameters;
- Execute each of the N code inputs;
- Process code results generated from running the N input code realizations to:
  - Characterize the range of realized variation for selected FOMs;
  - Correlate realized variability in FOMs with the uncertain input parameters to assess the contribution of the different input uncertainties to code output uncertainty.

2.2 DAKOTA Toolkit

DAKOTA (Design Analysis Kit for Optimization and Terascale Application) [29-32] is an open source software written in C++ and developed by Sandia National Laboratories (SNL) to perform sensitivity analysis, optimization, parameter estimation, parametric and UA in a fast and automatic way.

The DAKOTA toolkit is also provided as a plug-in [25] for SNAP [22], which is a graphical user interface designed to support the use of USNRC computer 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 SNAP's animation capability [1,23,24,33]. Through SNAP it is possible to set up a DAKOTA UA [22,25,27] and to perform all analytical steps automatically.

Figure 2-1 shows a schematic representation of a DAKOTA UA workflow within SNAP for MELCOR applications. Figure 2-2 shows the equivalent MELCOR/DAKOTA Uncertainty Job Stream within SNAP.

The DAKOTA plugin allows the following:

1) Enter the uncertain input parameters with their range and PDF,
2) Select the sampling method (direct Monte Carlo sampling or Latin Hypercube stratified sampling[7]),

[7] Direct Monte Carlo sampling is generally effective at adequately generating realizations of input parameters when a large number of samples are used. When a more limited number of samples are being used, Latin Hypercube stratified sampling is generally recommended because it ensures that input parameters will be sampled from the tails of each input parameter's PDF.

3) Enter the desired FOMs for the analysis, and
4) 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. Then, 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 UA and to characterize the relationship between input uncertain parameters and output parameters selected as FOMs.

Starting from the reference MELCOR input model, the selected uncertain input parameters (together with their range and PDF), and the FOMs, DAKOTA samples the uncertain input parameters creating a set of N MELGEN and MELCOR inputs. The minimum number of code runs, N, depends on the requested probability 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 the well-known Wilks formula [34][35], by solving the following equation with respect to N:

$$1 - \alpha^N = \beta \qquad \text{Eq. 1}$$

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 [36]:

$$\beta = \sum_{j=0}^{N-p} \frac{N!}{(N-j)!\,j!} \alpha^j (1-\alpha)^{N-j} \qquad \text{Eq. 2}$$

where p is the number of FOMs. More information on statistical aspects of traditional best estimate plus uncertainty analysis can be found in [37].

In the following sections, the different steps necessary to define the UA in a DAKOTA application in SNAP are described.

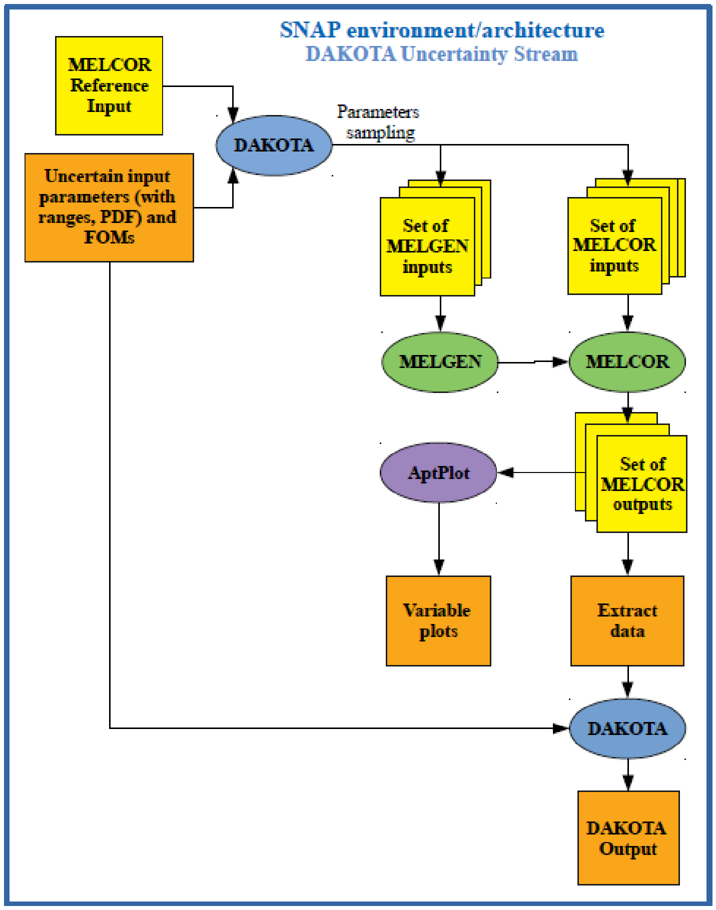

Figure 2-1 DAKOTA Uncertainty Analysis Workflow for MELCOR Code in a SNAP Environment/Architecture

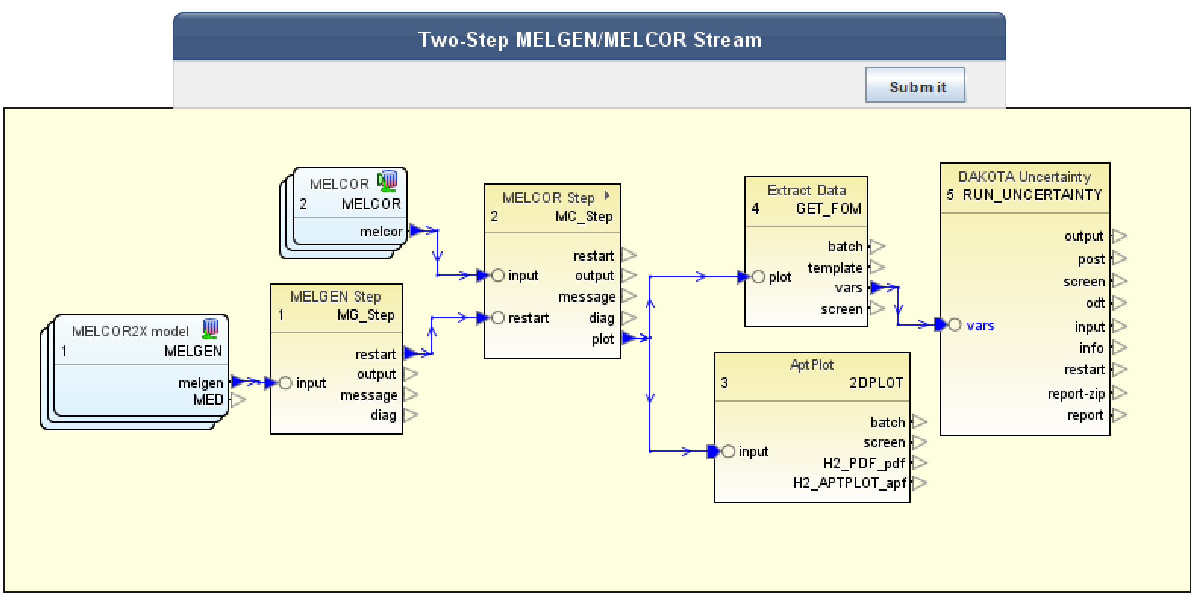

Figure 2-2 MELCOR/DAKOTA Uncertainty Job Stream Done in SNAP

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

In this section the primary steps to setup an UA with MELCOR and DAKOTA in the SNAP environment/architecture are presented. The base of this tutorial has been created in the 2018 with the SNAP Model Editor 2.5.7, by ENEA for preparing some explorative applications of MELCOR/DAKOTA coupling in a SNAP environment/architecture. The first tutorial information was shared by ENEA to USNRC and SNL [38].

3.1 Creation of DAKOTA Uncertainty Job Stream for a Two-Step MELGEN/MELCOR Stream

The first step is the creation of a new DAKOTA Uncertainty Job Stream that contains the MELCOR/MELGEN steps.

- In the *SNAP Model Editor* (Figure 3-1), right-click on *Job Streams*
- After right-clicking *Job Streams*, select *New* (Figure 3-2)
- From the *Job Stream* list, select *DAKOTA Uncertainty* (Figure 3-3)
- Within *DAKOTA Uncertainty*, select the *Two-Step MELGEN/MELCOR Stream* (Figure 3-4)[8].

A *Job Stream* with a basic configuration is automatically created. At this stage, it is now possible to view the job stream in a dedicated view (Figure 3-5).

3.1.1 Selection of MELGEN and MELCOR Executable

The next step is to select the MELGEN and MELCOR executables to be used in the *DAKOTA Uncertainty Job Stream*. Open the *DAKOTA Uncertainty Job Stream*, presently called *TwoStep_Stream*, (Figure 3-6) and then the *Stream Steps* (Figure 3-7). Select the *MELGEN Step* (Figure 3-8), then select the Application Button and the desired executable version (Figure 3-9) that will be visible in the *Select Application* Tab of the *MELGEN Step* Property View. Here all the executables, previously introduced in the Configuration Tool, are listed. Now the MELGEN executable will be visible in the *MELGEN Step* Property View (Figure 3-10). Repeat the same process for the MELCOR step and MELCOR executable (Figure 3-11, Figure 3-12, Figure 3-13, Figure 3-14).

[8] 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.

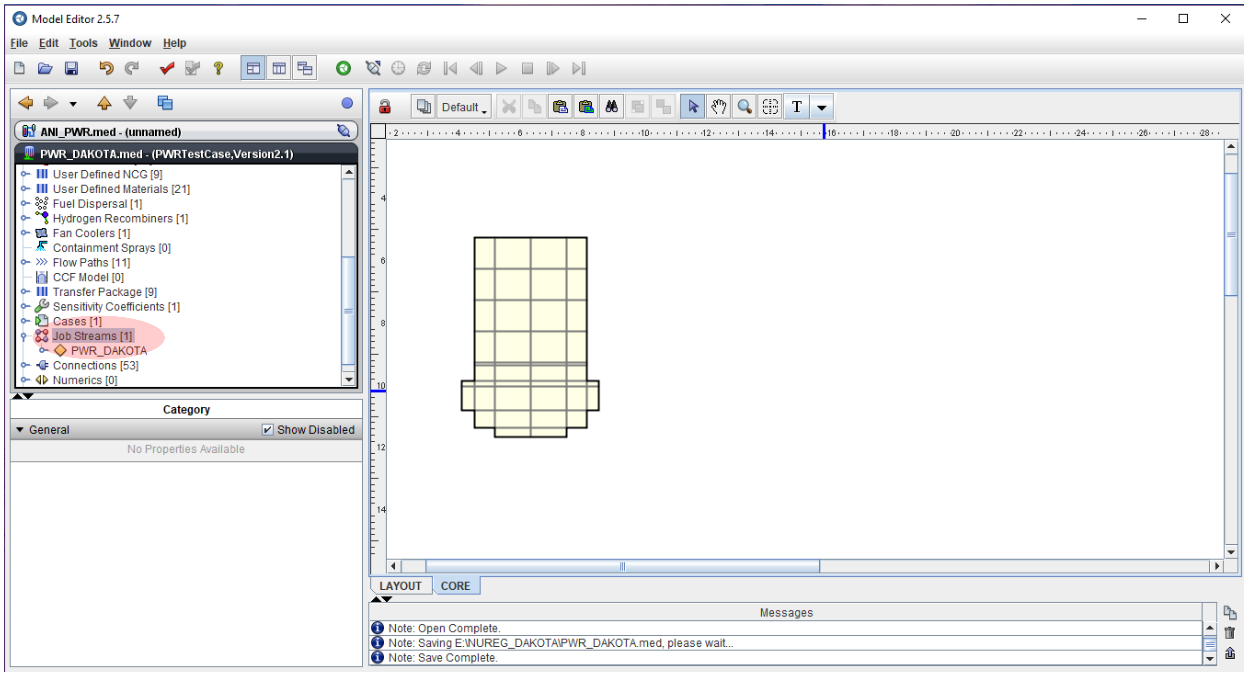

Figure 3-1 MELCOR Input Visualization and Job Streams Location in the Model Editor

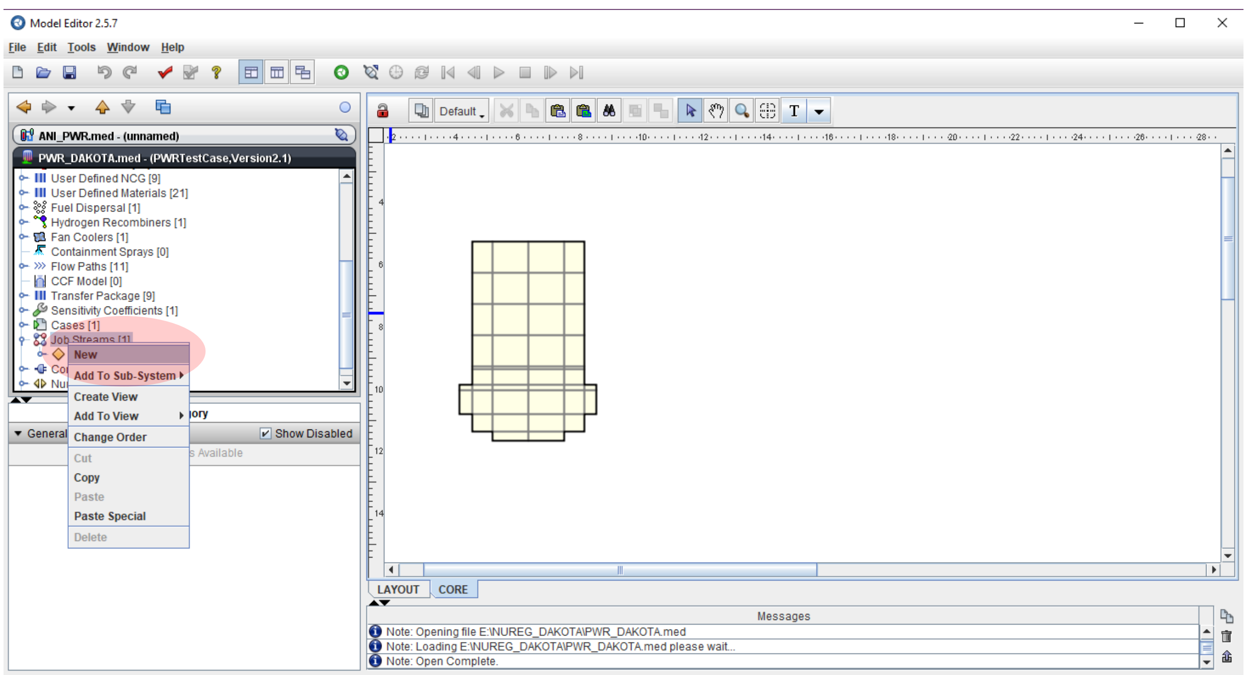

Figure 3-2 Creation of a New Job Stream

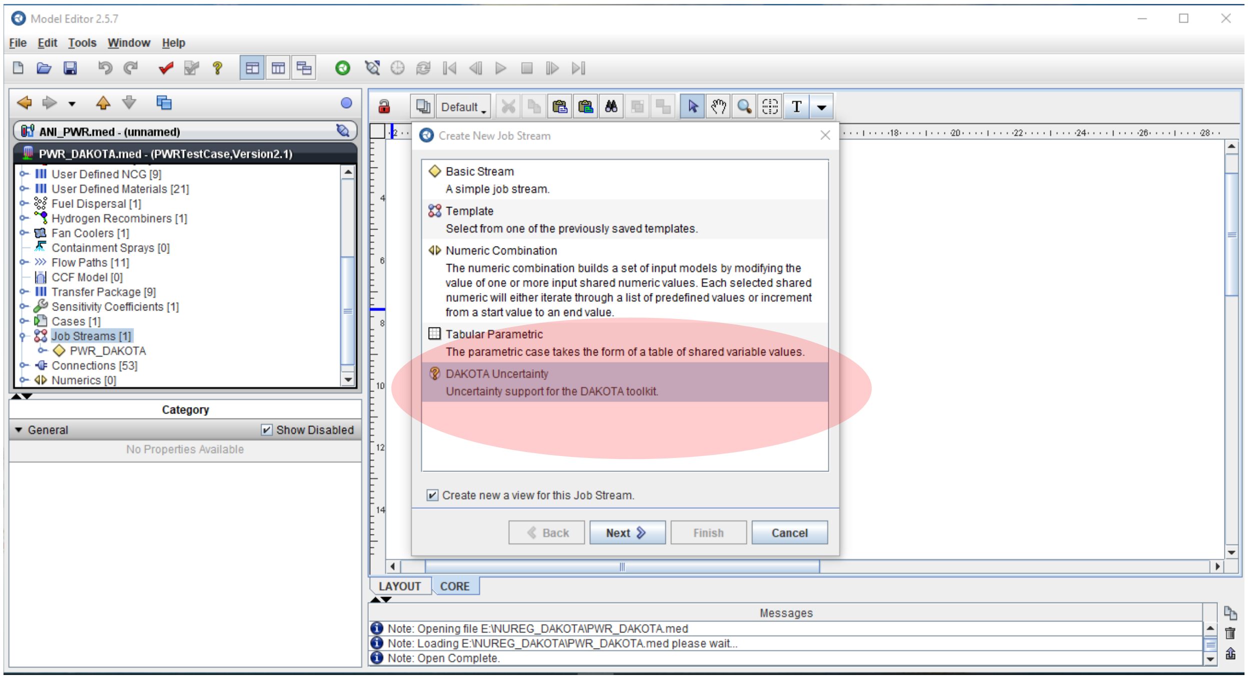

Figure 3-3 Selection of DAKOTA Uncertainty Job Stream

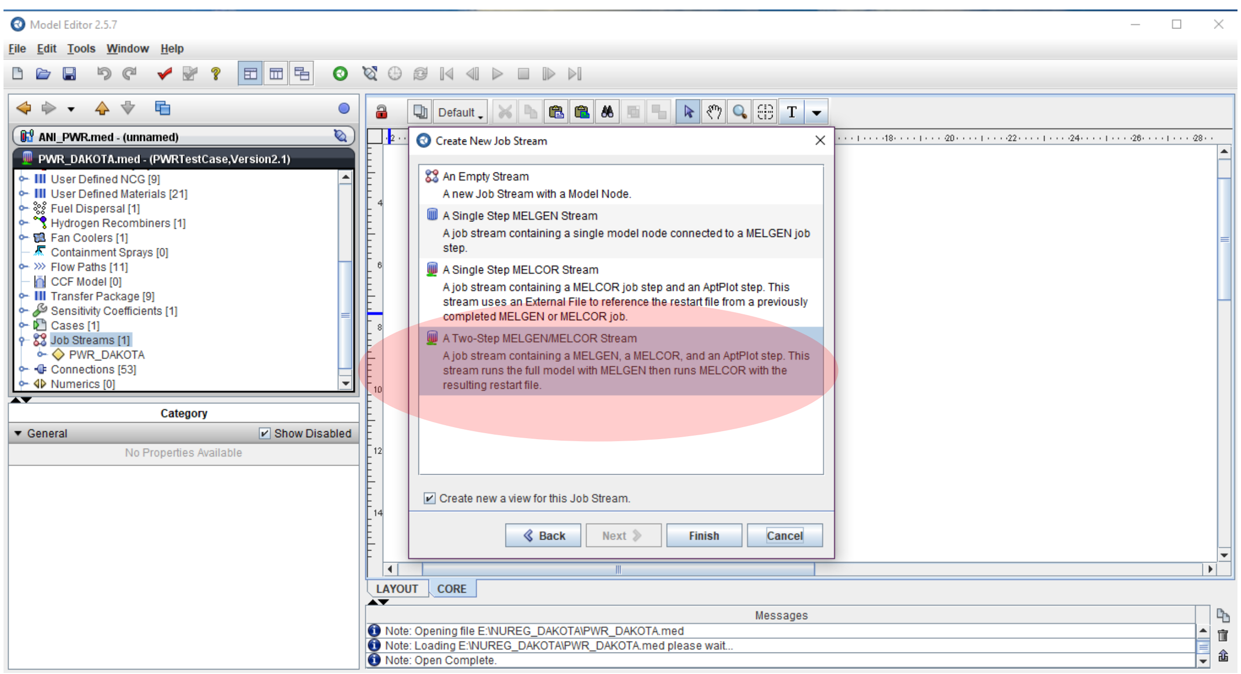

Figure 3-4 Selection of the Two-Step MELGEN/MELCOR Stream for the UA

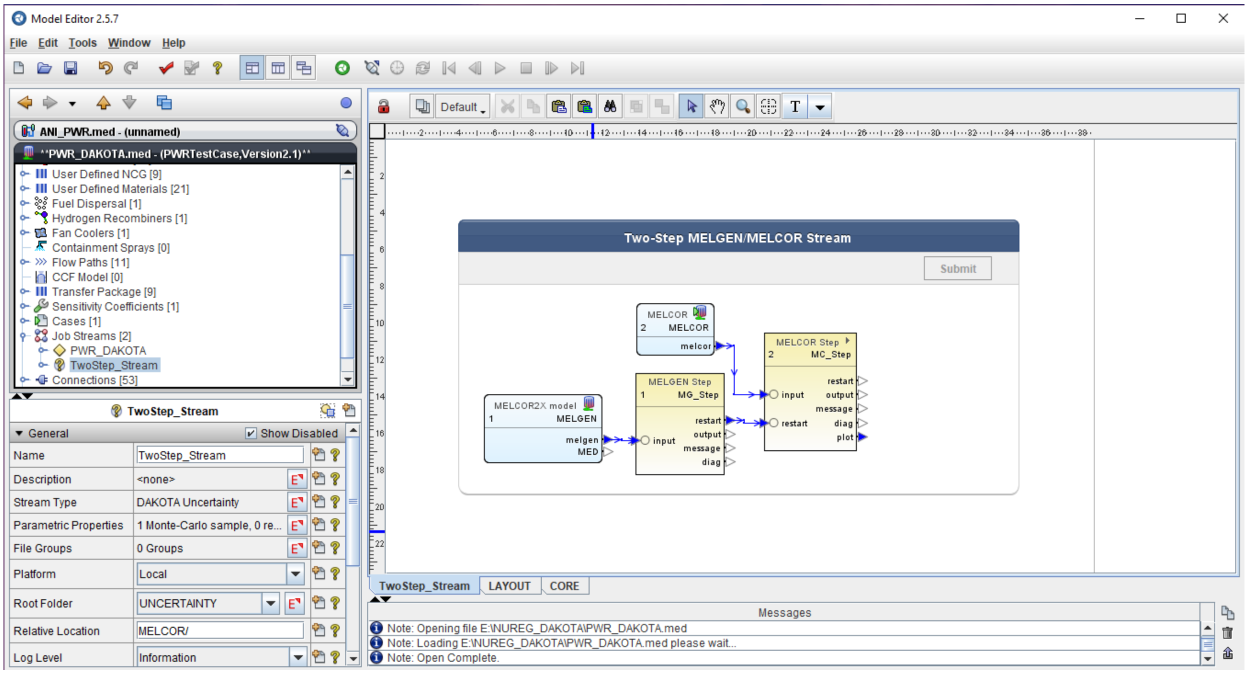

Figure 3-5 View of the Newly Created Two-Step MELGEN/MELCOR Stream for the UA

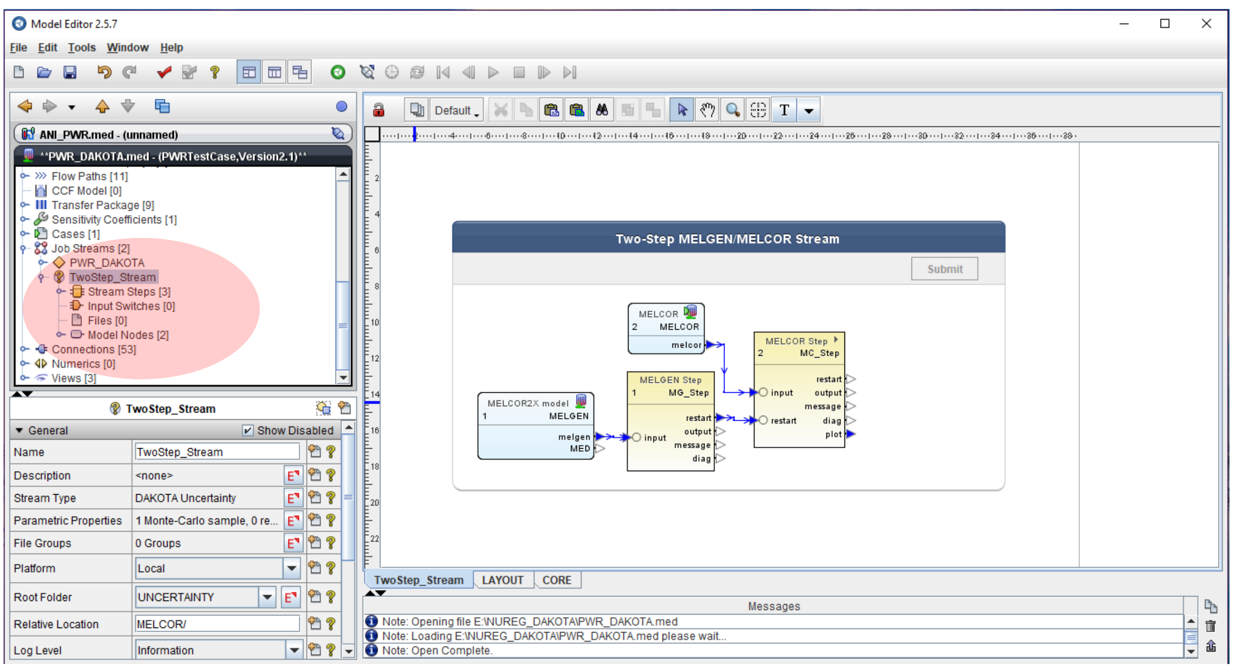

Figure 3-6 Selection of the DAKOTA Stream

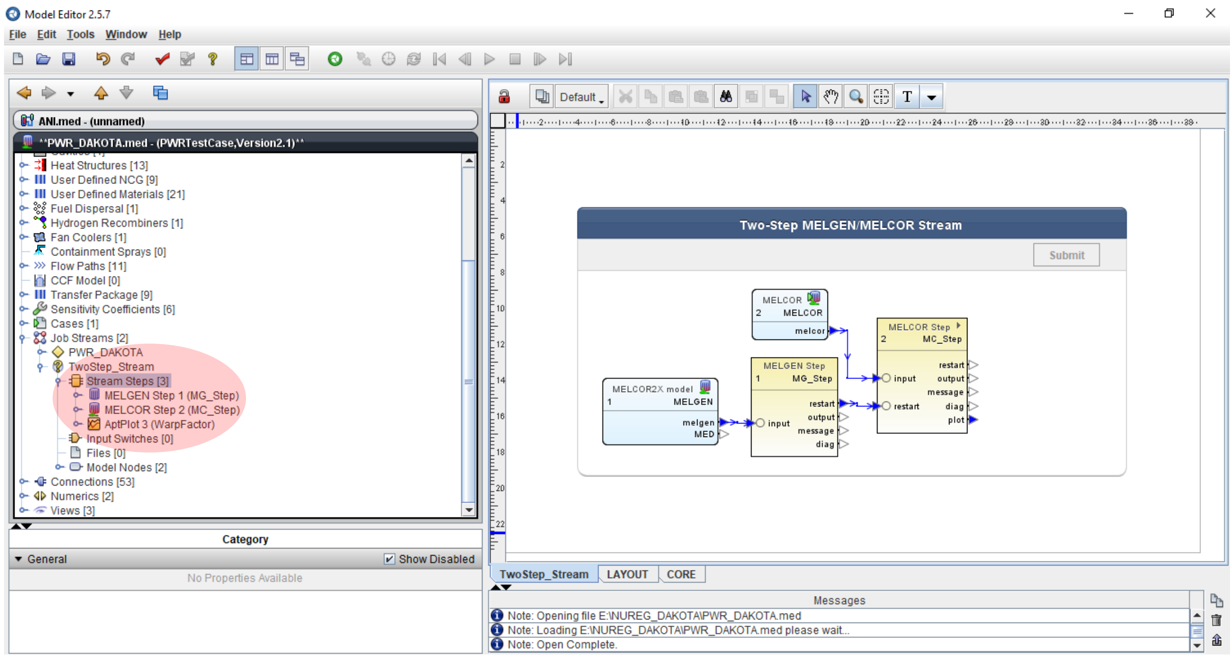

Figure 3-7 Visualization of the Stream Steps, at the Moment Available, of the DAKOTA Uncertainty Job Stream

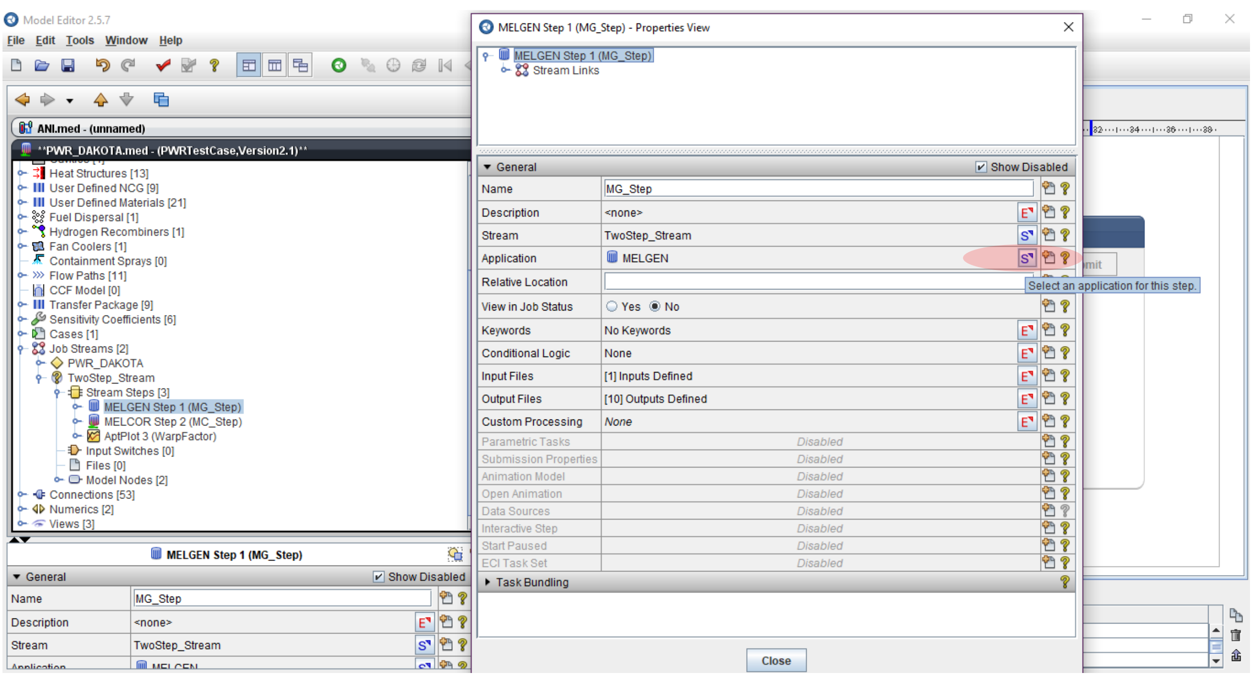

Figure 3-8 Selection of the Application Button of the MELGEN Step Property View

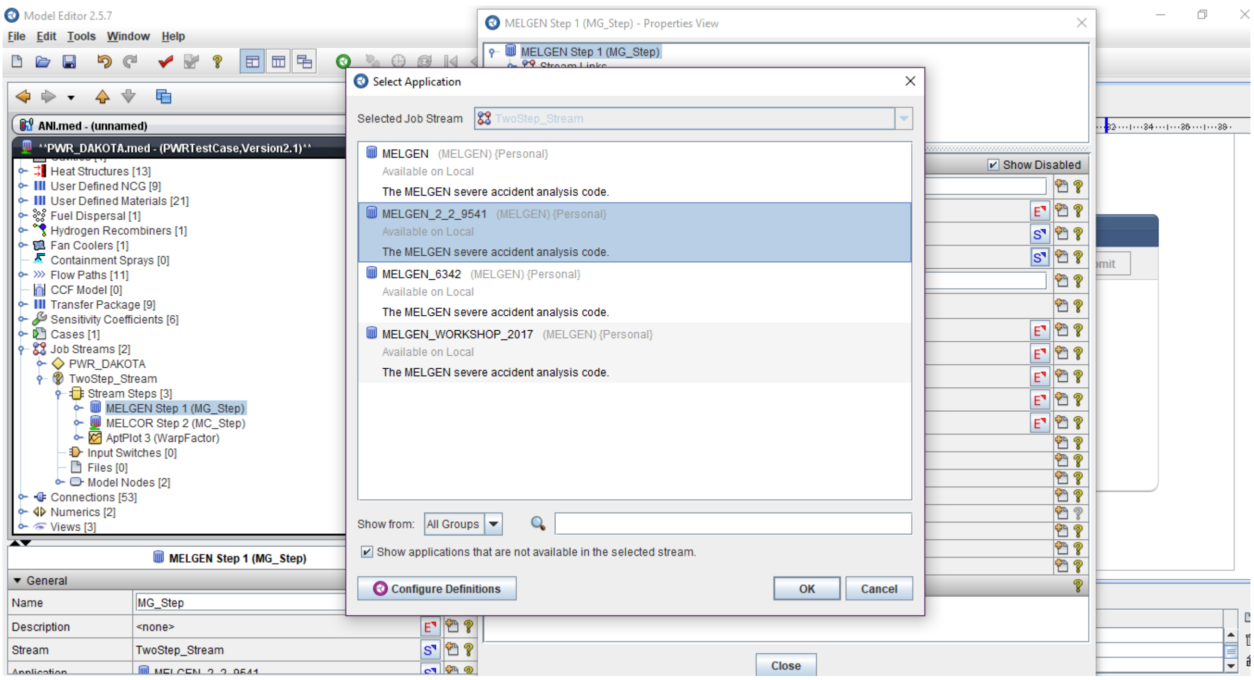

Figure 3-9 Selection of the Desired MELGEN Executable Version

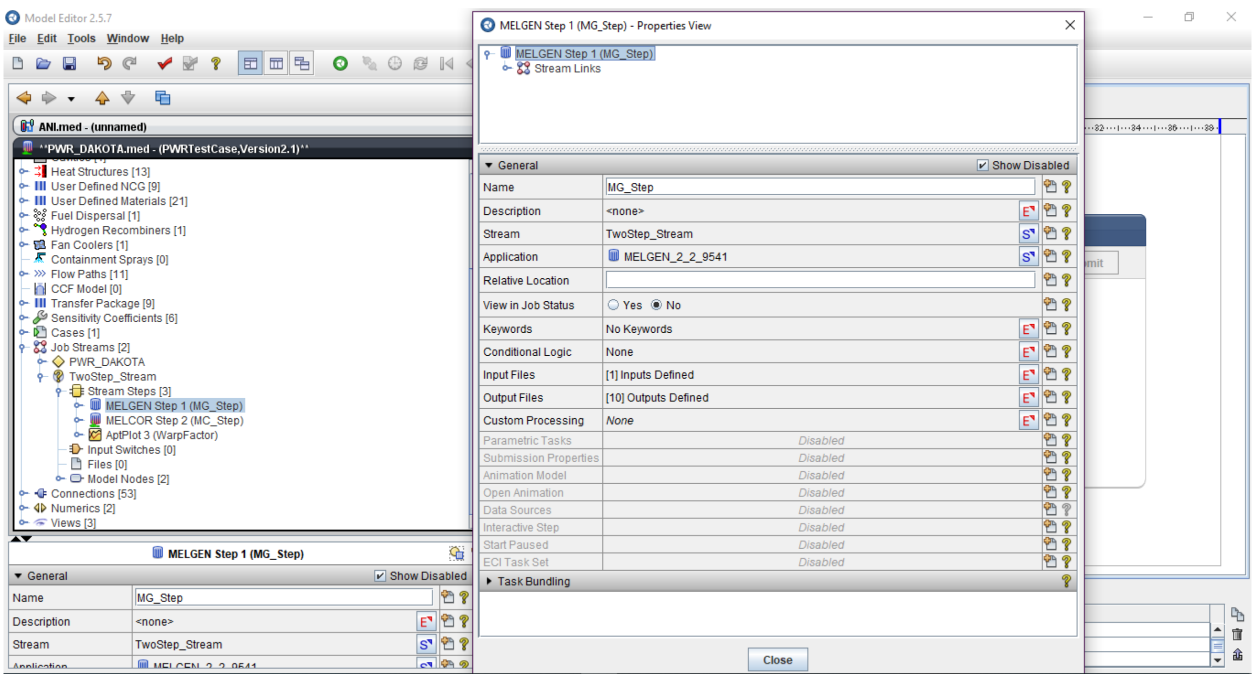

Figure 3-10 Desired MELGEN Executable Visualized in the MELGEN Step Property View

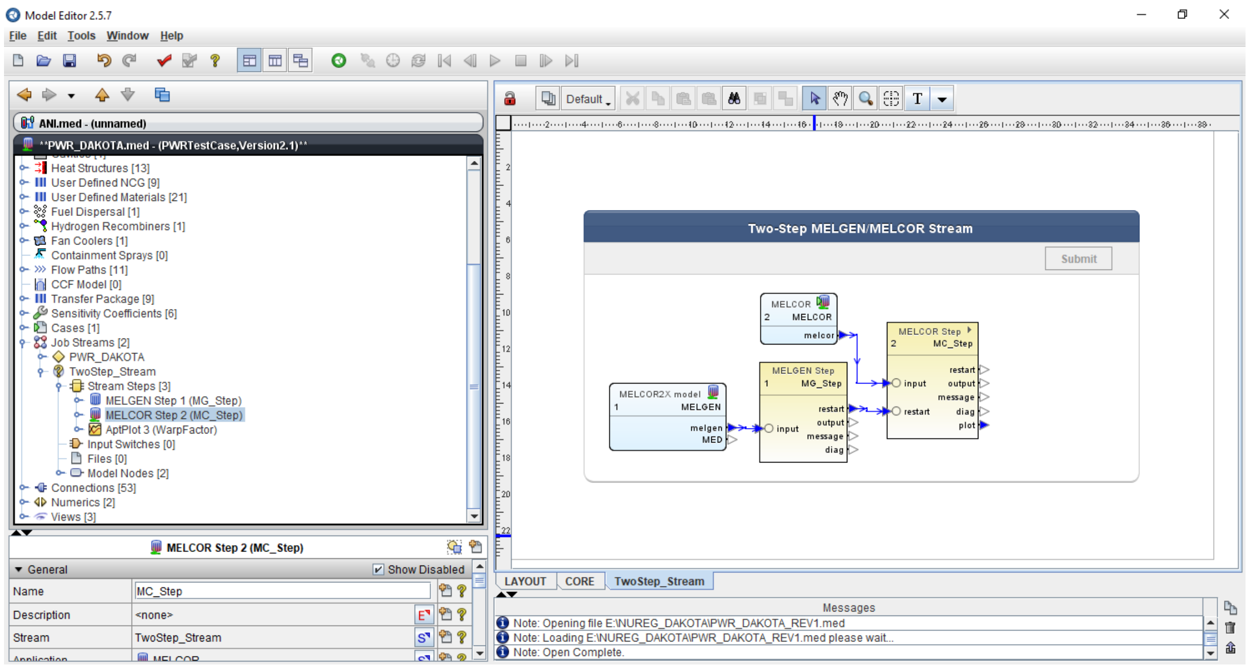

Figure 3-11 Selection of the MELCOR Stream Step

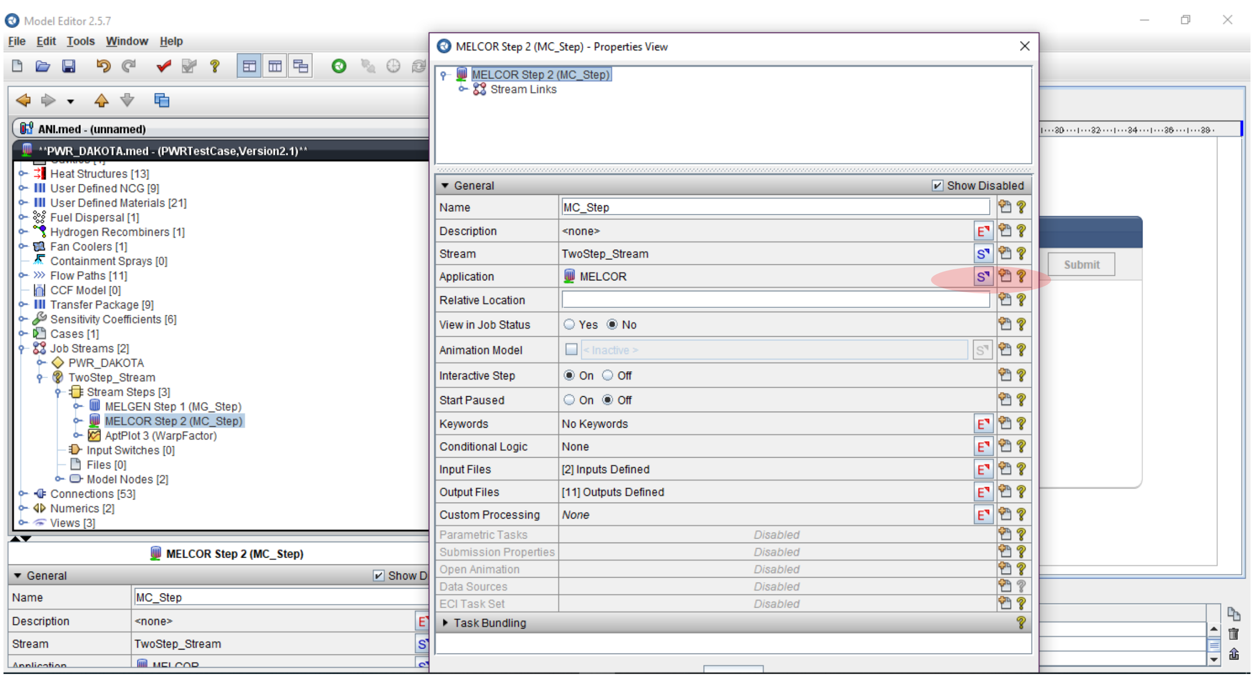

Figure 3-12 Selection of the Application Button of the MELCOR Step Property View

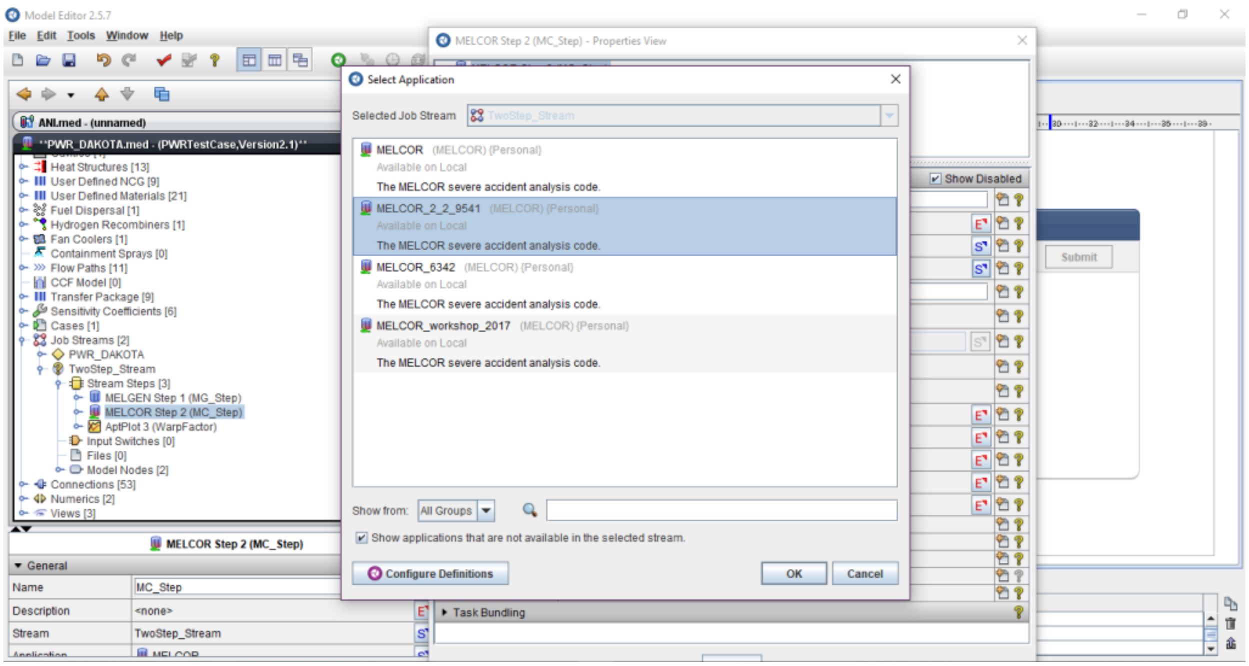

Figure 3-13 Selection of the Desired MELCOR Executable Version

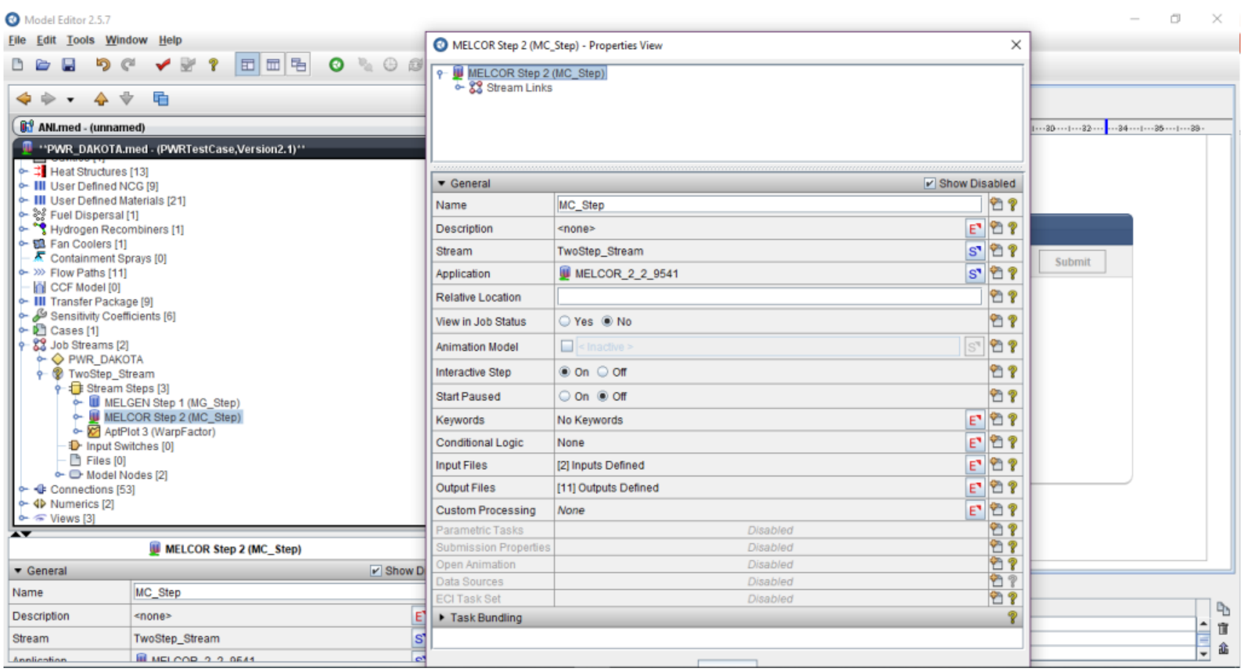

Figure 3-14 Desired MELCOR Executable Visualized in the MELGEN Step Property View

3.1.2 Setting-up DAKOTA Uncertainty Analysis

After setting up the MELGEN and MELCOR steps, the different uncertain parameters may be defined. From the Properties View of the *DAKOTA Uncertainty Job Stream* (Figure 3-15), various Tabs of the Parametric Properties allow the users to characterize the sampling process (e.g., number of required samples, sampling methods, etc.) by identifying uncertain input parameters and their respective PDF, identifying the FOMs, and specifying the aspects of the automatically generated report.

3.1.2.1 Definition of DAKOTA Application Properties

In this example, the Job Stream name has been changed to *PWR_UQ* (instead of *TwoStep_Stream*) (Figure 3-16). By selecting the *Parametric Property* Button, the user may in the first Tab Edit *Uncertainty Configuration/Dakota Properties* to specify the *Number of Samples*, *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, confidence level*, and *replacement factor*. 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. This evaluation is based on the Wilks method [25].

In the views shown in Figure 3-17 and Figure 3-18, the FOM for the UA can be specified and visualized. At this point, it is possible to rename the FOMs as desired (Figure 3-19). In this case, only one FOM has been defined—the total cumulative hydrogen production in the core from all oxidation processes (MELCOR/COR-DMH2-TOT). It is renamed in this example to the more descriptive label *H2_GEN*. As described in [25], “Figures of Merit” is approximately synonymous with the term “response function” that can be found in the DAKOTA literature. The *Time Dependent* field, as discussed in [25], enables computation of response correlation coefficients at selected instances of the transient. In this computation, the FOM is extracted at the selected times in the transient. The response correlations however can be defined also for only one instant in the transient, which is done for simplicity in this illustrative application.

3.1.2.2 Specification of Uncertainty Parameters and Distribution

In the second tab of the *DAKOTA Uncertainty Stream* configuration, *Edit Uncertainty Configuration/Variables* (Figure 3-20), it is possible to

- Add selected uncertain input parameters, previously defined in the MELCOR input deck, and
- Define characteristics of each input, such as probability distribution.

In this tab, it is possible to *Select New Variable Reference* to introduce an uncertain input parameter into the specification of the uncertainty model (see Figure 3-21). This type of variable is either a MELCOR sensitivity coefficient or a user-defined, real-valued variable. In the next tab of the *Select New Variable Reference*, as shown in Figure 3-22, different options/flags are available for the user to select the properties of the new distribution (Use an existing distribution; Scalar; Additive; Factor; Copy). When the uncertain input parameter is added, it is displayed in the variables list (Figure 3-23).

The third tab of the uncertainty model configuration, *Edit Uncertainty Configuration/Distribution*, provides the means to specify the input uncertainty distributions previously defined. A user may define the Distribution Type (Normal, Lognormal, Uniform, Loguniform, Triangular, Exponential, Beta, Gamma, Gumbel, Frechet, Weibull, Histogram) and the associated distribution parameters (Figure 3-24). Similarly, it is possible to enter the input uncertainty parameters in the *Edit Uncertainty Configuration/Variable* tab (Figure 3-25) and to specify the underlying distributions in the *Edit Uncertainty Configuration /Distribution* tab (Figure 3-26).

Each of the following will be displayed:

- Variables (e.g., VFALL),
- Distribution identifier or label (e.g., d3),
- MELCOR Variable Type (e.g., User-defined Reals),
- Nominal value,
- Variable units (e.g., velocity having units of m/s),
- Distribution type (e.g., Scalar), and
- Distribution parameters.

At this point, if the number of samples has not been previously specified, finalizing the UA will not be permitted. Clicking on OK will result in a warning message indicating that the number of samples must be specified in order to perform the analysis (Figure 3-27). To enter the required number of samples, it is necessary to return to the first tab (Figure 3-28) and click the *Calculator* Button highlighted in Figure 3-29. The required number of tasks given the *Order*, *Probability*, and *Confidence* selected by the user (Figure 3-29) is then calculated according to Wilks' method [25]. The number of samples will be automatically updated (Figure 3-30).

3.1.2.3 Specification of Automatic UA Reporting

In the fourth tab, *Edit Uncertainty Configuration/Report*, it is possible to specify the report configuration, automatically generated by DAKOTA, and the plot variables in the Plotted Values Table (such as following sets of data pairs: uncertainty parameter and iteration index, FOM and input uncertain parameters, FOM and iteration index). In this tab, it is possible to enter the title page, the front matter, header, footer, miscellaneous information, as shown in Figure 3-31 and Figure 3-32. Addition of desired plots to the report is shown in Figure 3-33. Different options are present for *Plotted Values*: selected input parameters as function of the iteration index (Figure 3-34), the FOM as a function of a selected input parameter (Figure 3-35 and Figure 3-36) and the FOM as function of the iteration index. At this point the properties of the DAKOTA *Uncertainty Job Stream* are completely set.

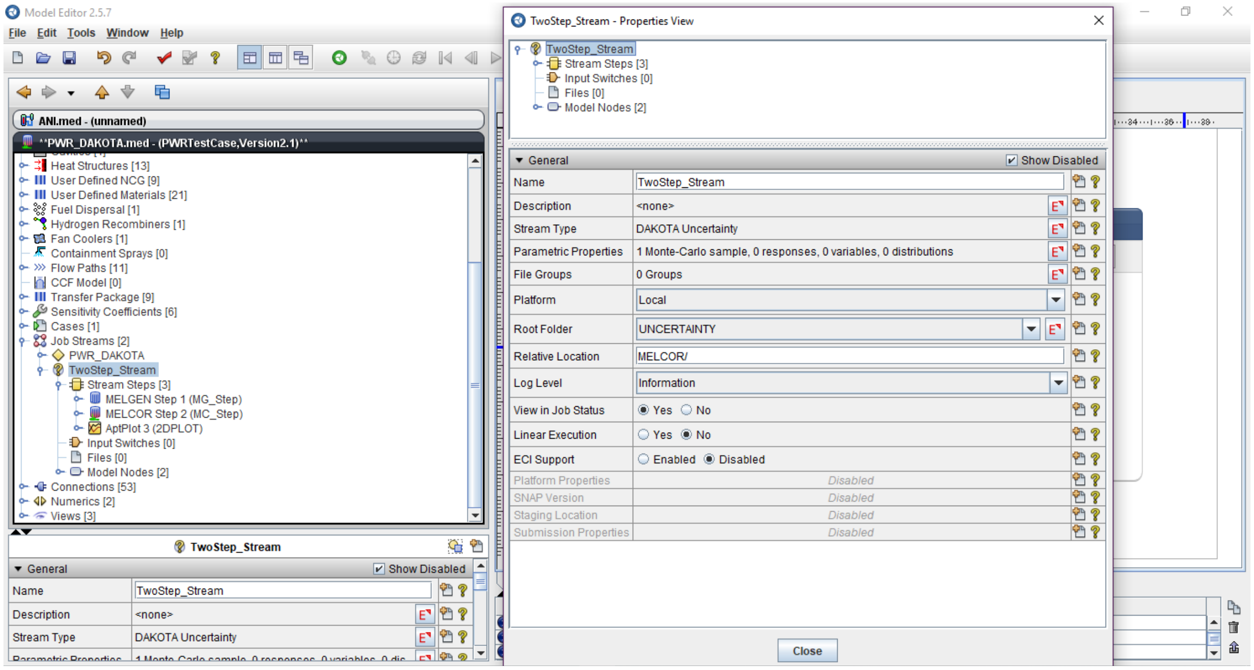

Figure 3-15 Property View of the DAKOTA Uncertainty Job Stream

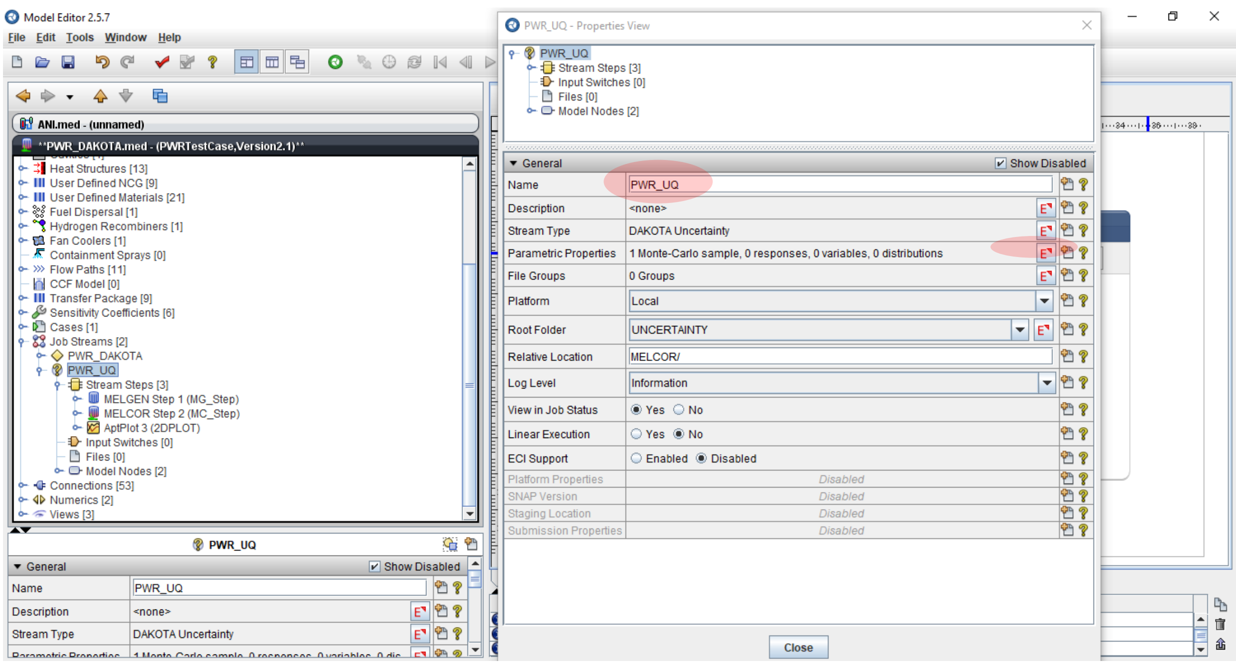

Figure 3-16 Naming the DAKOTA Uncertainty Job Stream and Parametric Properties Selection

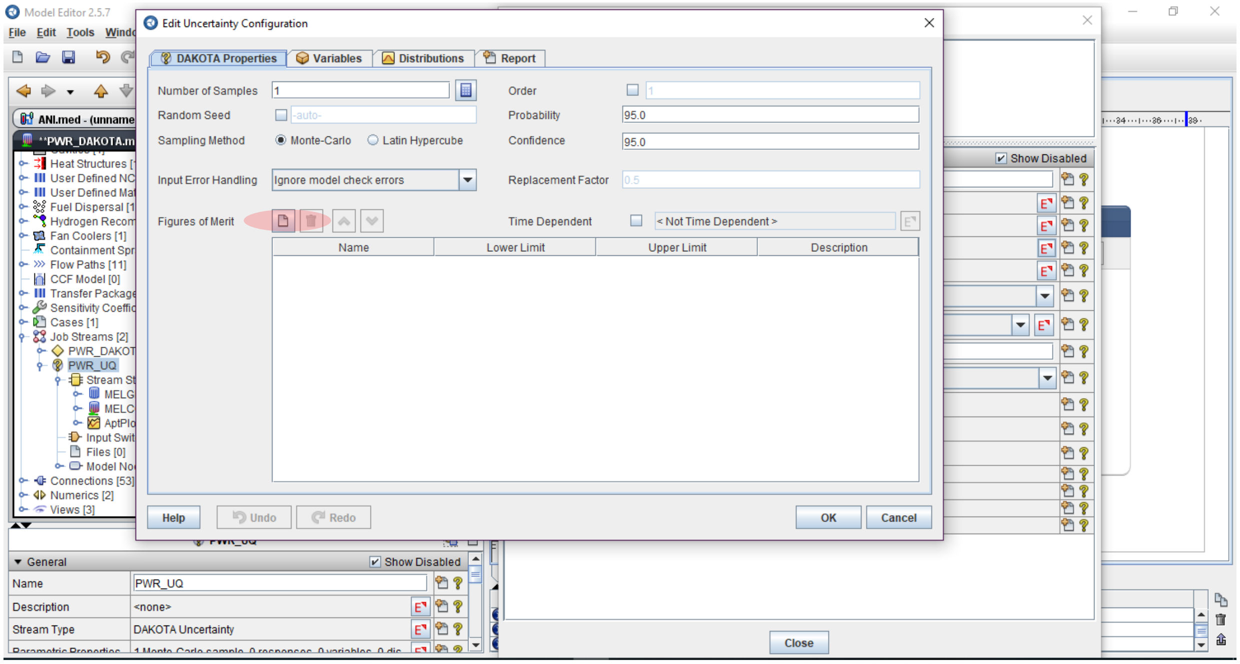

Figure 3-17   Add the FOM Target of the DAKOTA UA

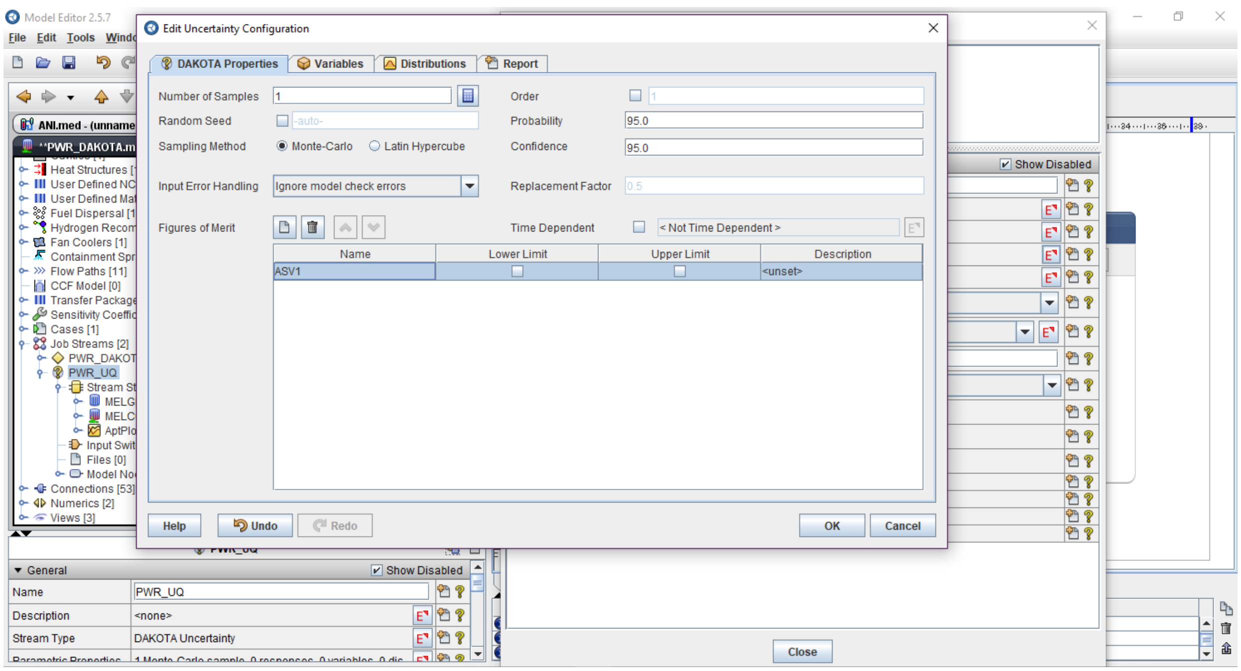

Figure 3-18   FOM Added for the DAKOTA UA

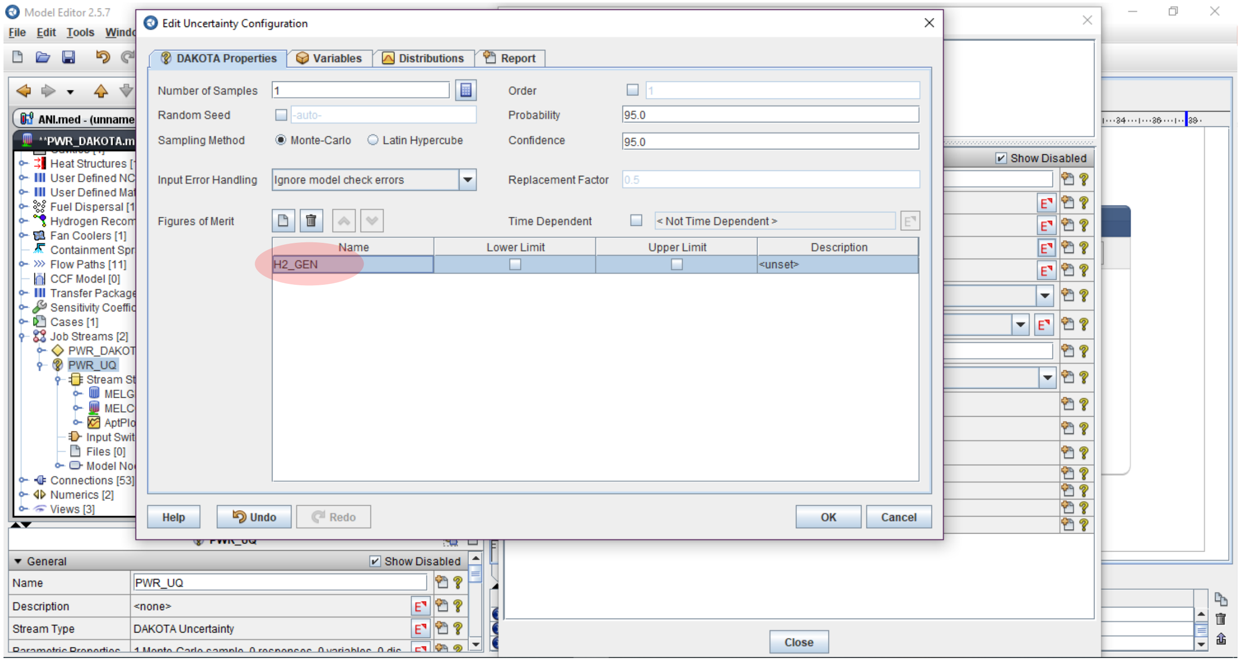

Figure 3-19 Renaming of the FOM Previously Added

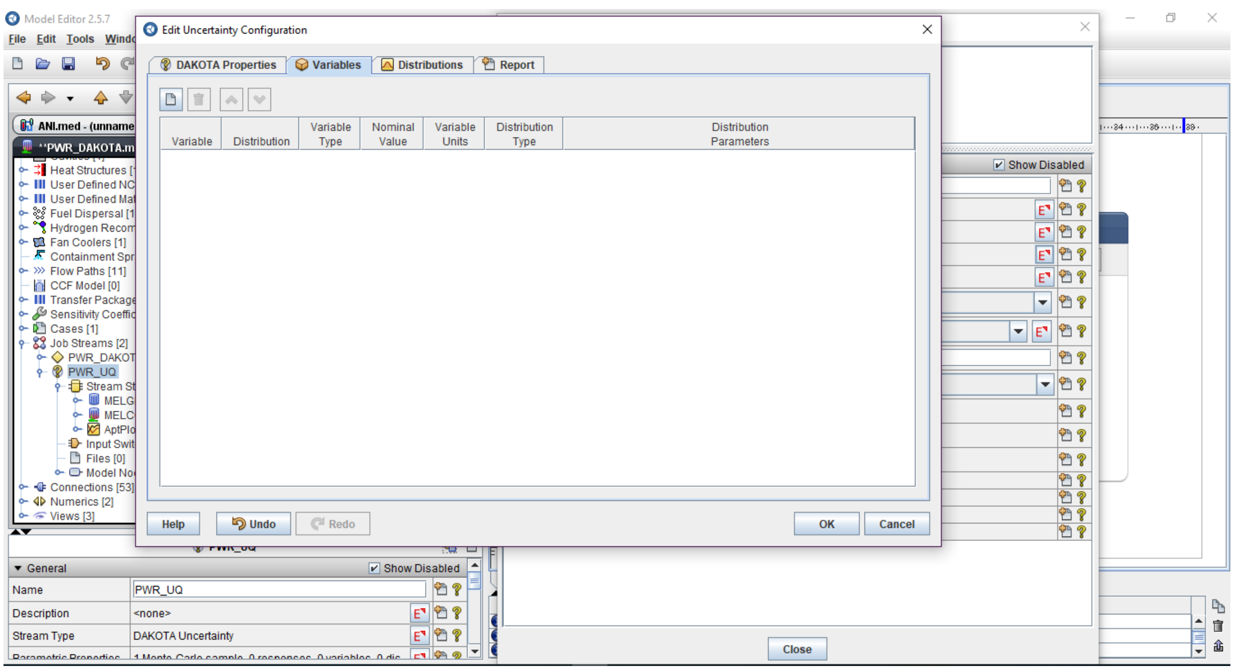

Figure 3-20 Opening of the Edit Uncertainty Configuration/Variables Tab

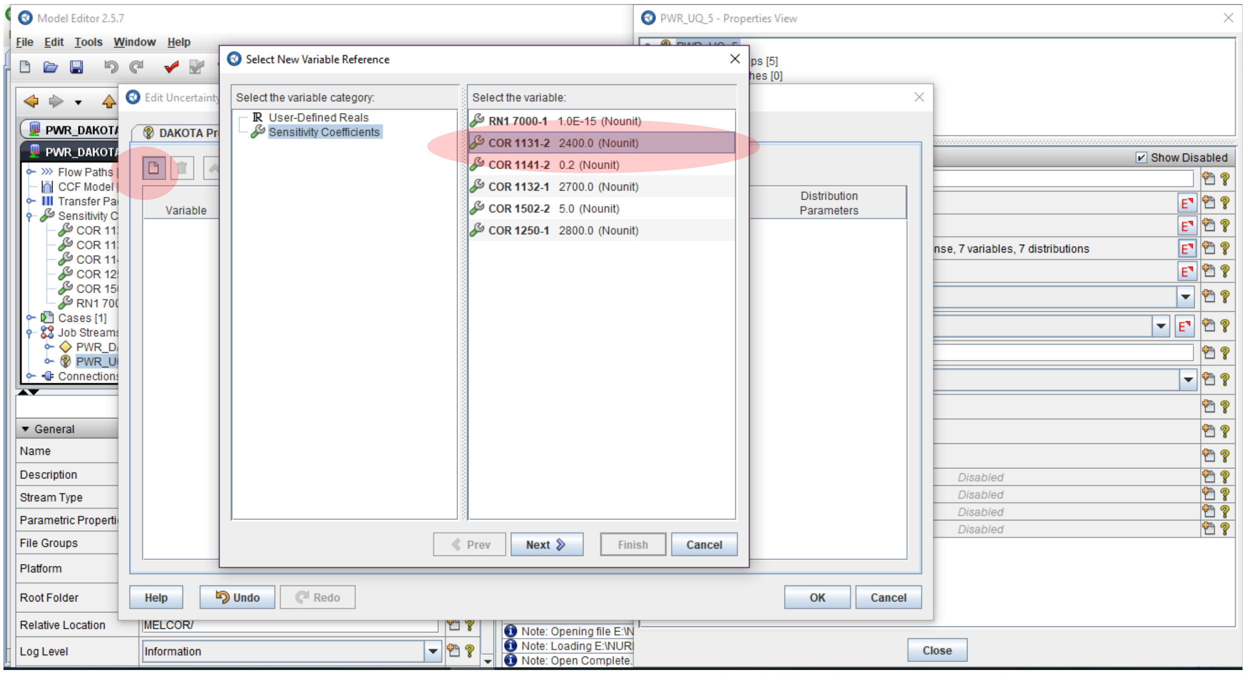

Figure 3-21 Select New Variable Reference/Select Variable Category/Select the Variable Tab

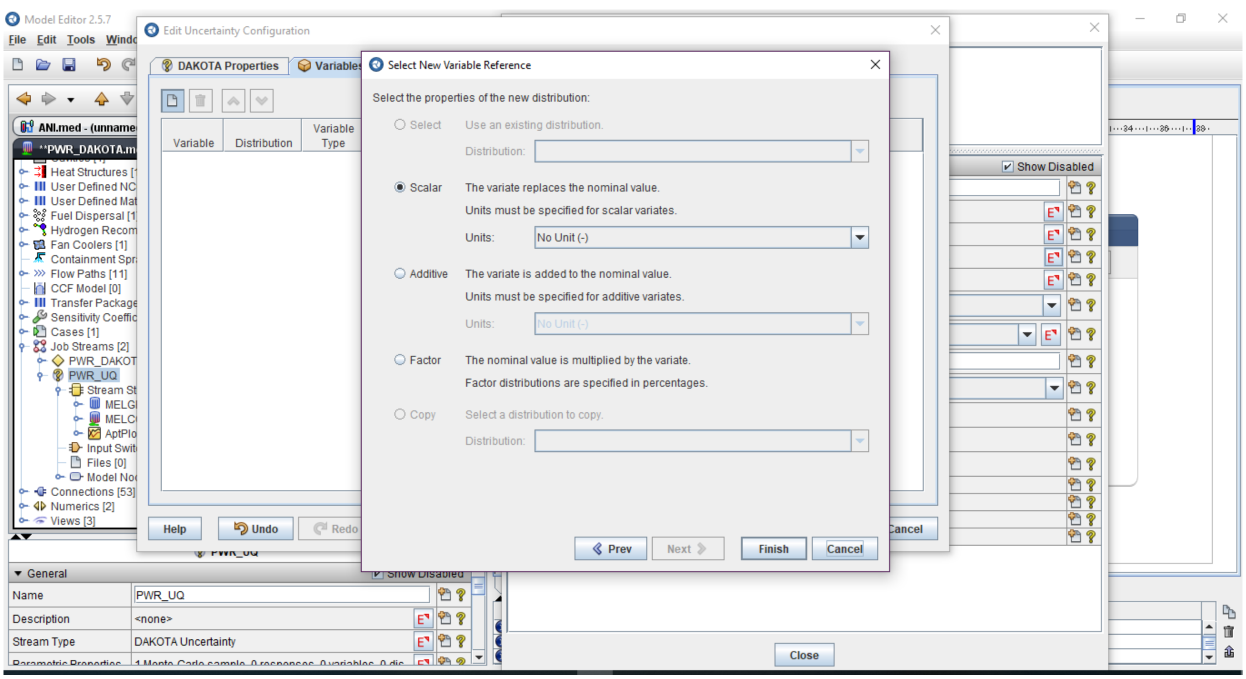

Figure 3-22 Select New Variable Reference/Select the Property of the New Distribution Tab

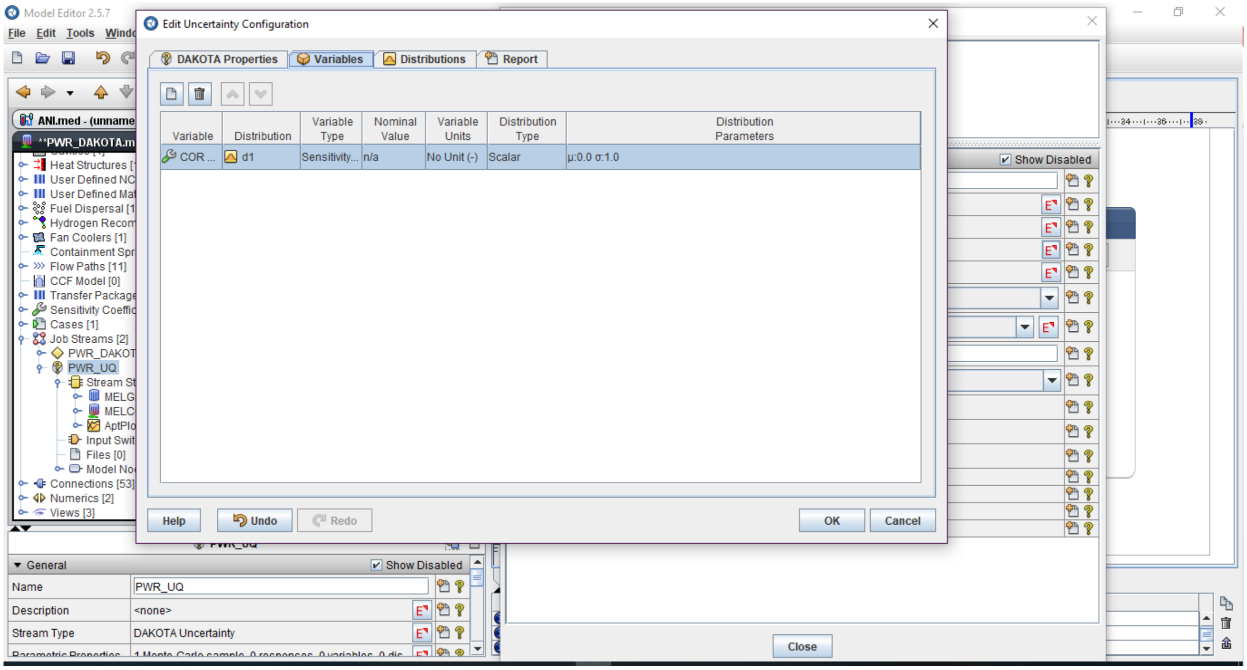

Figure 3-23 View of the Newly Created Uncertain Input Parameter

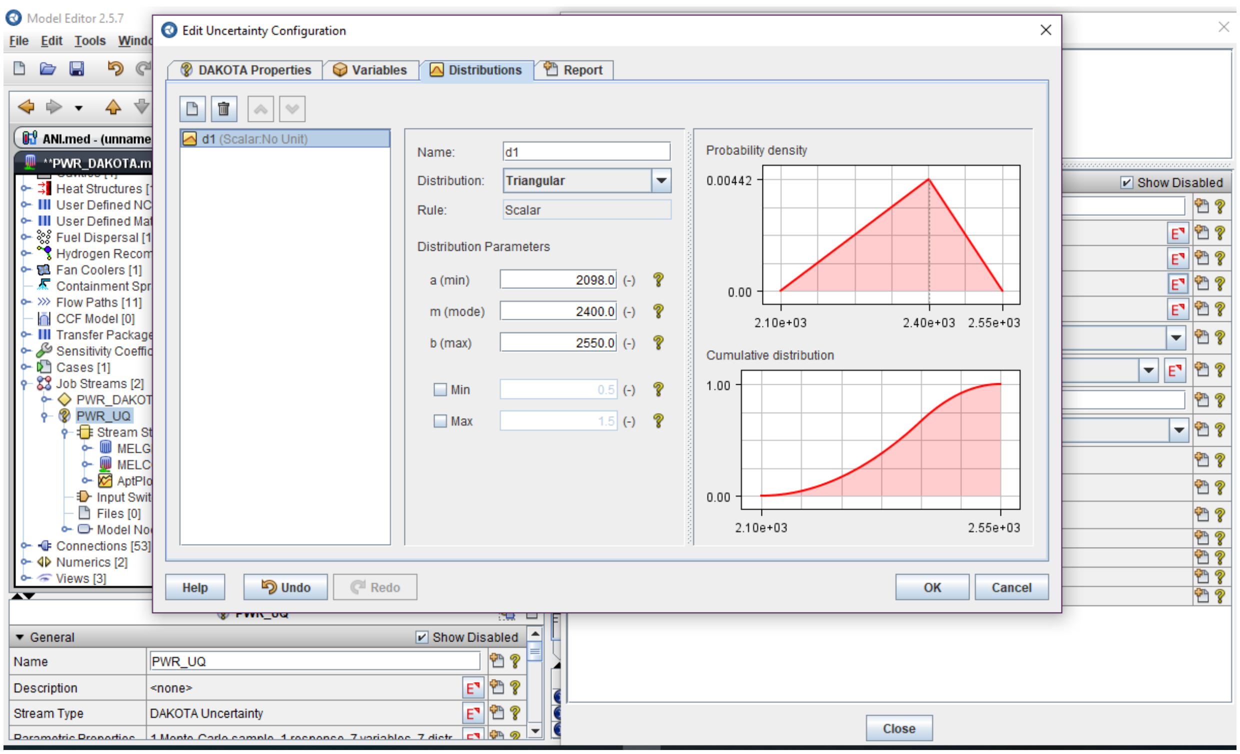

Figure 3-24 Definition of the Distribution Properties of the Uncertain Input Parameters

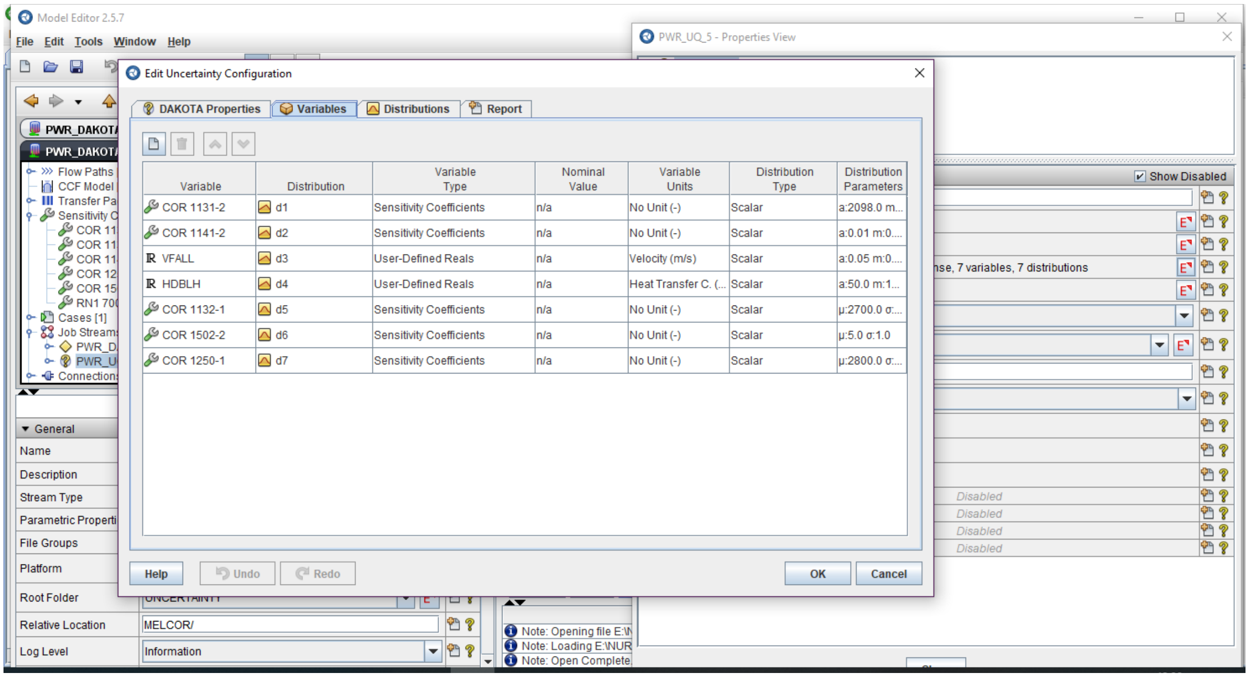

Figure 3-25 View of the Uncertain Input Parameter Final List

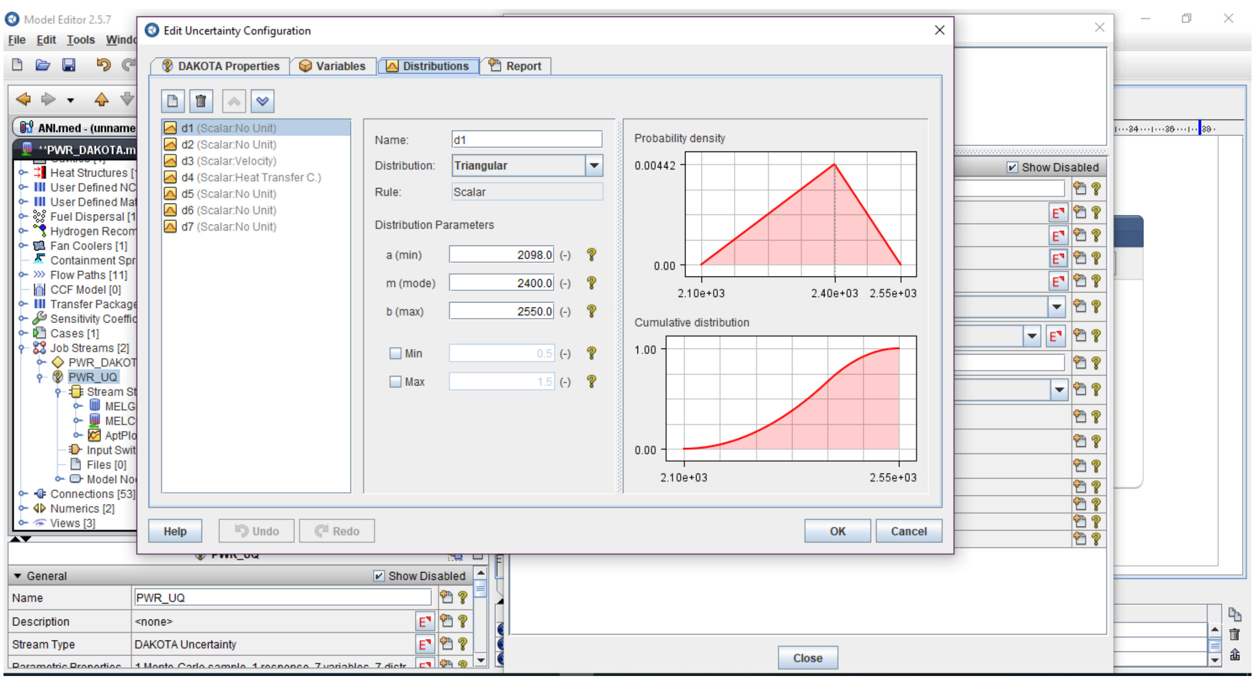

Figure 3-26 Example of Input Uncertain Parameter Distribution Representation in the Tab (all the parameters previously selected for this application are listed)

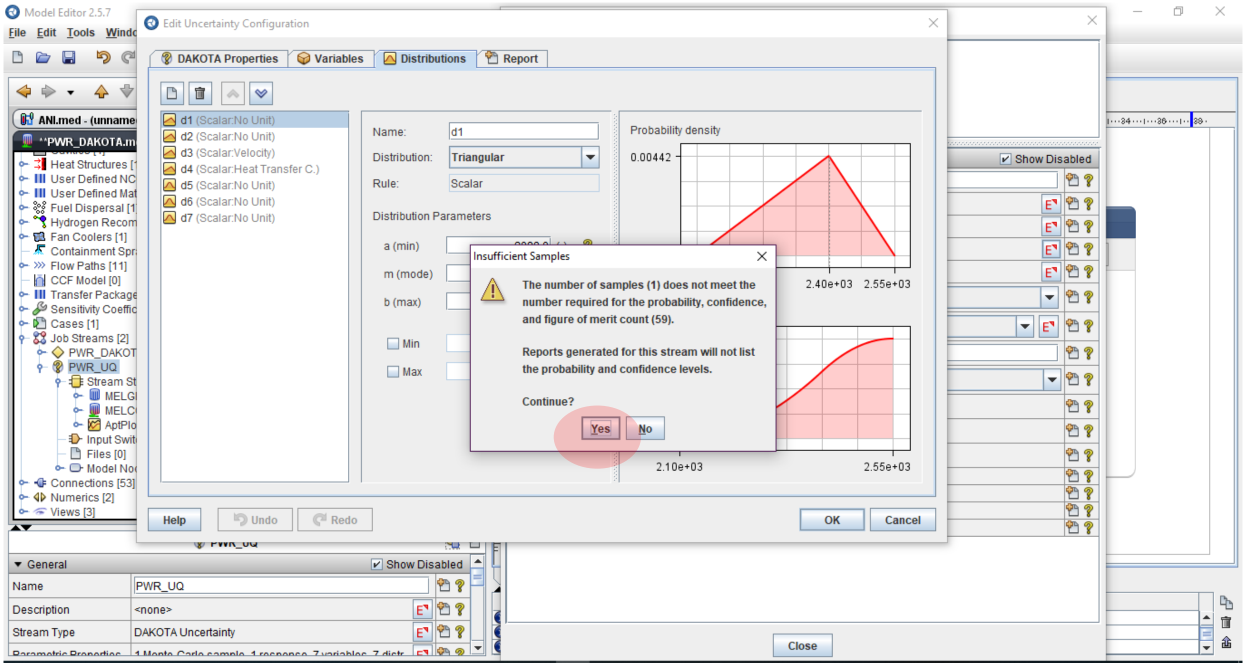

Figure 3-27 Insufficient Number of Sampling Automatic Warning

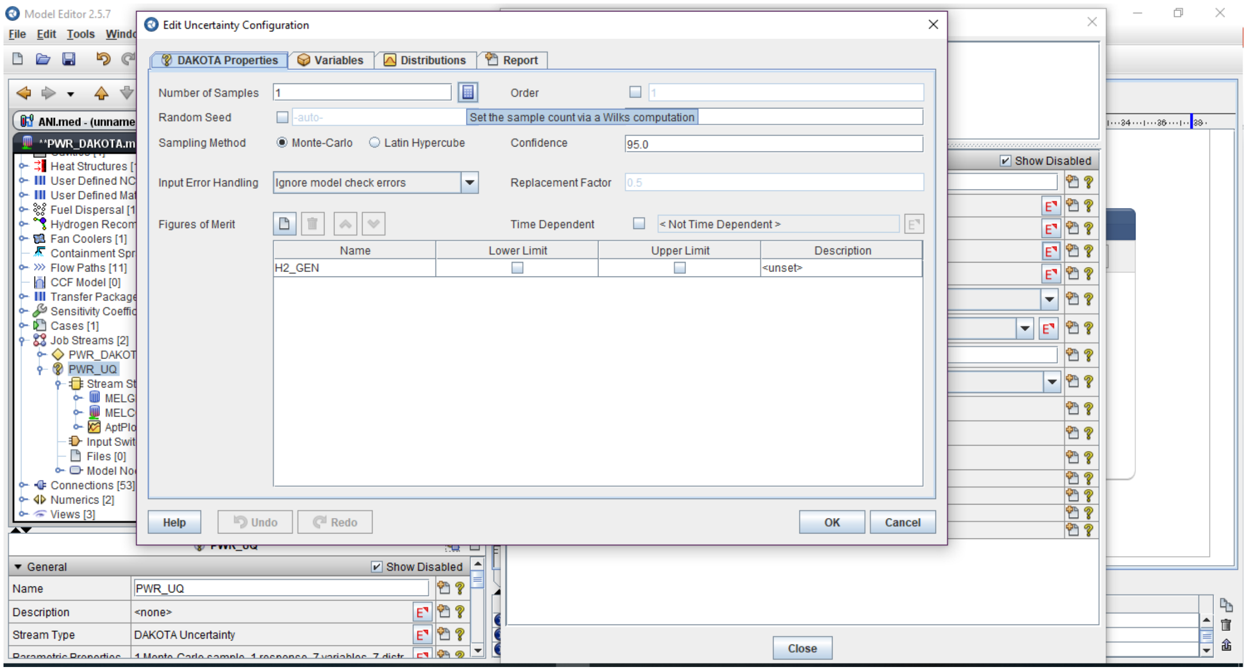

Figure 3-28 Enter the Desired Number of Samples in the Edit Uncertainty Configuration/DAKOTA Properties Tab

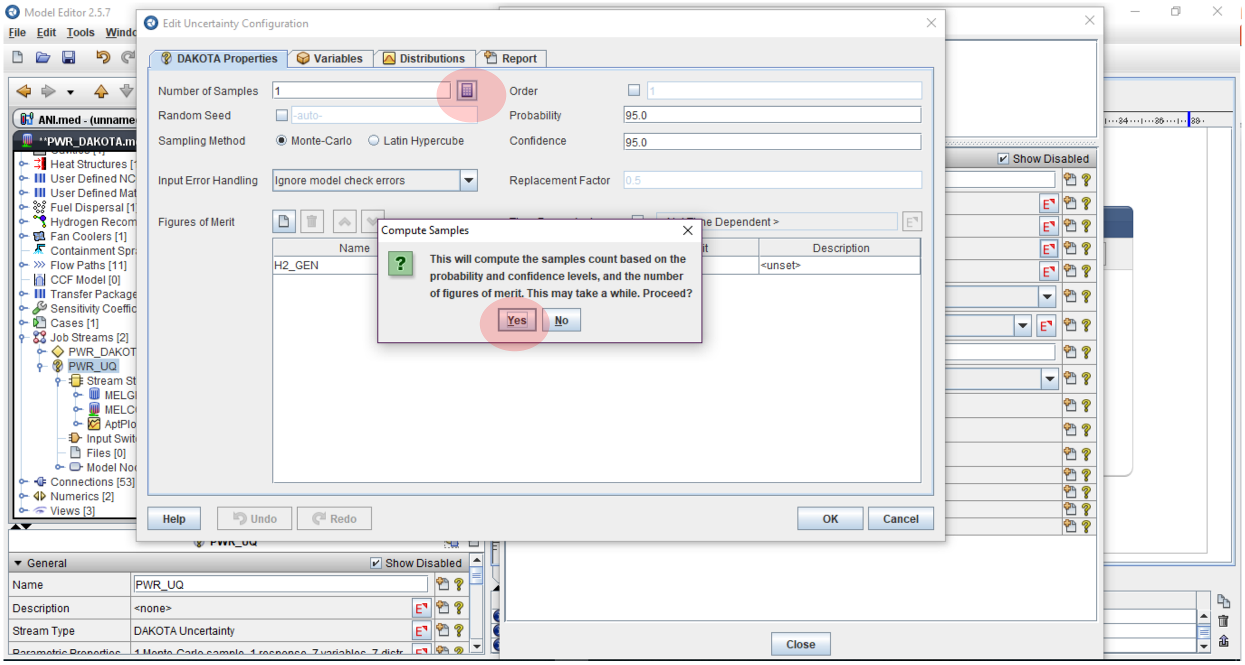

Figure 3-29 Automatic Computation of the Required Samples to Meet the Specified Probability and Confidence Level

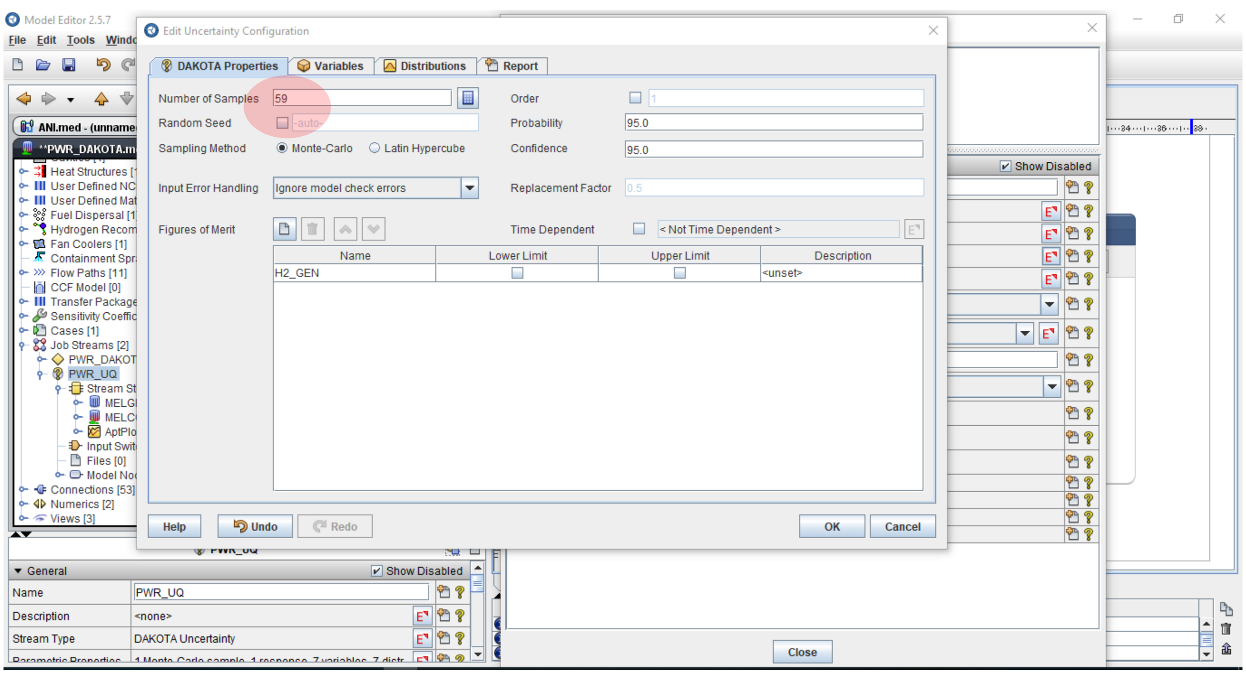

Figure 3-30 Updated Number of Samples for the UA

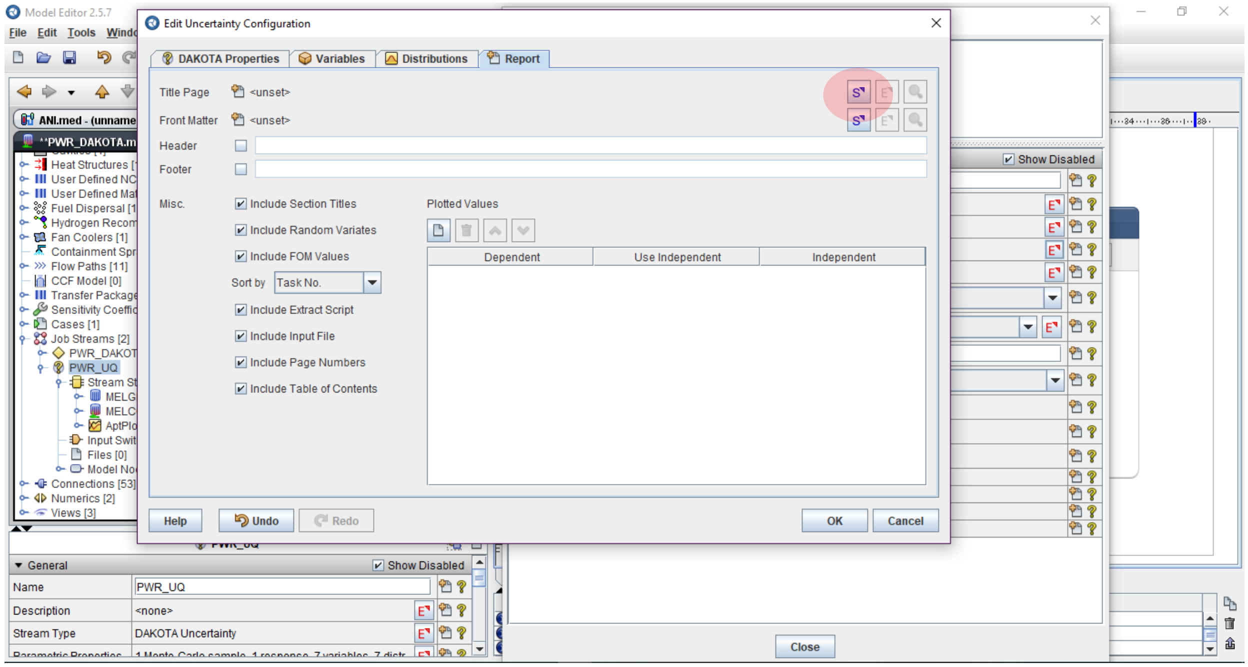

Figure 3-31 Setting the Title Page of the DAKOTA UA Final Report

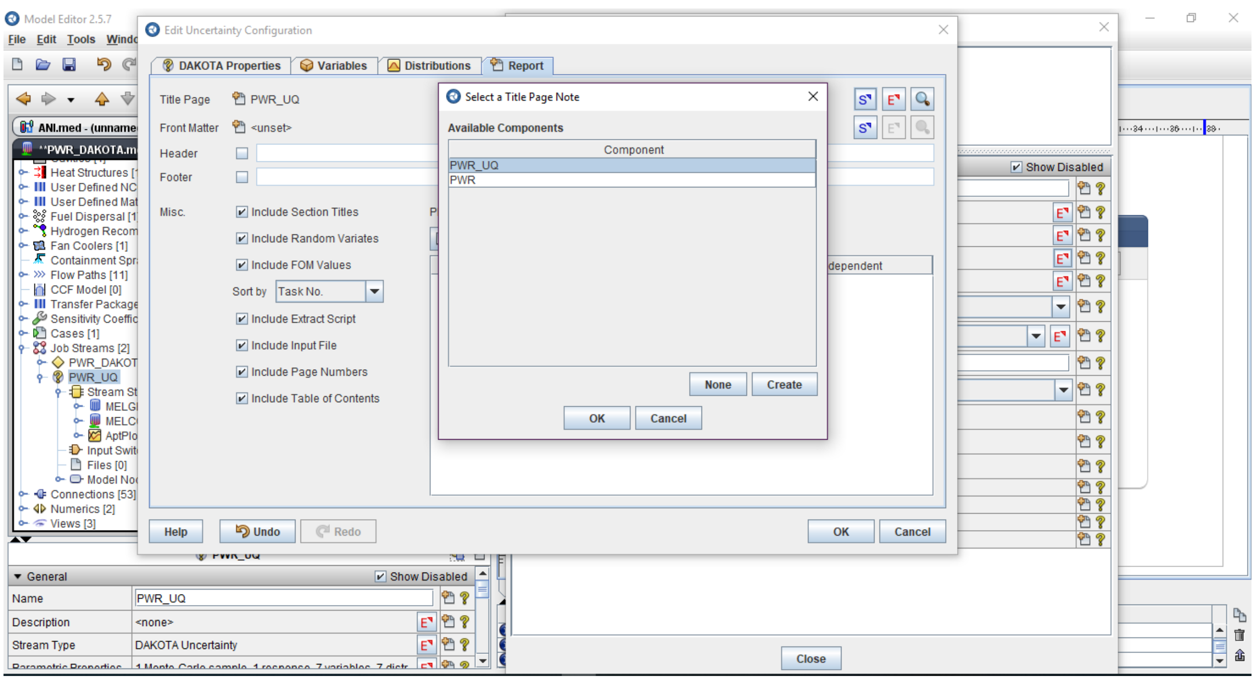

Figure 3-32 Selection of the Title Page of the DAKOTA UA Final Report

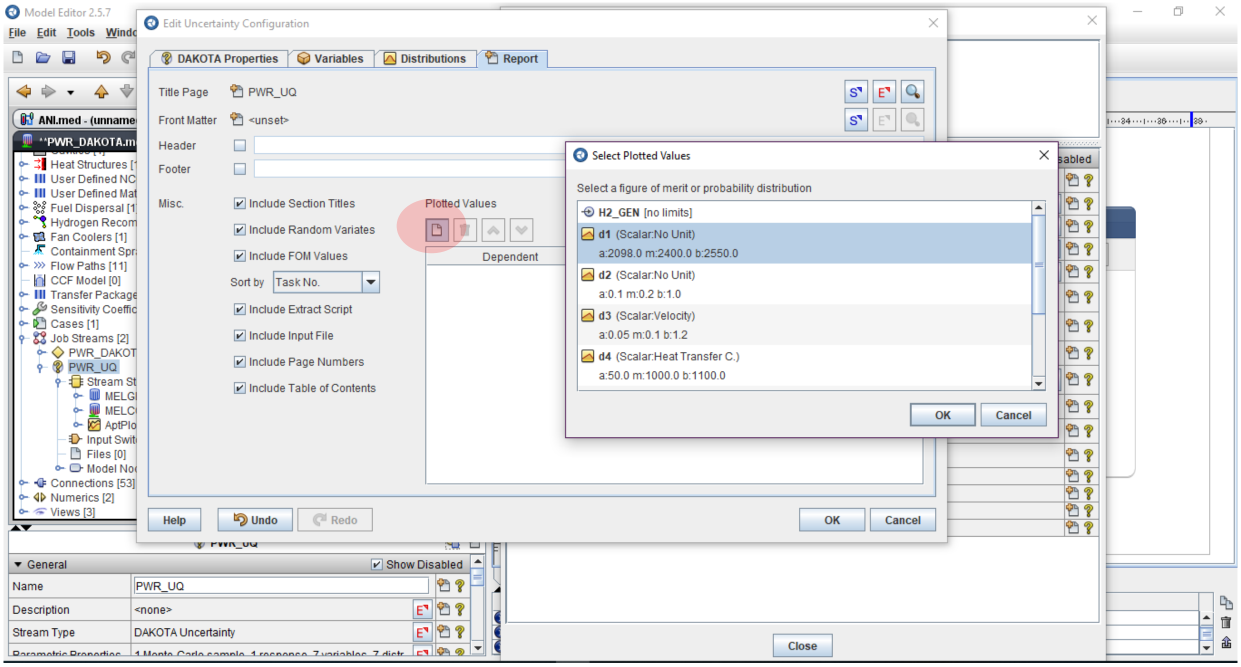

Figure 3-33 Addition of Plots to the DAKOTA UA Final Report

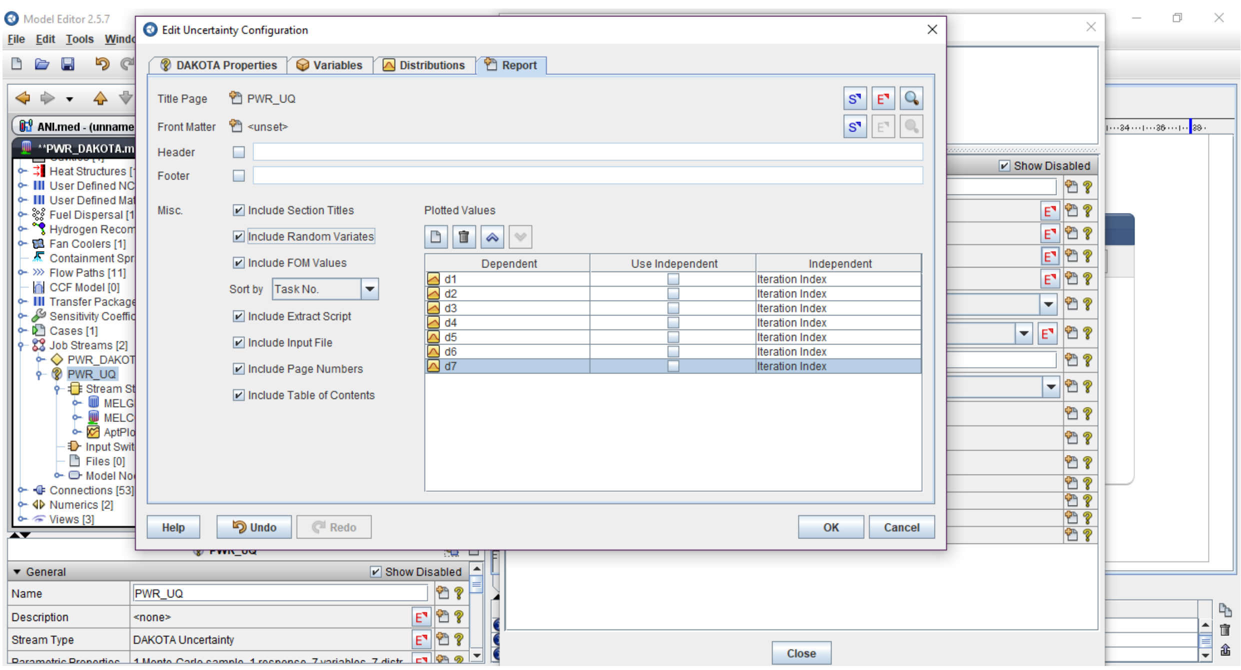

Figure 3-34 View of All the Uncertain Input Selected Parameters Plotted as Function of the Iteration Index

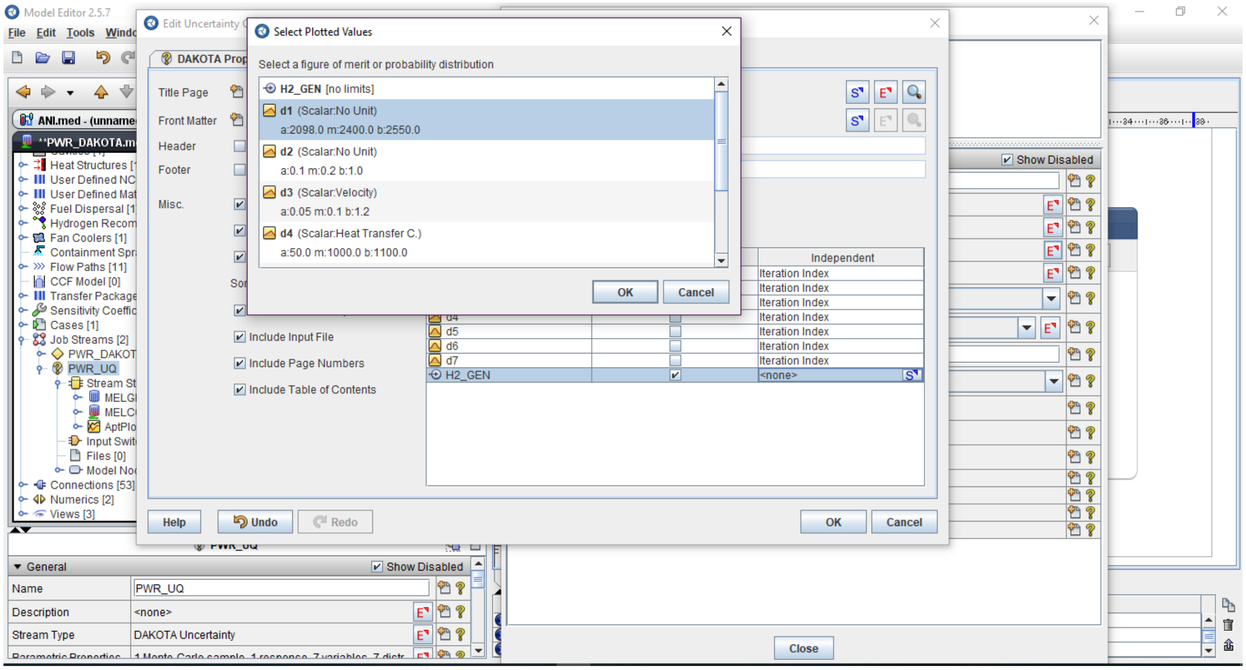

Figure 3-35 Plot of the FOM as Function of a Desired Input Distribution

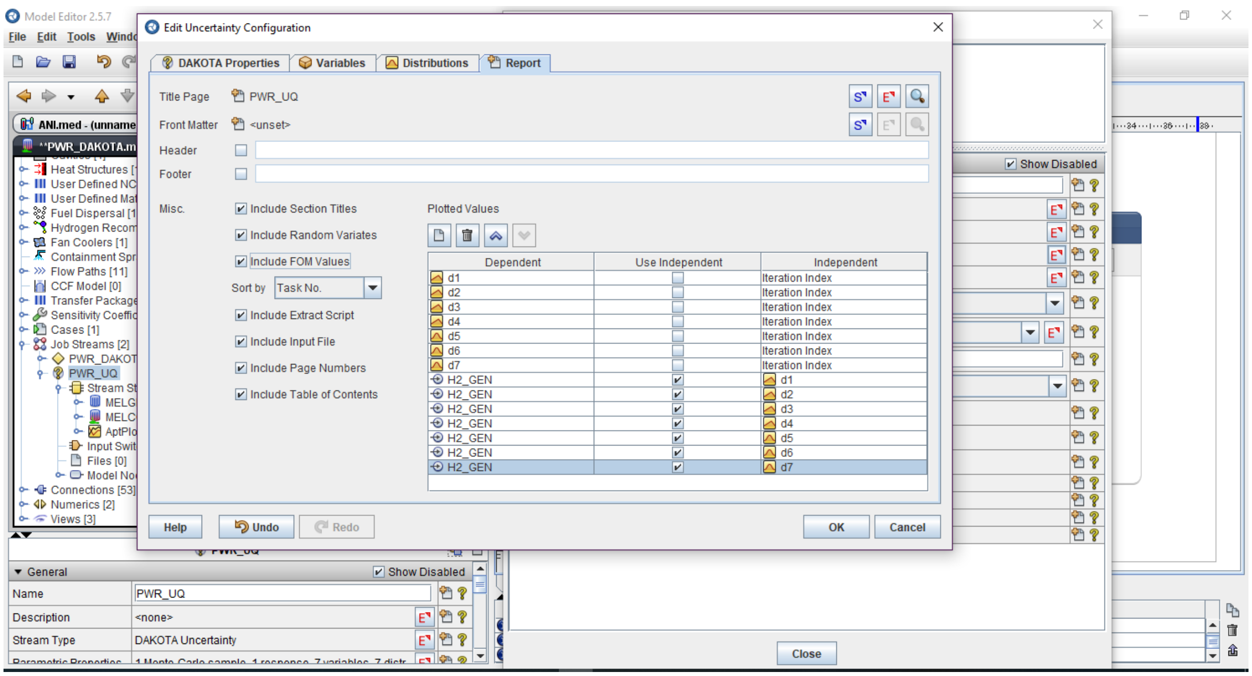

Figure 3-36 View of the FOM Plotted as Function of the Input Uncertain Parameters

3.2 Setting-up the Plotting Step

Similar to the MELGEN/MELCOR steps, creation of the two-step job stream has automatically created an AptPlot step (in more recent SNAP versions the AptPlot stream step is automatically generated with the Three-step MELGEN/MELCOR/APTPLOT stream) for plotting the results (Figure 3-37). The setup of the UA allows at this point the definition of the properties of the AptPlot step. From the AptPlot Properties View (Figure 3-38) it is possible to change the step name (in this case we decide to call it 2DPLOT). Also, by selecting the Plot Inputs Definition Button (Figure 3-39), the File Set flag should be set to True (Figure 3-40).

Open the AptPlot step properties by click on the Plot button (Figure 3-41). In the Edit Plot Properties View it is possible to edit the properties of the plot (Figure 3-42), the graph (Figure 3-43), and the uncertain input parameters data sets (Figure 3-44). In the Edit Plot Property View it is possible to specify the parameters for the plot which could include FOMs as well as other parameters. The reader may note that only one set is displayed at this moment and not all the sets correspondent to the set of uncertainty code runs. In order to add all the sets, it is necessary to set the model nodes as parametric. In the Uncertainty Job Stream open the Model Nodes Views followed by the MELGEN step (Figure 3-45) and set the Parametric flag to True (Figure 3-46). Repeat the same process for the MELCOR step (Figure 3-47 and Figure 3-48). Returning to the AptPlot Edit Plot Properties View, the reader may note that all sets are now displayed (Figure 3-49) and it is possible to open each set (Figure 3-50). The user may add all desired plots at this point.

Finally, the AptPlot step should be connected to the calculation results of the MELCOR step. In the Stream Steps right-click on the AptPlot step and add it to the stream view (Figure 3-51)[9]. It should already be connected to the Plot output of the MELCOR step (Figure 3-52).

[9] In more recent Model Editor version (e.g. 3.1.3) this step is already done, if it is selected the Three-Step MELGEN/MELCOR/APTPLOT stream.

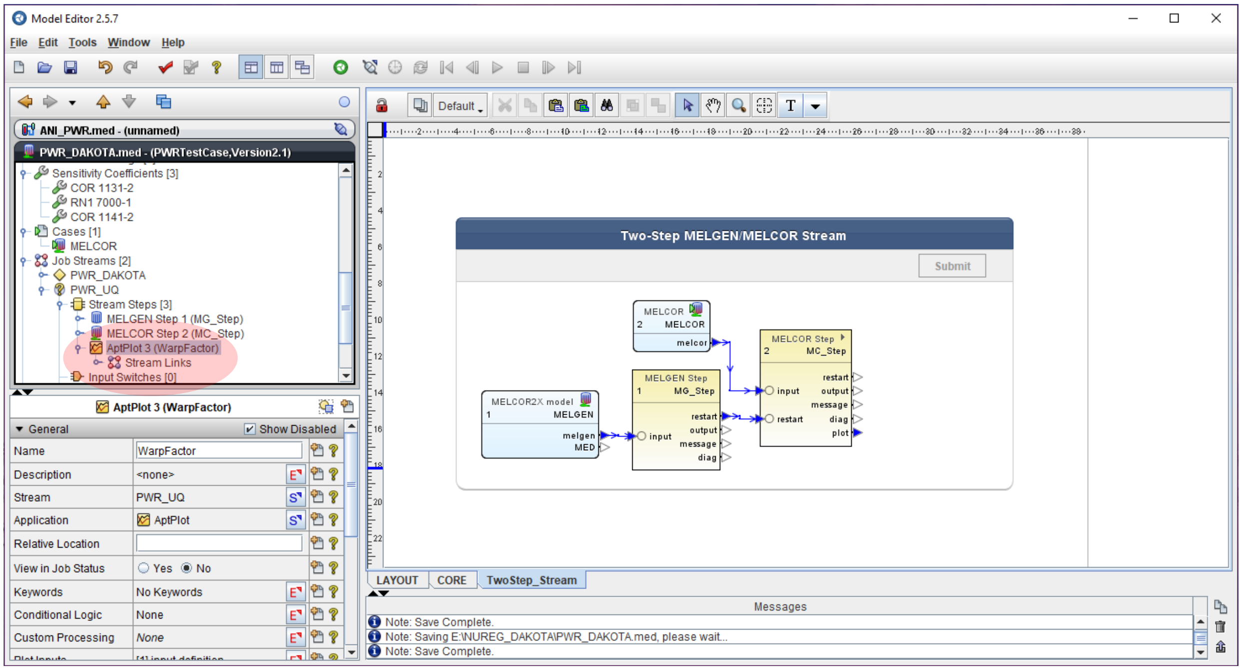

Figure 3-37 Selection of the AptPlot Stream Step

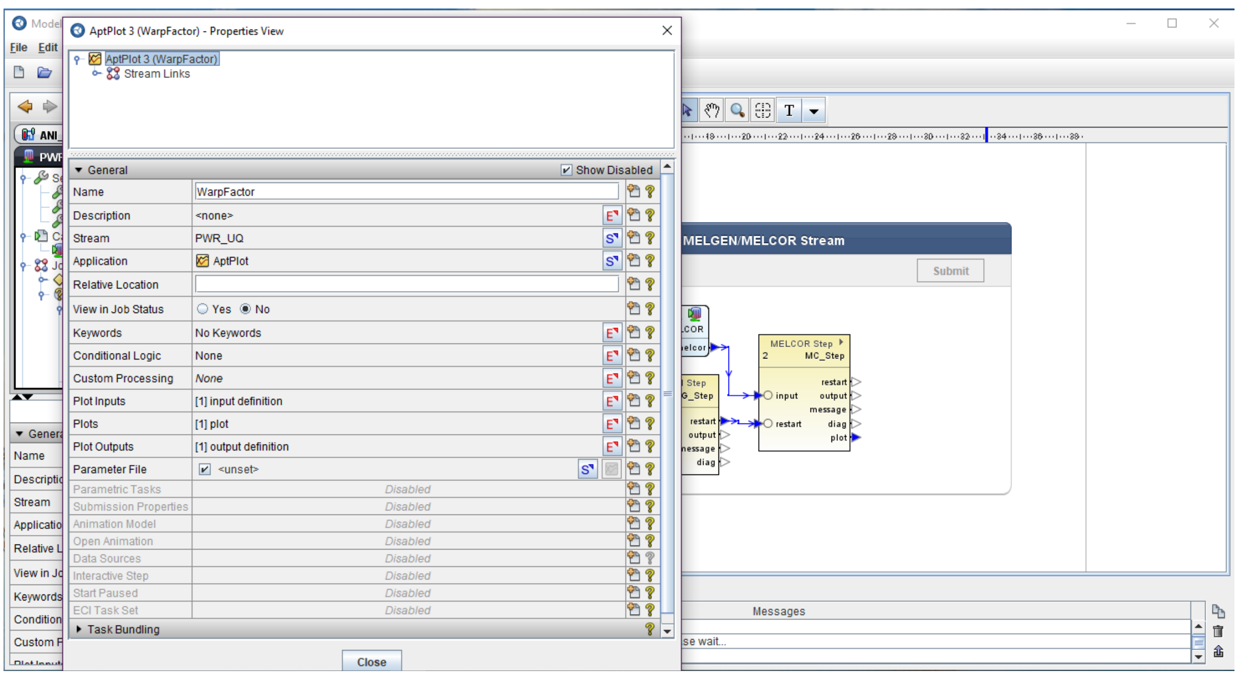

Figure 3-38 Properties View of the AptPlot Stream Step

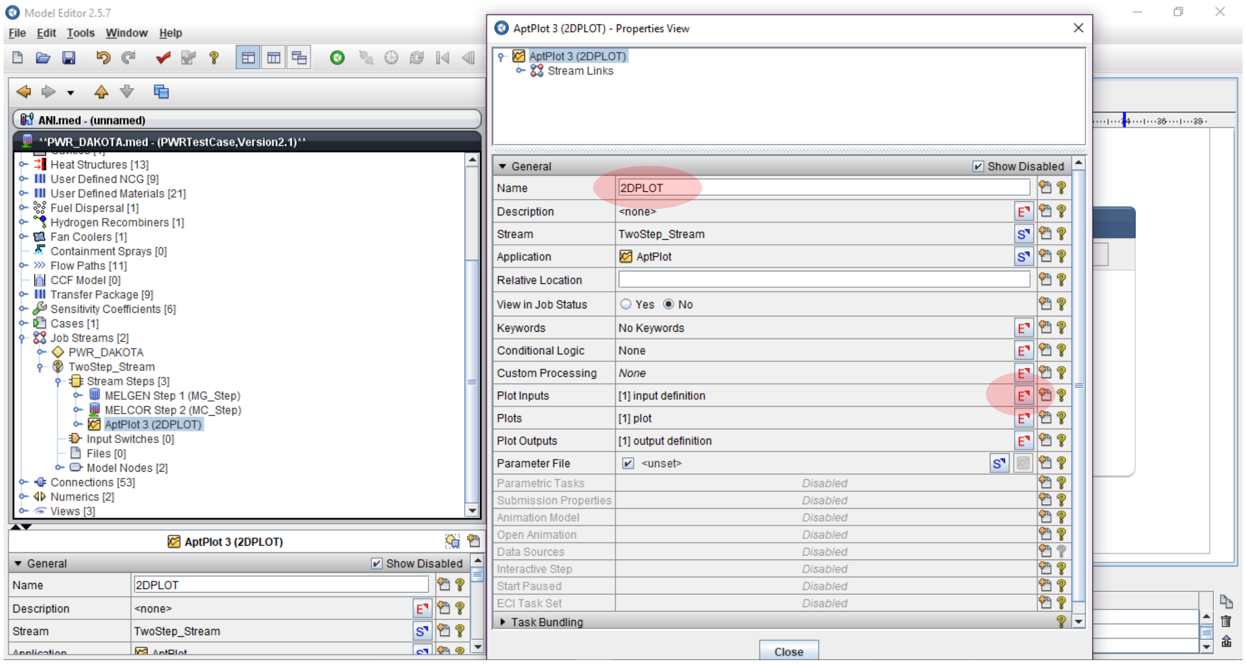

Figure 3-39 Naming of the AptPlot Stream Step and Selection of Plot Inputs Button for the AptPlot Stream Step Input Definition

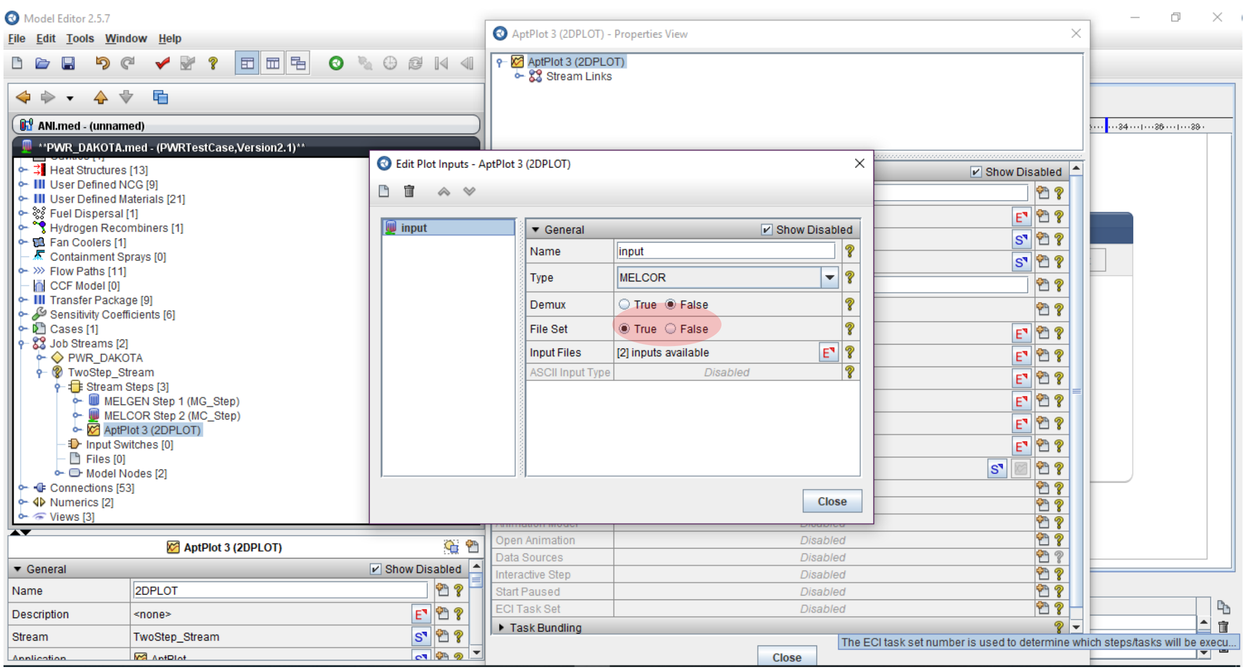

Figure 3-40 Setting the File Set as True in the Edit Plot Inputs Tab of the AptPlot Stream Step

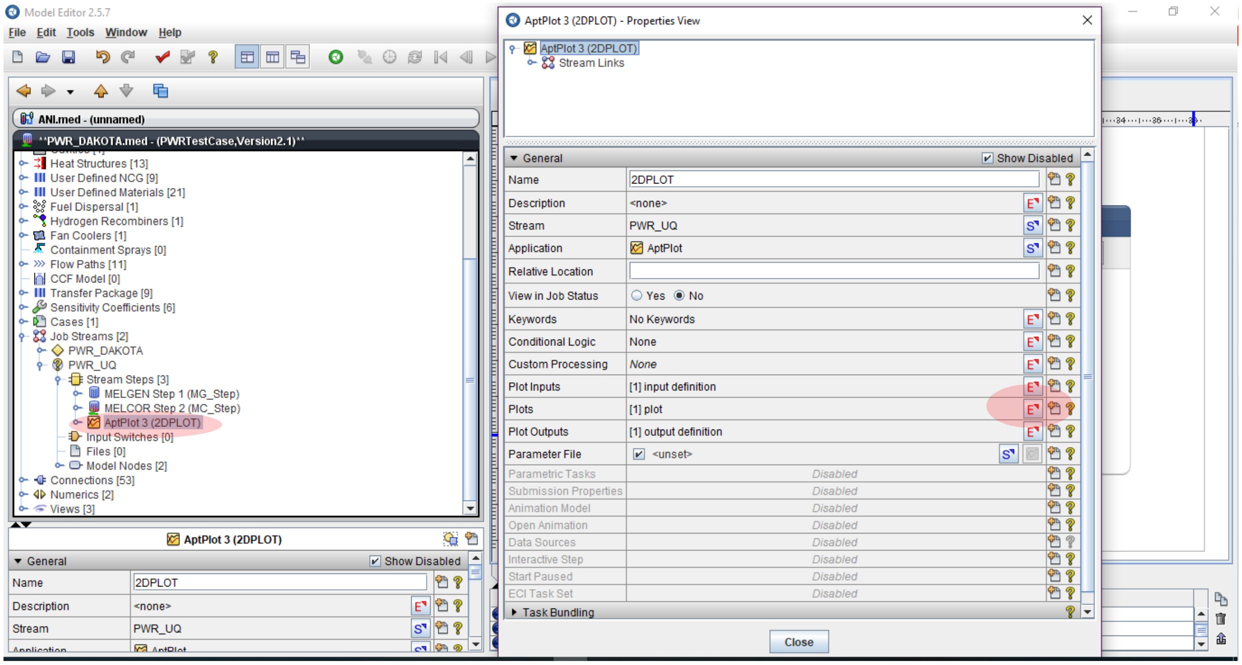

Figure 3-41 Definition of the Plots in the AptPlot Step

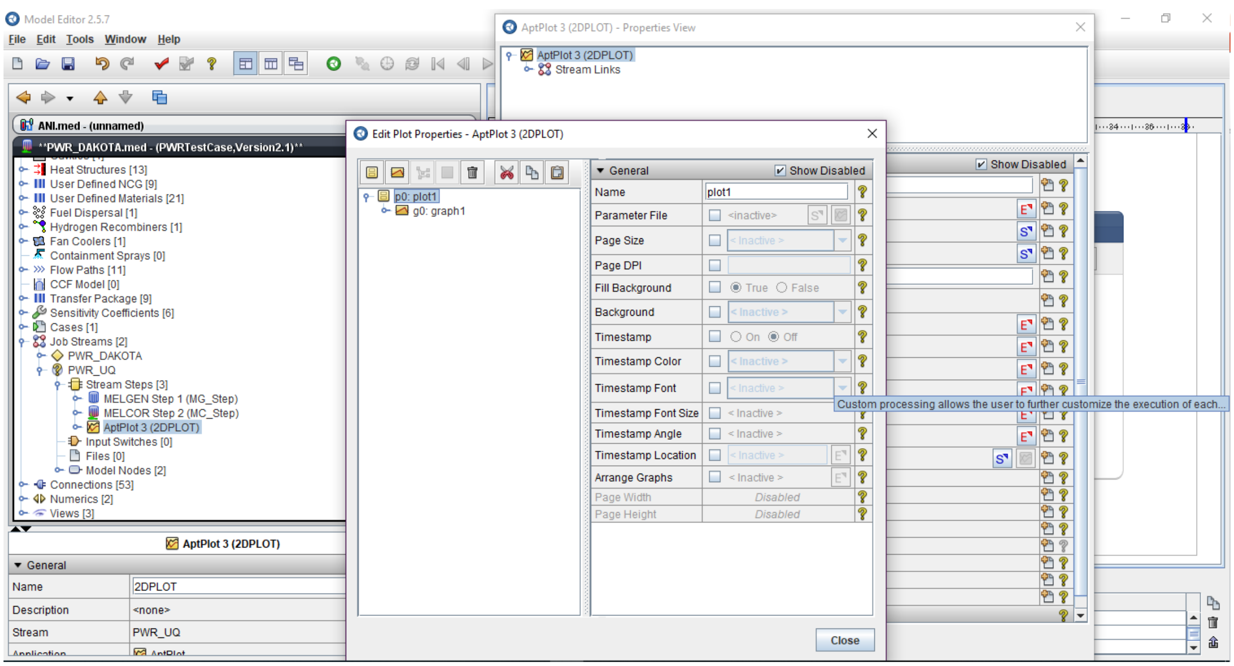

Figure 3-42 Editing of Plot Properties

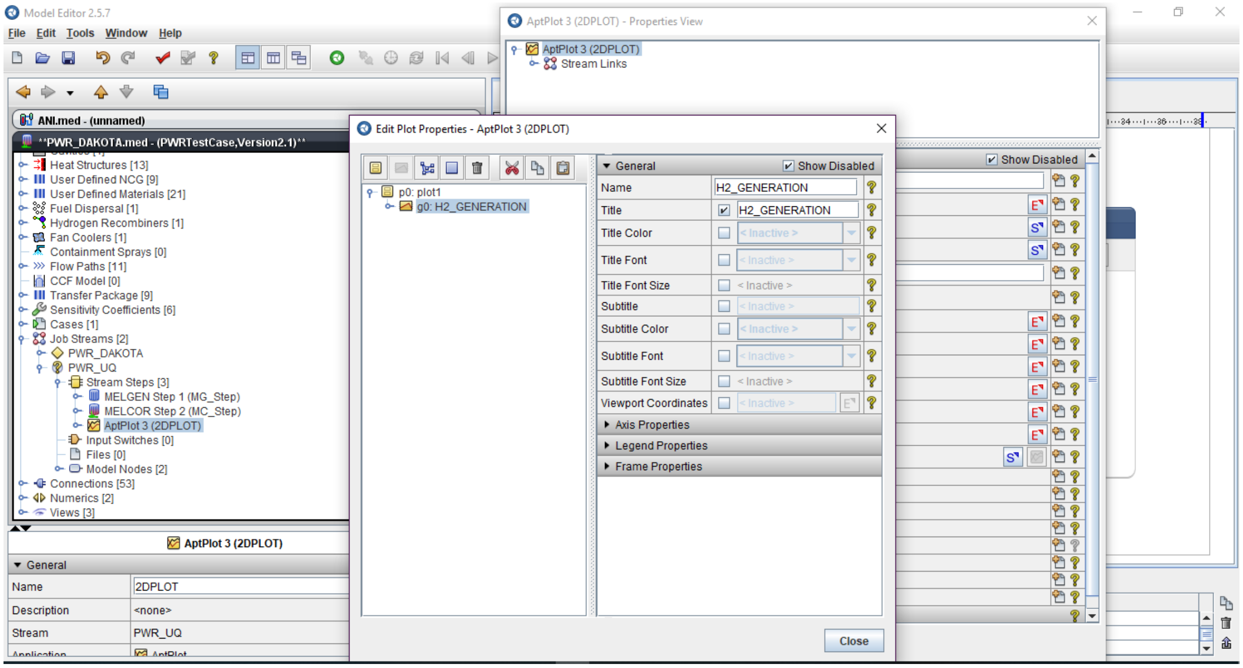

Figure 3-43 Editing of Graph Properties

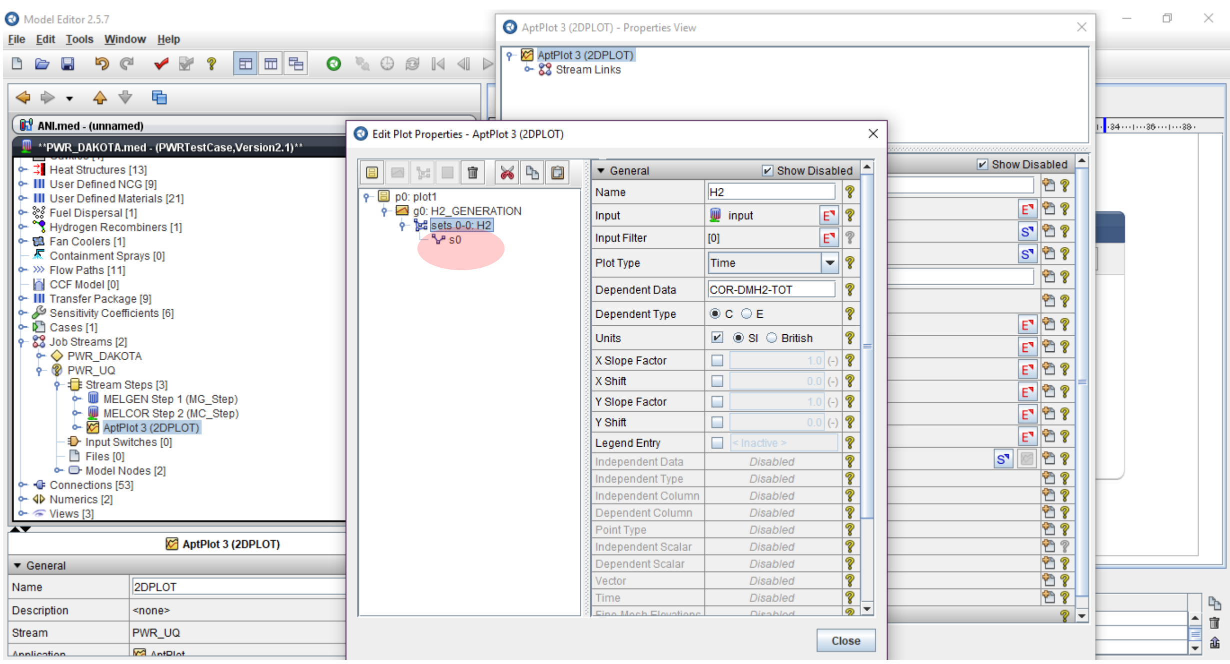

Figure 3-44 Visualization of the Set in the Graph (only one set is displayed at this point)

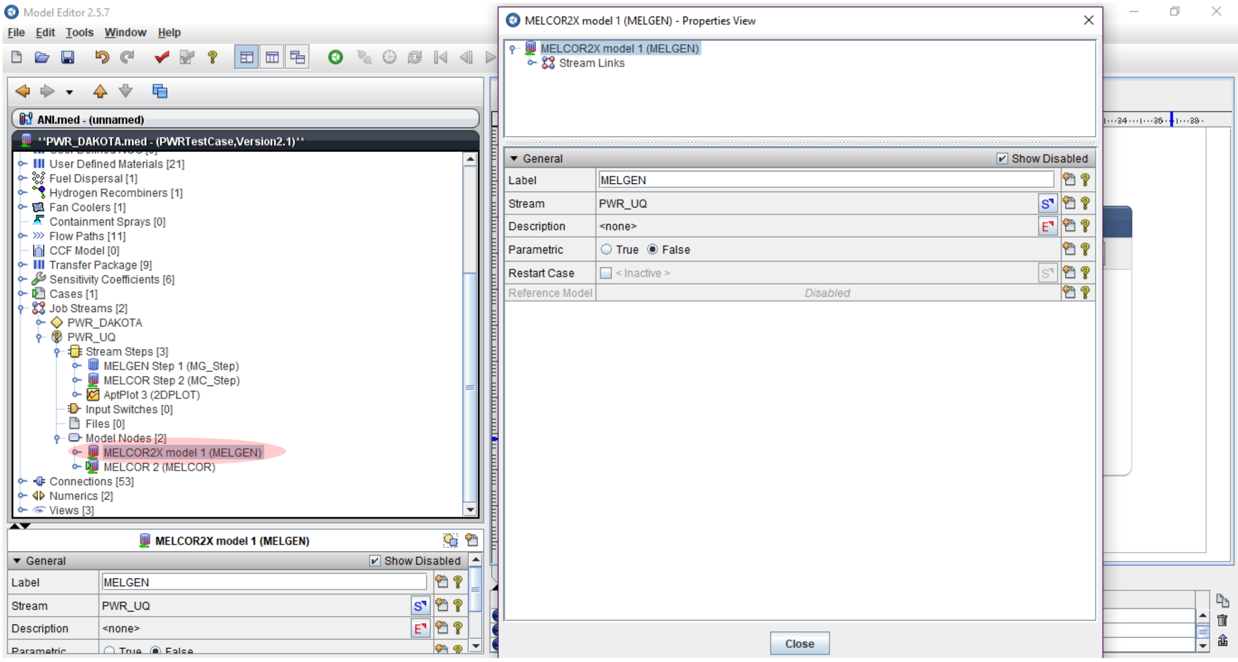

Figure 3-45 Selection of the Parametric Option for the MELGEN Step

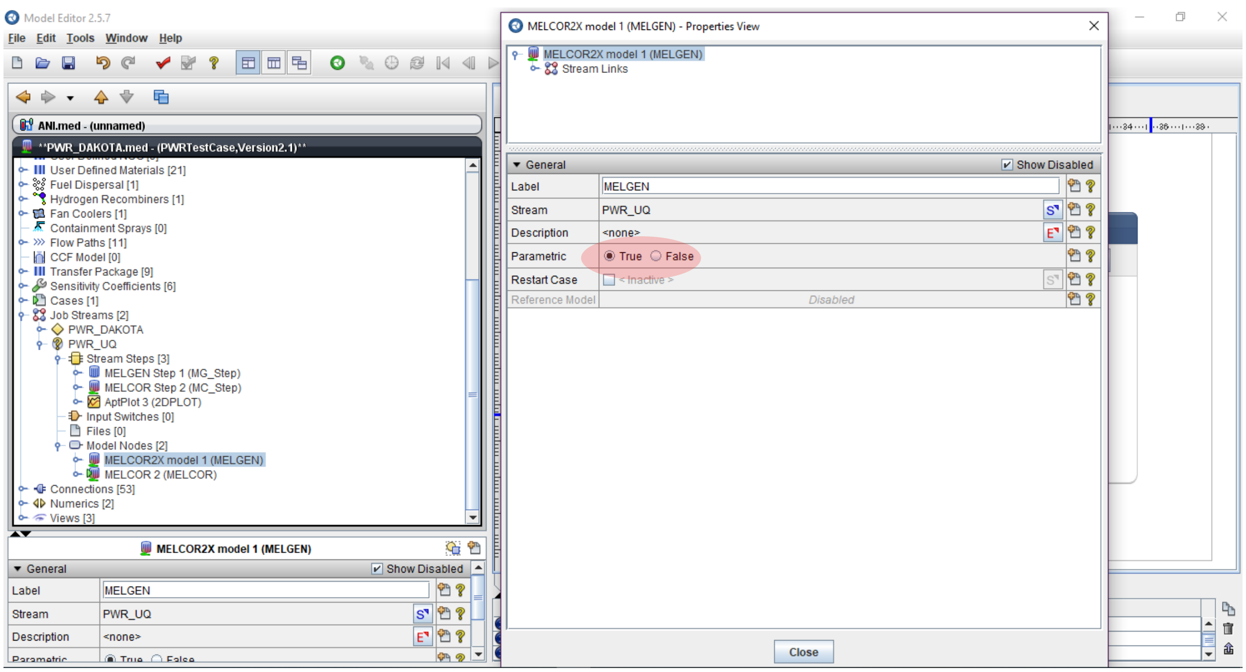

Figure 3-46 Parametric Set as True in the MELGEN Step

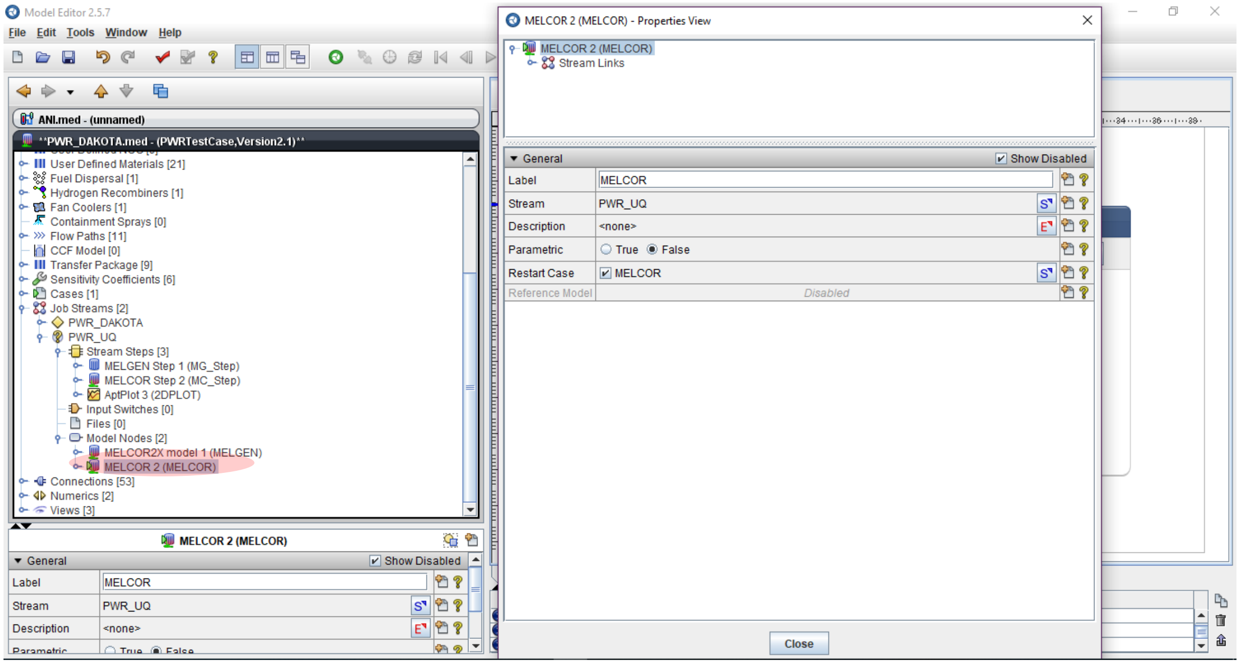

Figure 3-47 Selection of the Parametric Option for the MELCOR Step

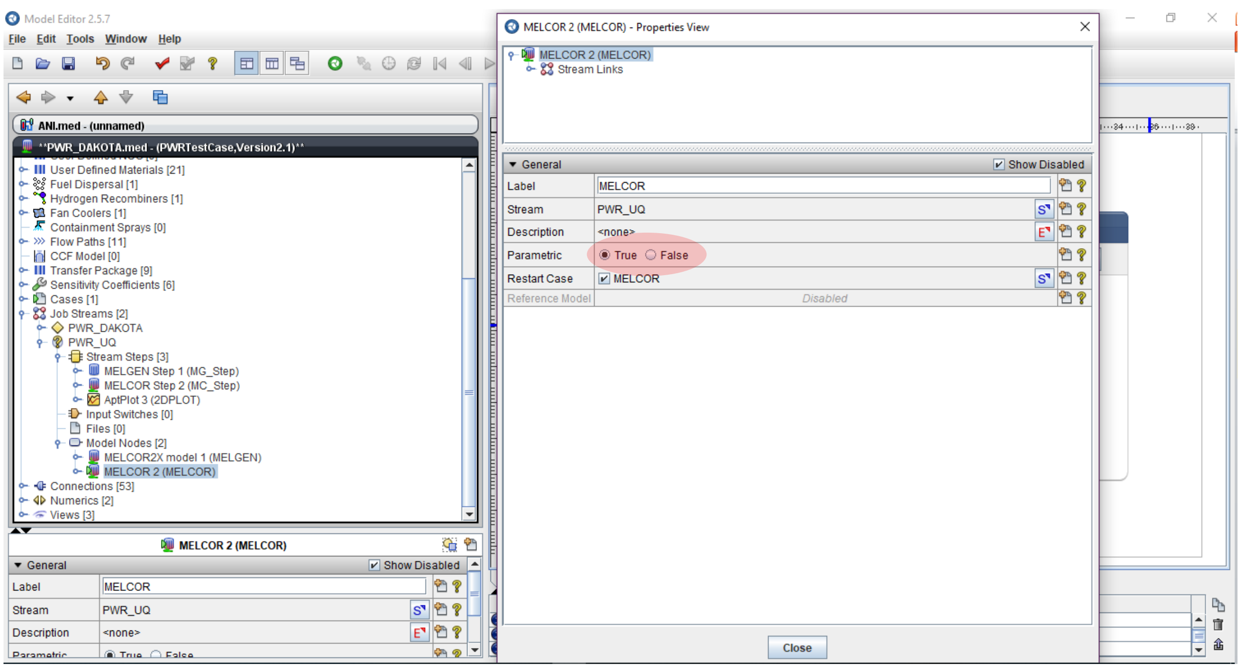

Figure 3-48 Parametric Set as True in the MELCOR Step

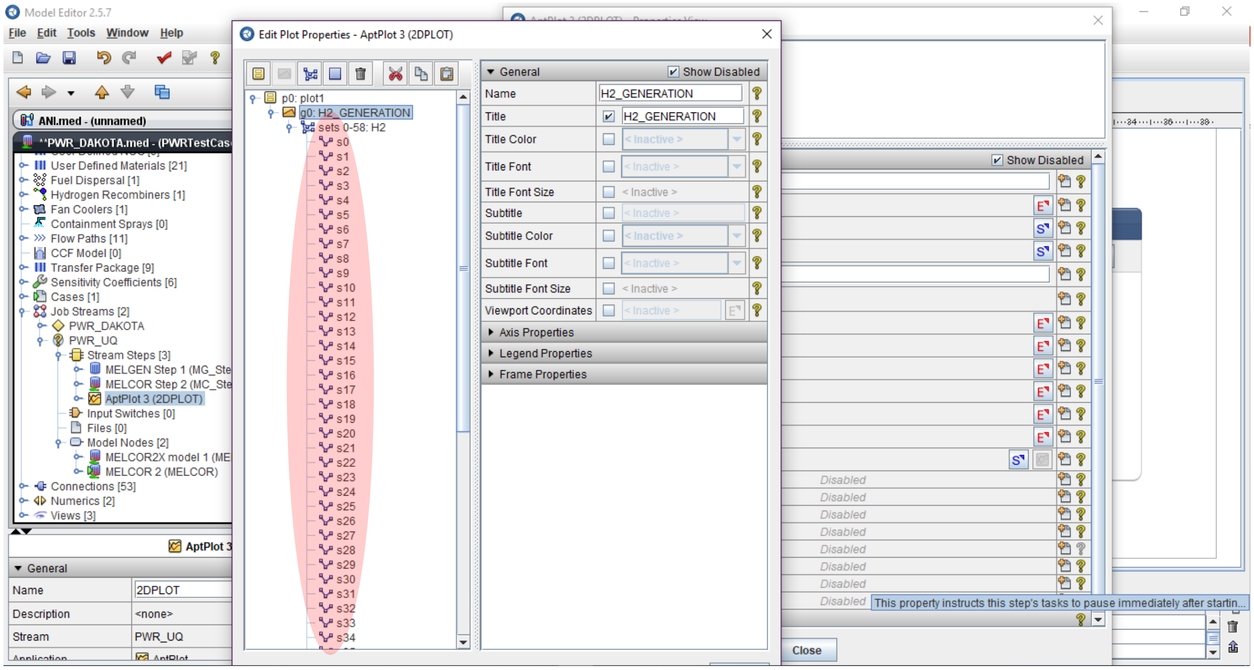

Figure 3-49 Visualization of the Sets in the Graph (all the sets are now displayed)

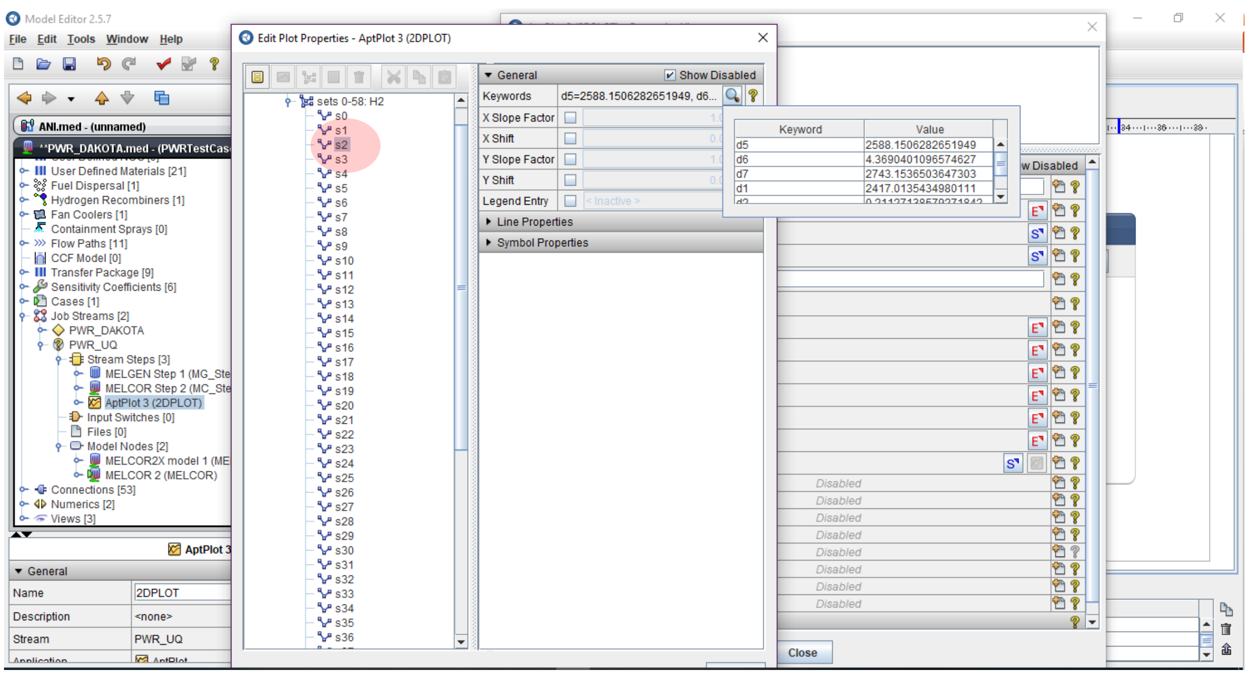

Figure 3-50 Visualization of a Specific Set

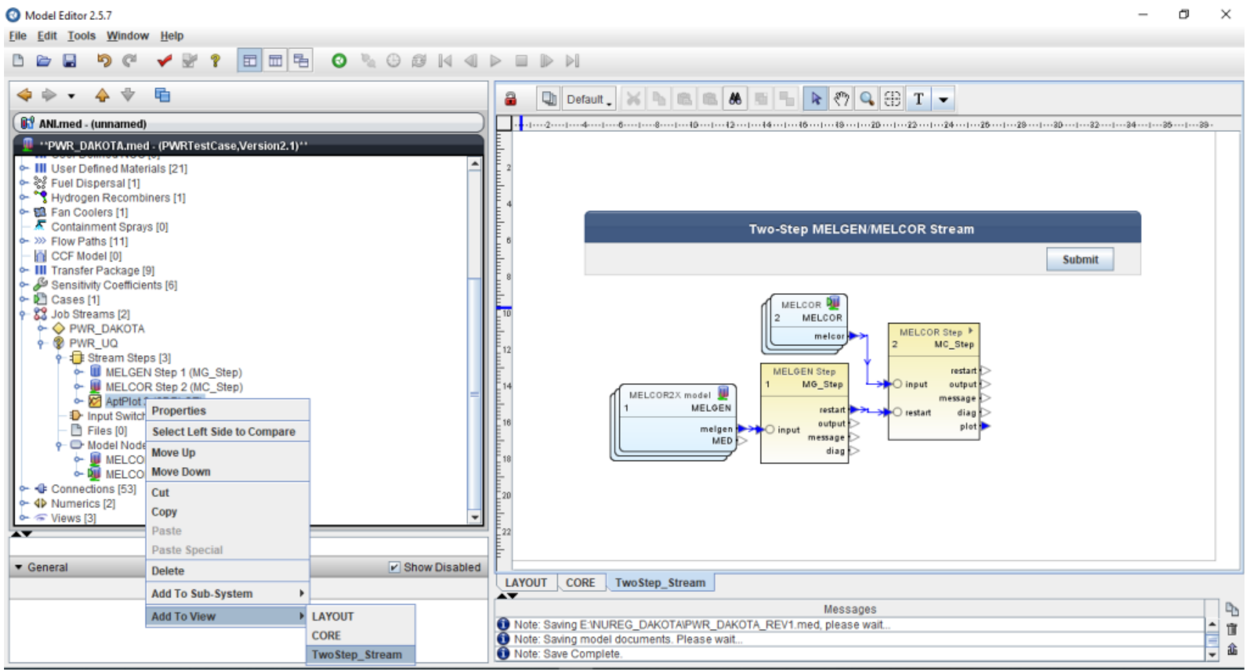

Figure 3-51 Adding the AptPlot Step in the Stream View

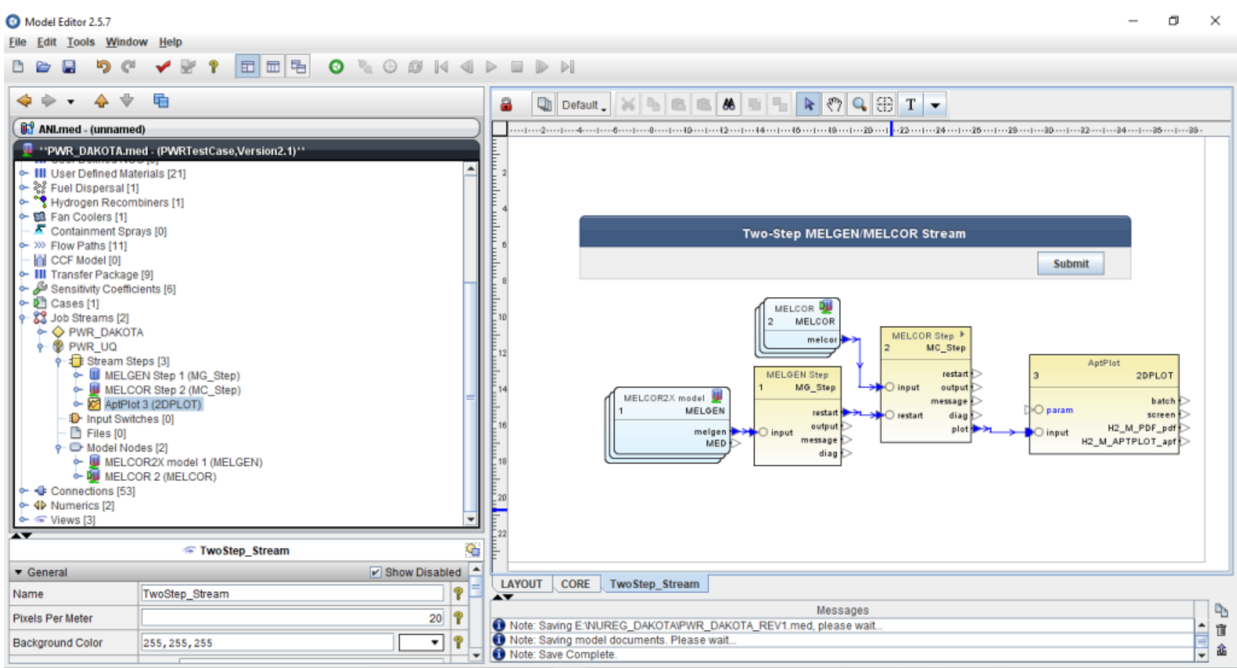

Figure 3-52 Connecting the AptPlot Step to the Output of the MELCOR Step

3.3 Setting-up Data Extraction Step

The necessary inputs for DAKOTA to create a set of code inputs for the required number of tasks and for the AptPlot plotting step have been defined and described in the previous sections. At this point, results extraction from the simulation output is necessary.

In the Job Stream, right-click on the Stream Steps and select New (Figure 3-53) and then Extract_Data (Figure 3-54). Open the properties of the newly created Extract data step and select the Plot Type File MELCOR (Figure 3-55). The reader should note that the Input File field indicates missing files are required. By clicking the related button, the Define Input Files For Extract Data Tab is opened and the Source is indicated as disconnected and is red (Figure 3-56). By opening the related selection window, it is possible to Select Input Source; then MELCOR Step 2 plot is selected (Figure 3-57) and will be visible in the input file window (Figure 3-58).

The required variable to be extracted is still missing and an AptPlot script is needed to perform the extraction. The script can be entered by opening the AptPlot Script window (Figure 3-59) and an AptPlot command should be entered by the user in the central part of the script window (Figure 3-60). The variable to be extracted should be inserted by the user in the central part of the script (Figure 3-61). Several extraction possibilities are available in AptPlot. In this case we have decided to extract the value of the FOM at 24000s. The last process is to add the Extract Data Step to the Job Stream View. By right-clicking on it and selecting Add to View (Figure 3-62), it will be automatically connected to the plot output of the MELCOR step (Figure 3-63).

3.4 Setting-up DAKOTA Uncertainty Step

The final task to be completed for the UA setup is the DAKOTA Uncertainty Quantification Step that produces the output of the analysis. In the Job Stream Steps, right-click and select new, then select DAKOTA (DAKOTA Uncertainty Quantification) (Figure 3-64). Then, the DAKOTA uncertainty step will be created, and its properties edited within the Properties View (Figure 3-65). The DAKOTA step should be added to the Uncertainty Job Stream View (Figure 3-66) and then connected to the vars output of the Extract Data step (Figure 3-67, Figure 3-68 and Figure 3-69).

At this point the UA setup is completed and it is possible to run the Job Stream.

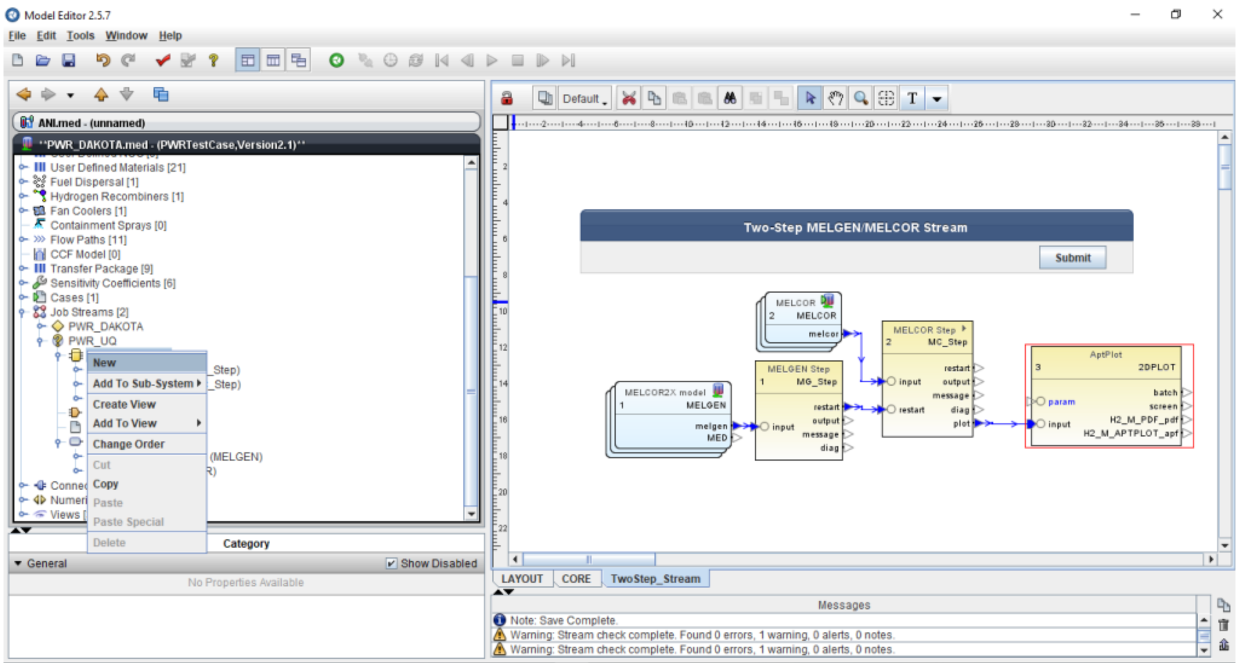

Figure 3-53 Creation of a New Step in the Job Stream Step

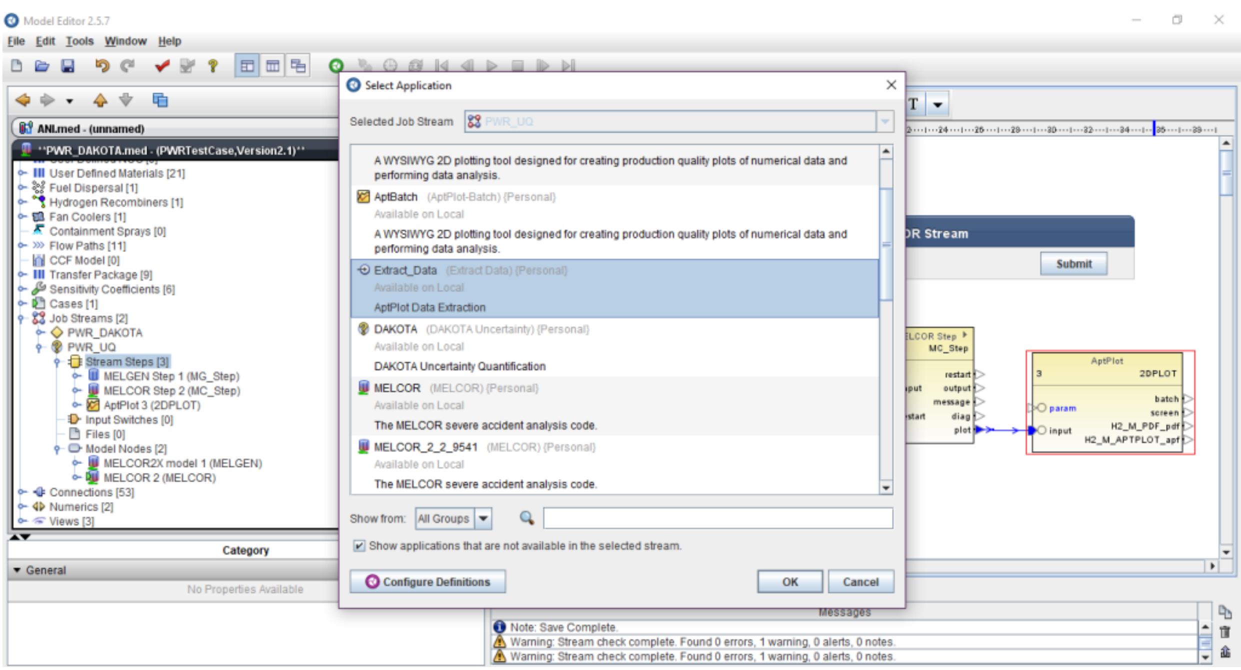

Figure 3-54 Selection of an Extract Data Step

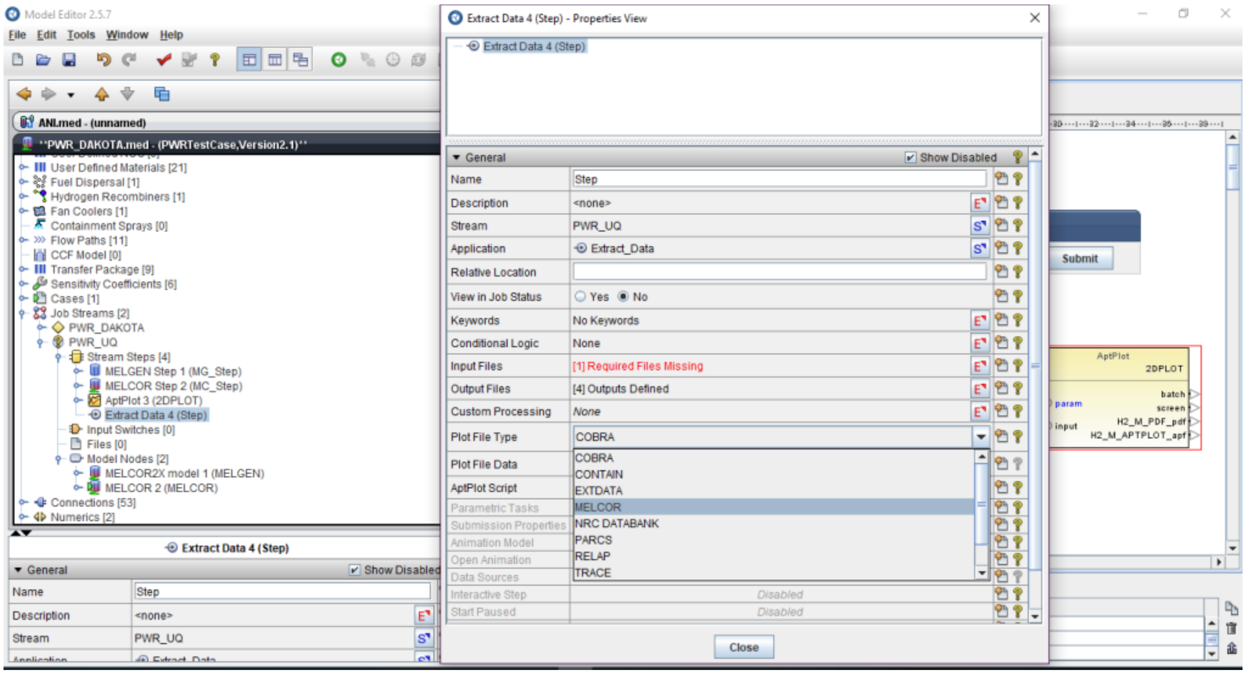

Figure 3-55 Selection of the Plot File Type in the Extract Data Step

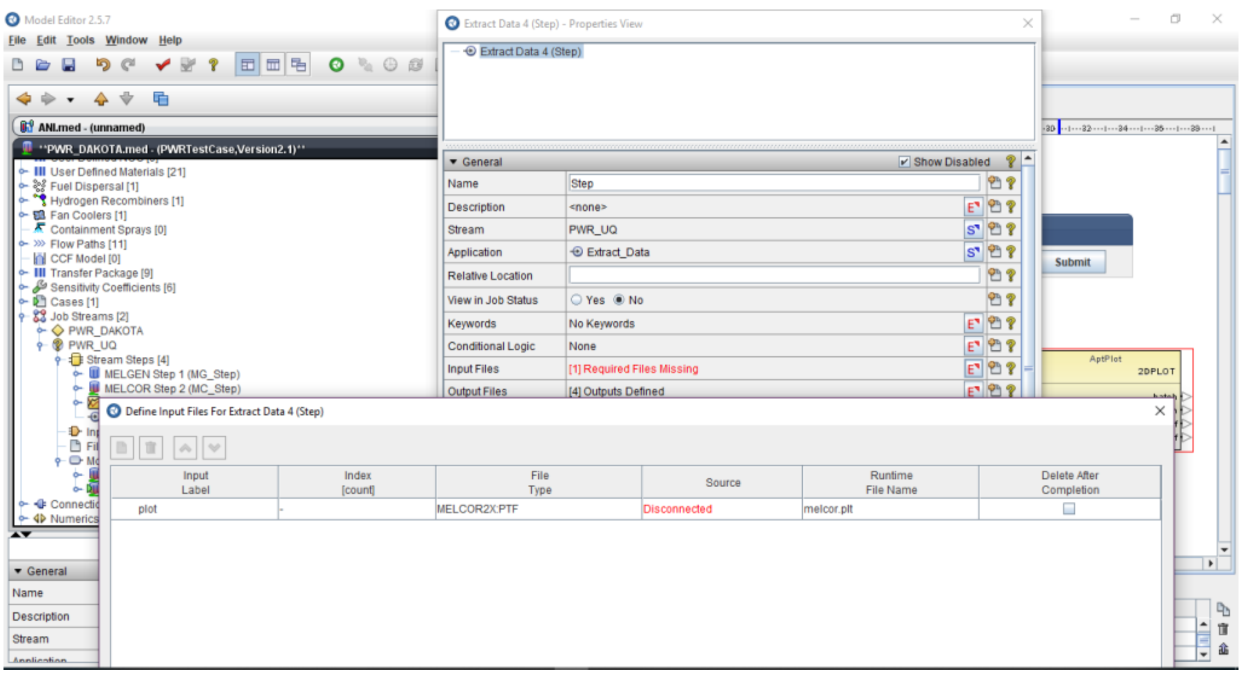

Figure 3-56 Definition of the Input Source for the Extract Data Step

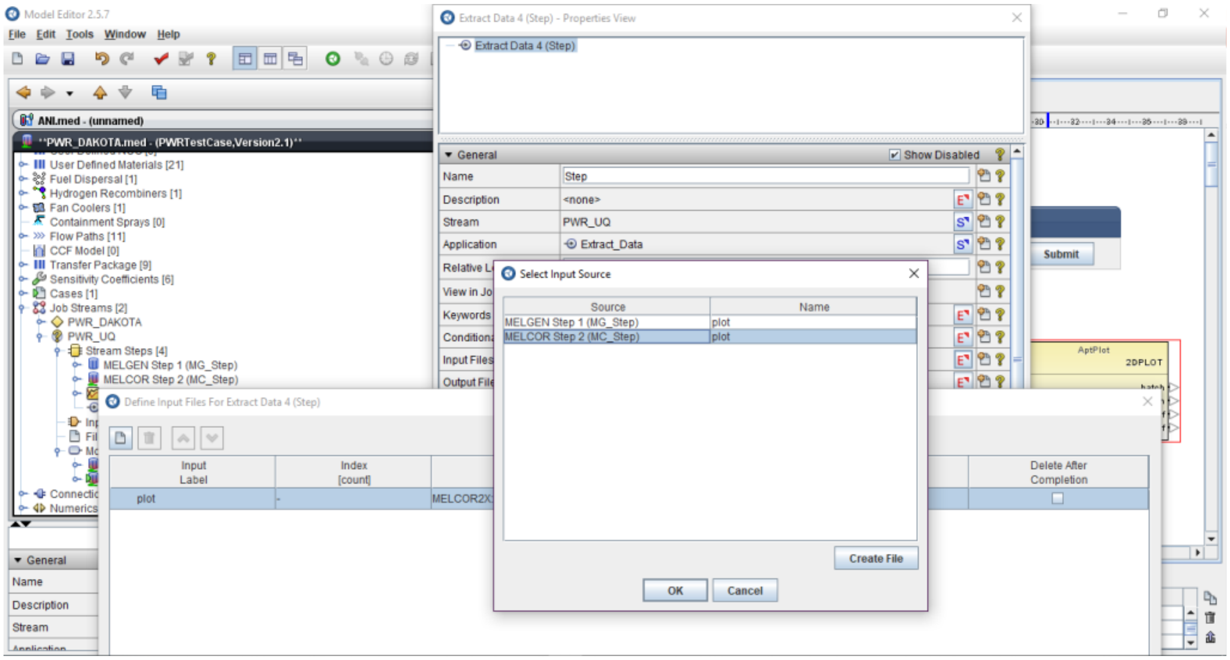

Figure 3-57 Selection of the Desired Input Source

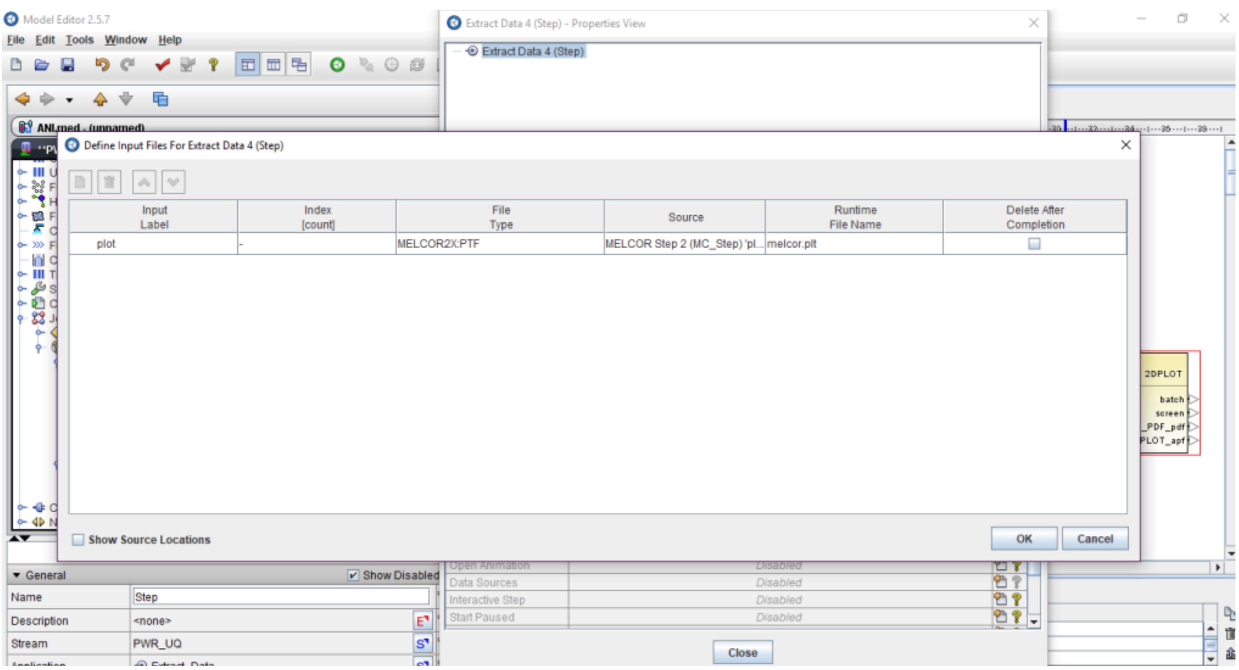

Figure 3-58 Selected Input Source for the Extract Data Step

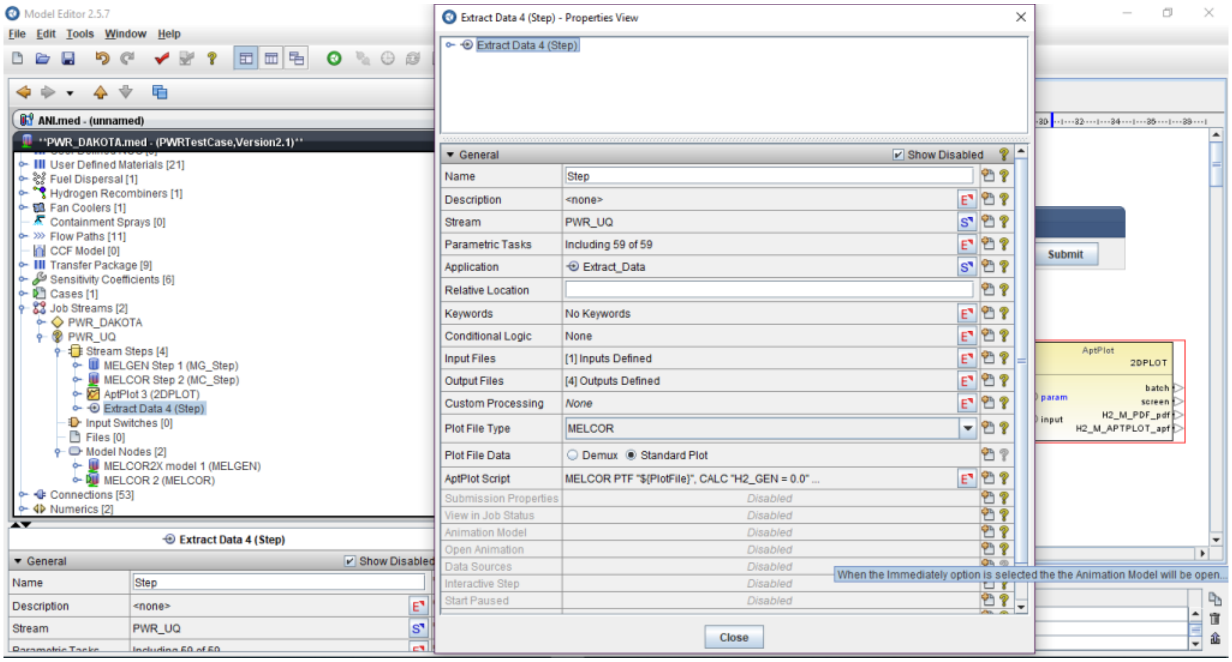

Figure 3-59 Opening of the AptPlot Script Window

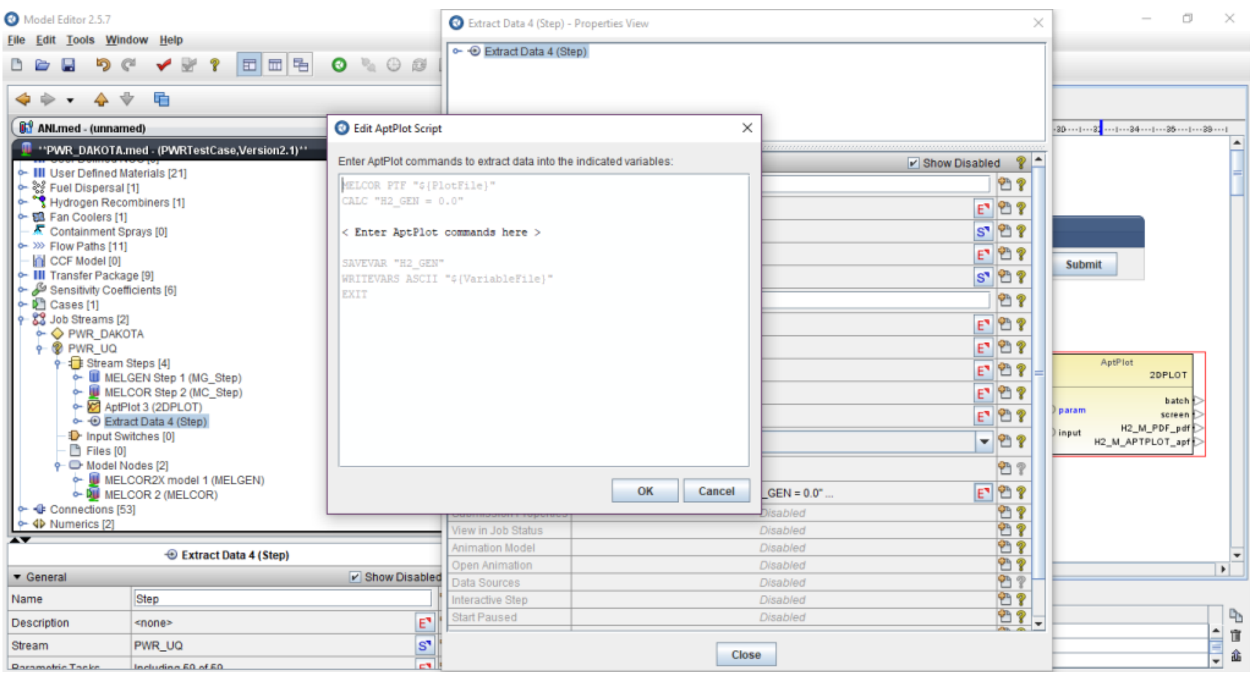

Figure 3-60 The AptPlot Script Window

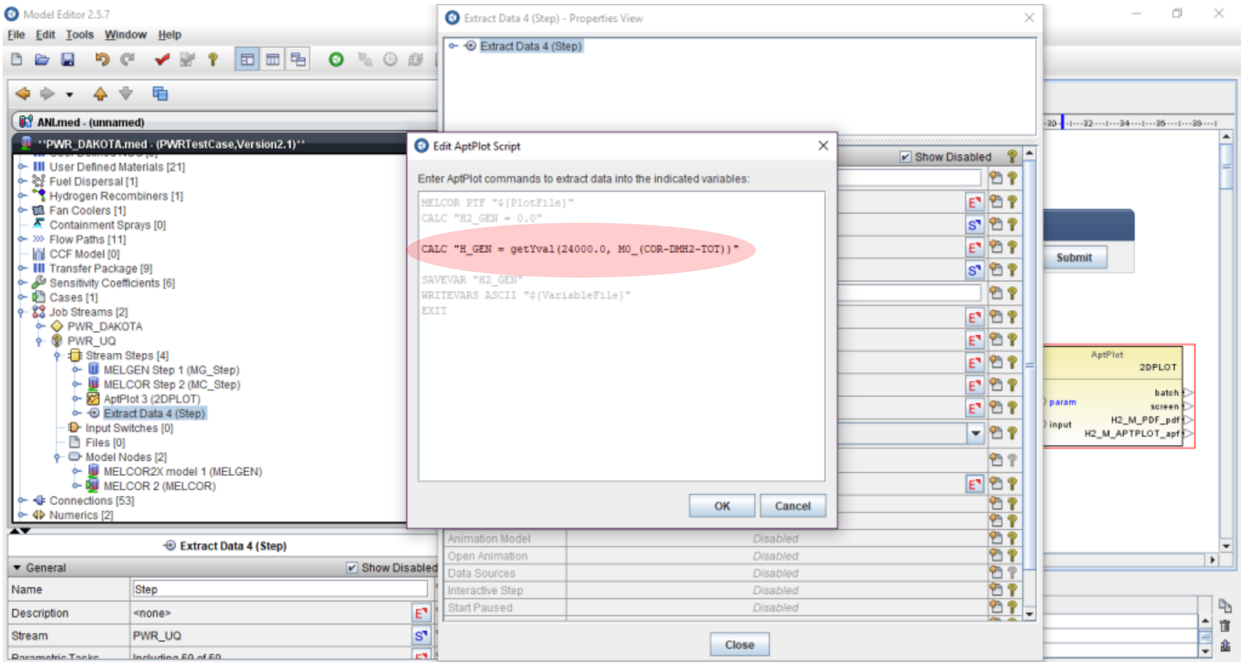

Figure 3-61 The Script for the Extraction of the Calculation Results for the DAKOTA UA

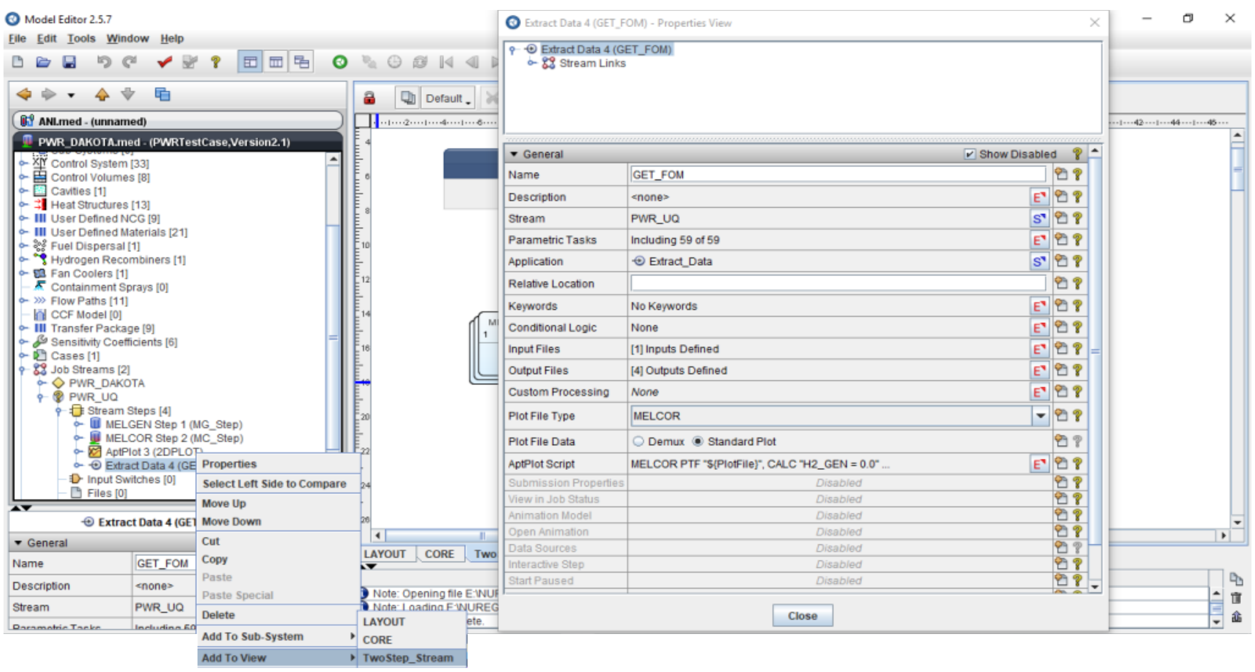

Figure 3-62 Adding the Extract Data to the Uncertainty Stream View

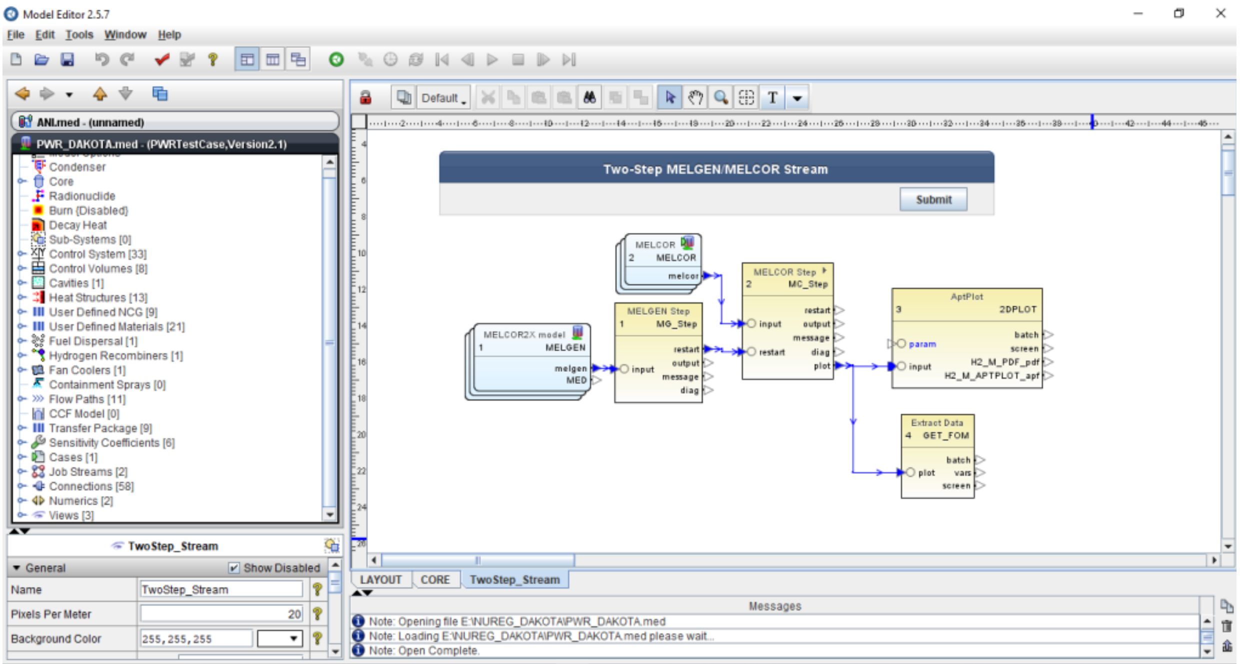

Figure 3-63 The Job Stream After the Connection of the Extract Data Step

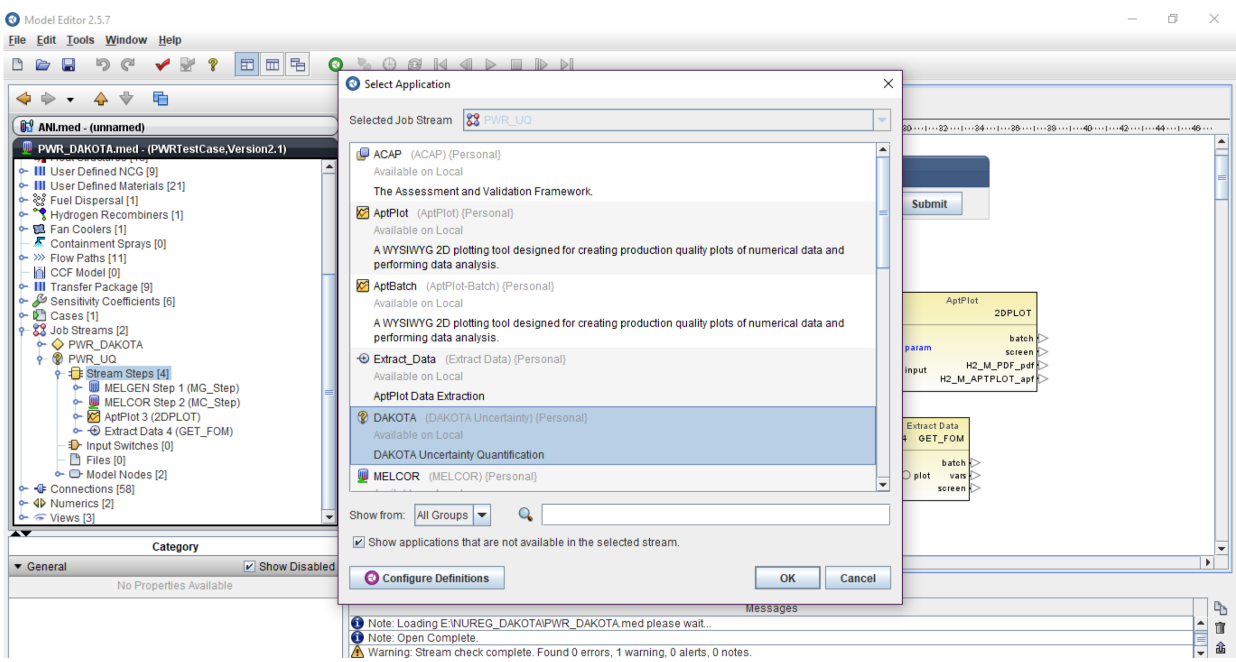

Figure 3-64 Adding the DAKOTA Uncertainty Step

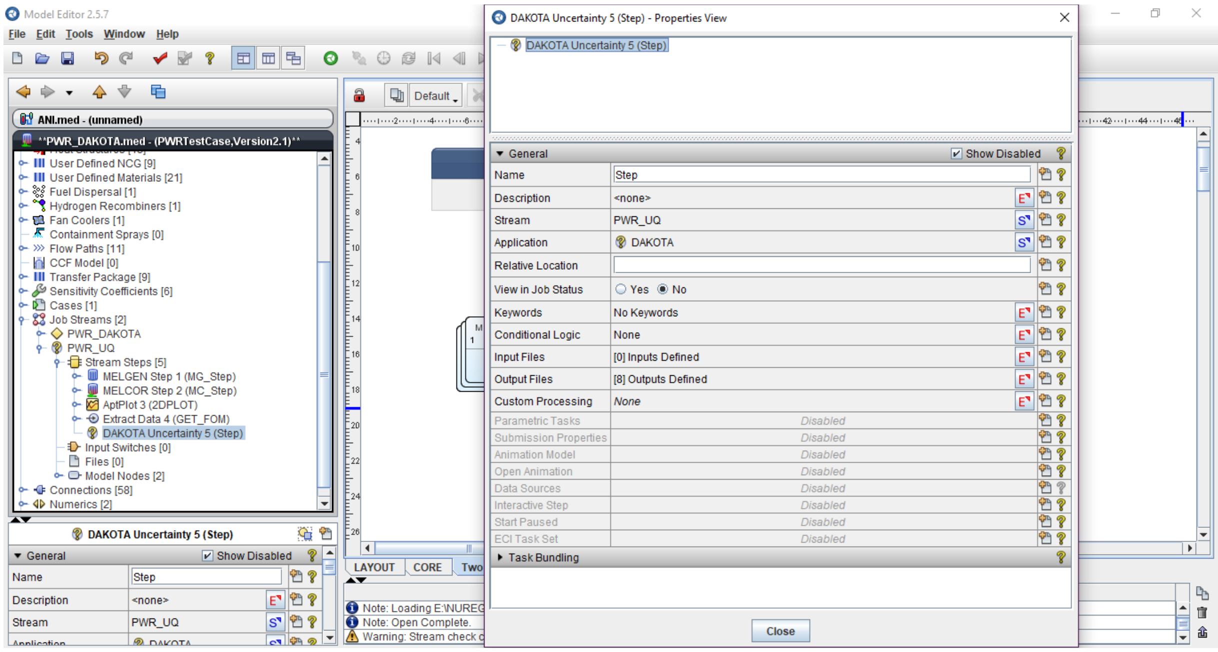

Figure 3-65 Properties of the DAKOTA Uncertainty Step

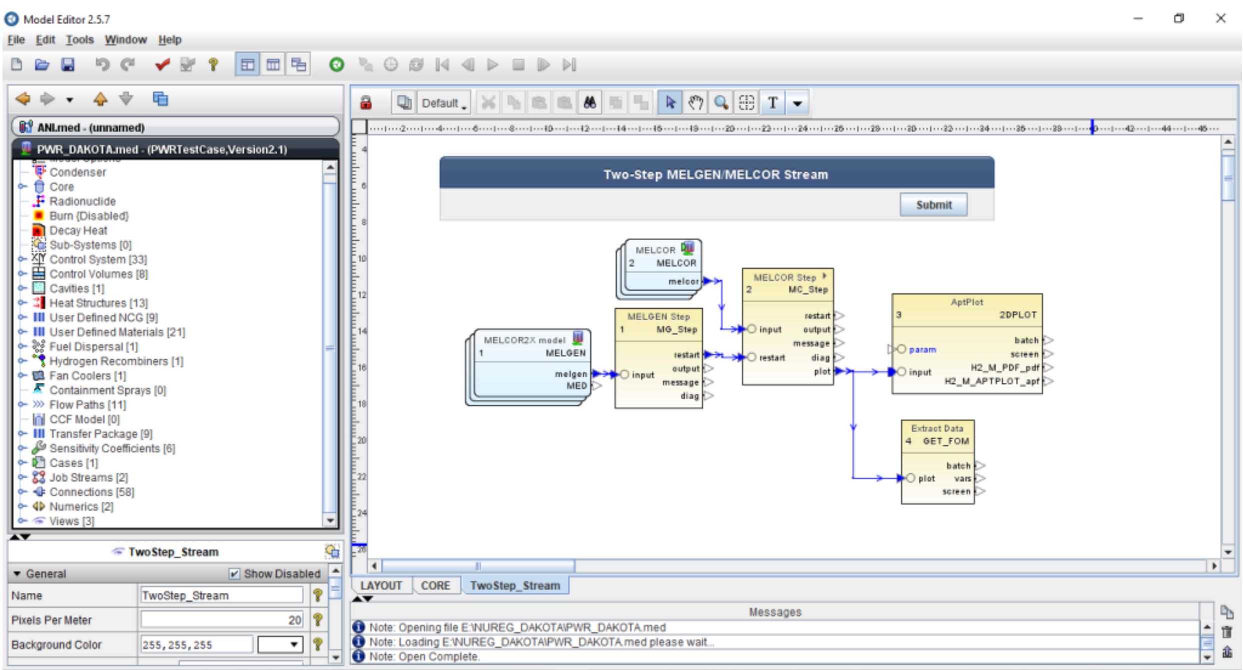

Figure 3-66 Adding the DAKOTA Step to the Uncertainty Stream View (DAKOTA step missing)

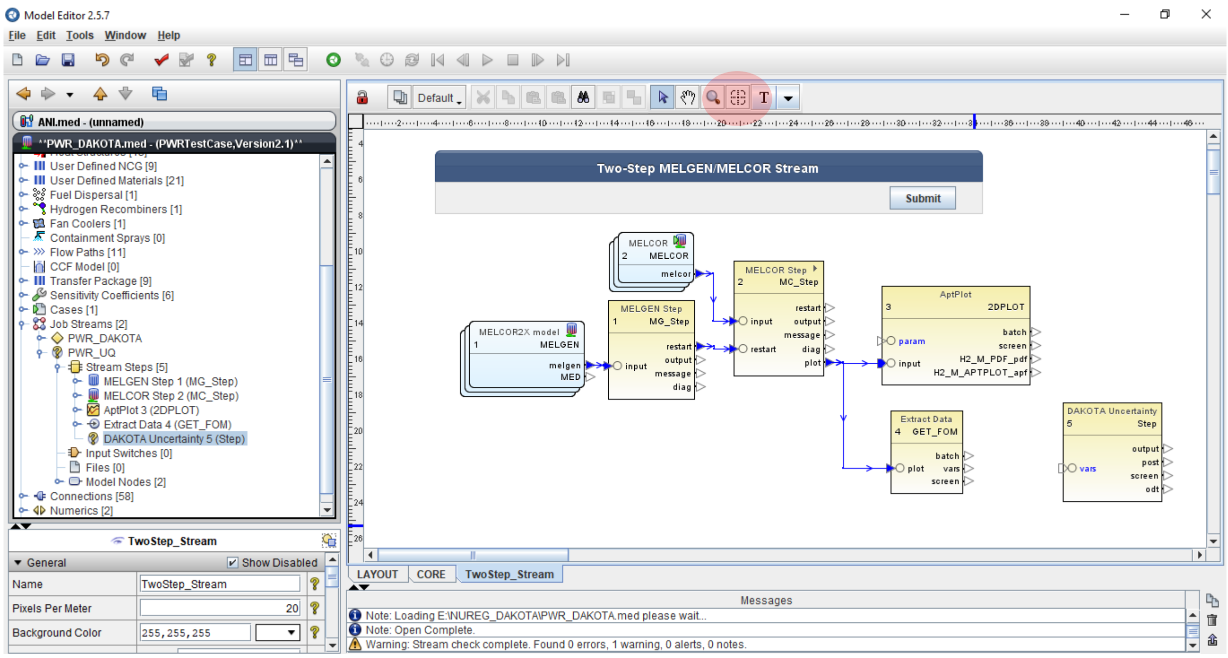

Figure 3-67 View of the Uncertainty Stream with the DAKOTA Step Unconnected

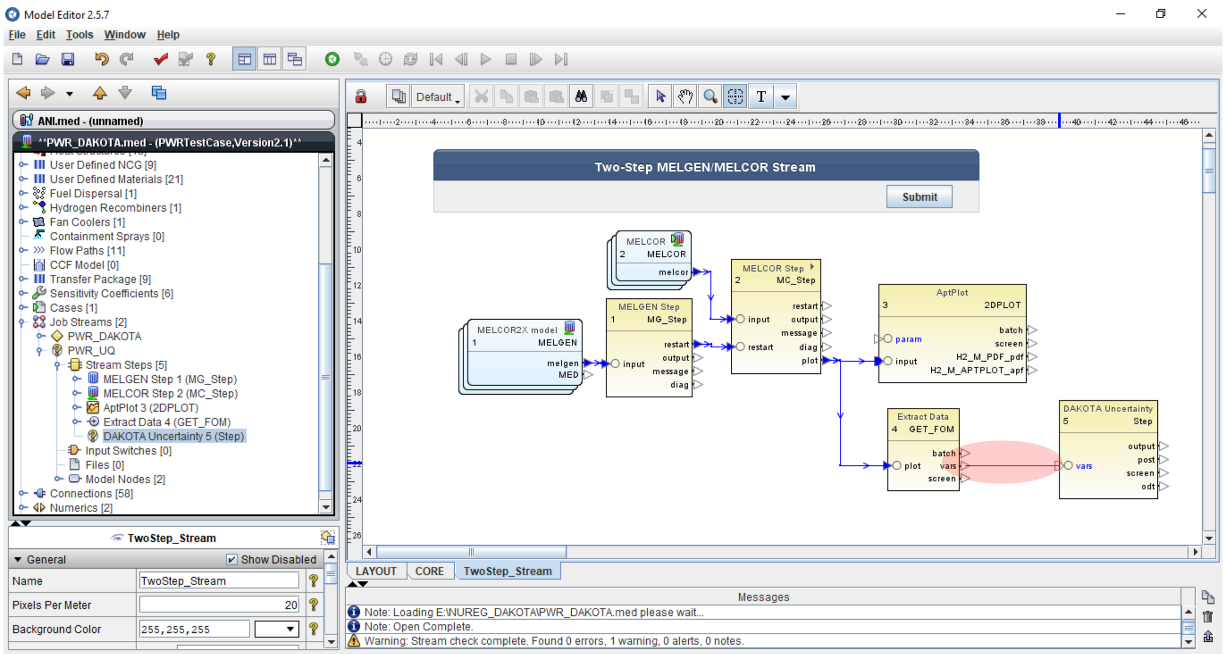

Figure 3-68 Adding the Connection between the Extract Data Step and the DAKOTA Step

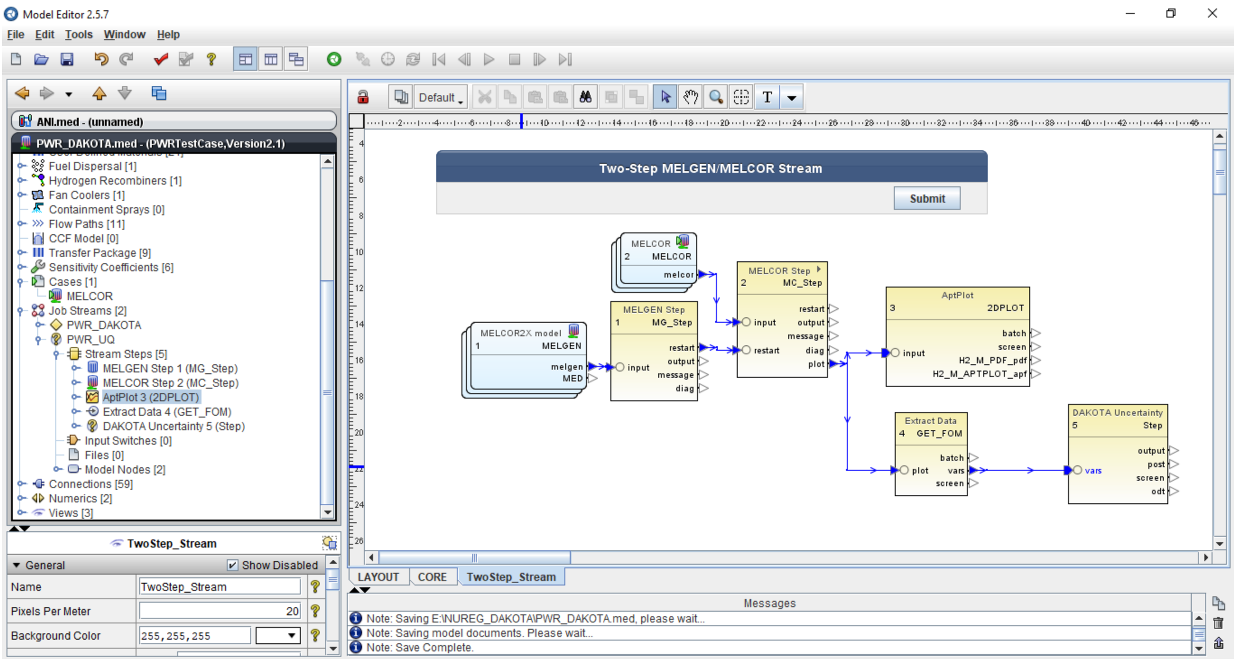

Figure 3-69 View of the Uncertainty Stream with the DAKOTA Step Connected

3.5 Execution of the Uncertainty Analysis

The execution of the UA Job Stream is performed similarly to a normal Job Stream. Click on Tools to selected Submit Job and then select the UA Job Stream (Figure 3-70) and click OK (Figure 3-71). The Job Status window will be opened (Figure 3-72) showing all the steps of the Job Stream (MELGEN/MELCOR steps, plotting step, data extraction and DAKOTA step).

Once all the steps have been completed, the DAKOTA output file is created together with all plots requested in the AptPlot step (Figure 3-73).

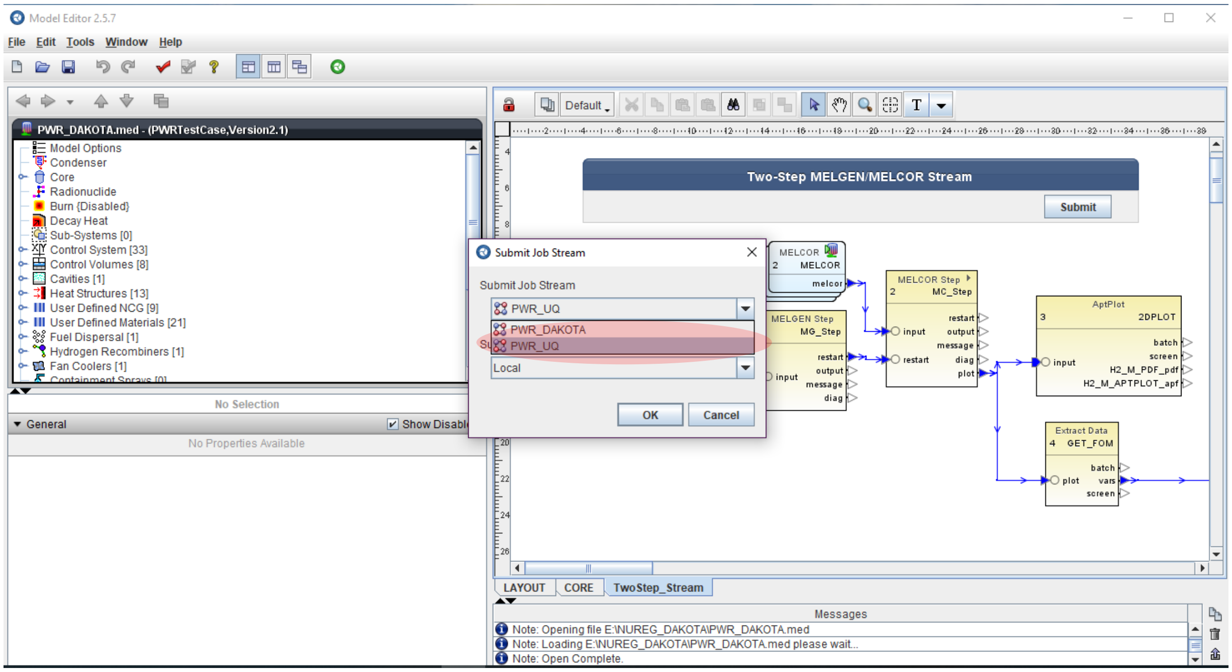

Figure 3-70 Selection of the Uncertainty Job Stream to be Submitted

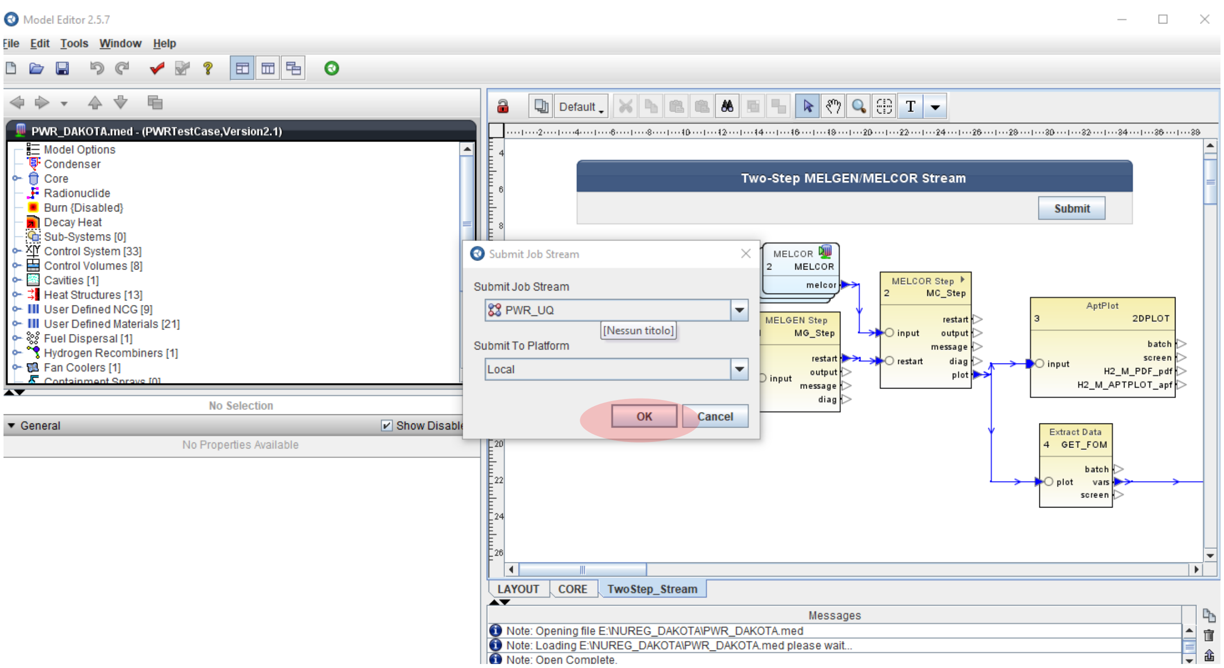

Figure 3-71 Submission of the Uncertainty Job Stream

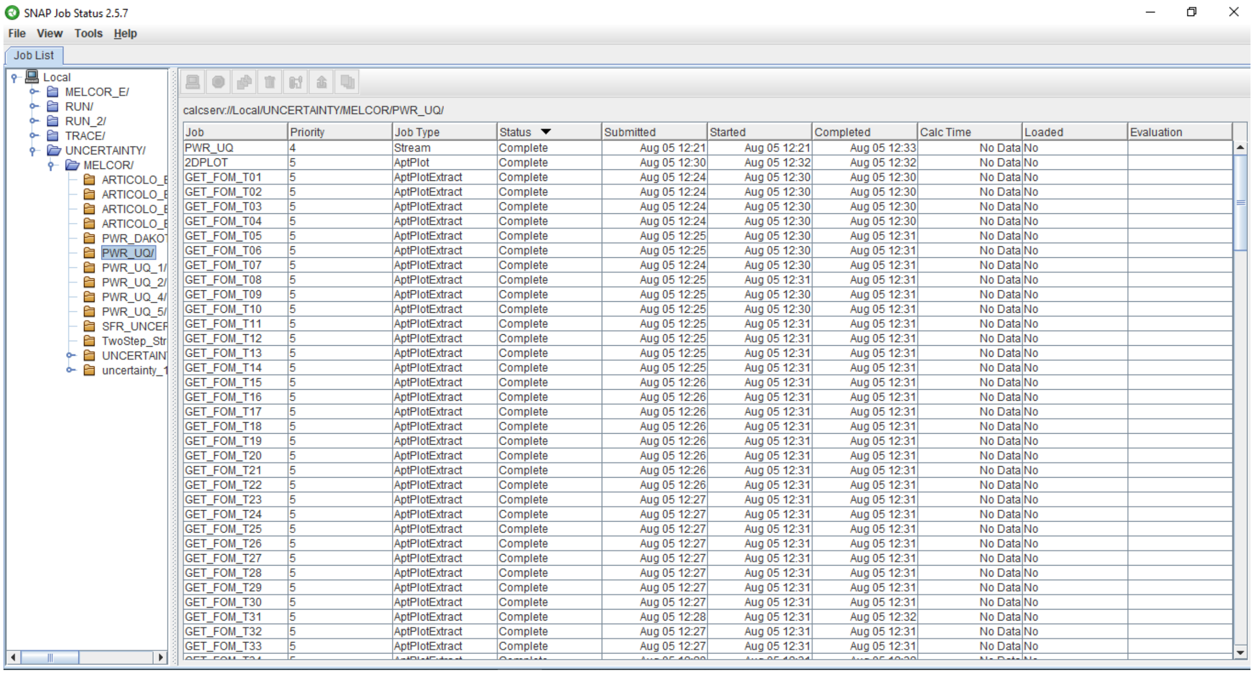

Figure 3-72 View of the Job Status in the Data Extraction Step Section

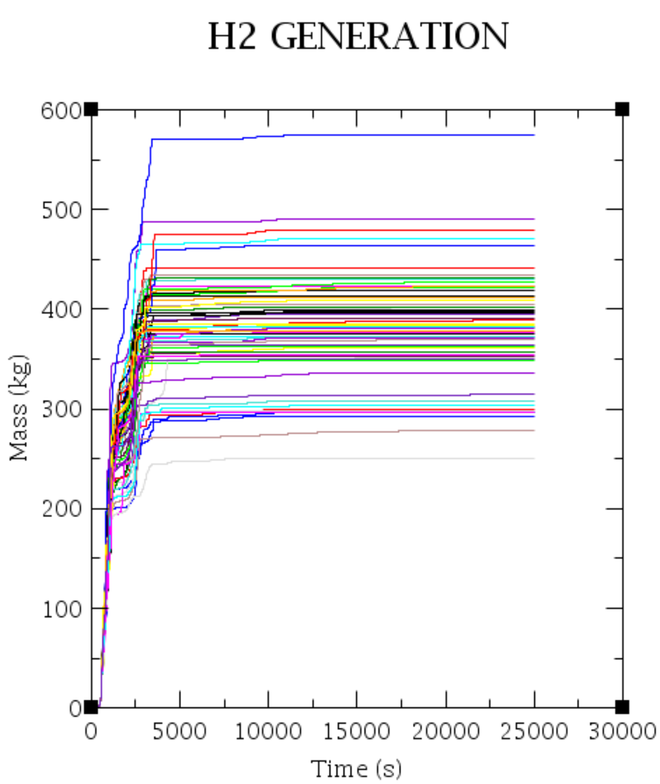

Figure 3-73 Plot of the Hydrogen Generation for all the Cases in the UA (result of the AptPlot step)

4 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:

- Table of contents,
- Introduction section,
- Uncertainty quantification input options section,
- Variate and response data section,
- DAKOTA Results:
  In this section the following information are reported for each FOM:
  - the Cumulative Distribution Function (CDF) and PDF plot,
  - the statistical results, and
  - the response correlations.
- DAKOTA Input File:
  The input file used in a *pre_run* DAKOTA invocation to generate the random variates.

The presence of eventual failed calculations may prevent the creation of the DAKOTA UA report. A solution to overcome this issue is the adoption of the Python directed job stream (see Appendix A).

4.1 Report: Uncertainty Quantification Input Options Section

The Uncertainty quantification input options section includes:

- A tabulated summary of the main information characterizing the UA application (e.g., Table 5-1).[10],
- A tabulated summary of distributions, their characteristic parameters, and the selected model variables (e.g., Table 5-2),
- A table listing the application used in the job stream is reported (e.g., Table 5-3), and
- User identified FOMs in the analysis.

4.2 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 (e.g. Figure 5-2, Figure 5-3) and
- Variate data (input uncertain parameters value for each task) and response data table (FOM value for each task).

[10] For a matter of convenience, we refer to the table discussed in Section 5.

As shown in Figure 2-1, a first DAKOTA run is performed using the specified input uncertain parameters to generate a set of variates for each task. The individual tasks are then performed and the FOMs are extracted from the completed calculations.

The plots present in the DAKOTA automatically generated report are:

- Input uncertain parameter against iteration index (e.g. Figure 5-2),
- FOM VS input uncertain parameter (e.g. Figure 5-3), 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.

4.3 Report: DAKOTA Results

As shown in Figure 2-1, a second DAKOTA run was performed using the variate and extracted FOM values to obtain the statistical results and a CDF for the FOM. DAKOTA also calculates the response correlations for the FOM.

In relation to the DAKOTA statistical results of the FOM, the following information can be found in the automatically generated report:

- Plots (e.g. Figure 5-4, Figure 5-23 on the right):
    - CDF and
    - PDF

- Tabulated Data (e.g. Table 5-4, Table 5-16)
    - Statistical results:
        - Min value and the related task,
        - Max value and the related task,
        - Mean value,
        - Median value and the related task,
        - Standard deviation, and
        - Coefficient of variance.

4.4 Report: Uncertainty Analyses Response Correlation

As a result of the uncertainty analysis, DAKOTA computes four response correlation coefficients [25,30,39]: simple, partial, simple rank and partial rank. The simple coefficient is related to the actual input and output data. The simple coefficient r between an input variable x and an output variable y, in n samples, is computed using the Pearson's correlation. It is a measure of the degree of linear correlation between the two variables and its value is comprised between -1 and 1. If $r<0$ the correlation is negative (an increment of x leads to a reduction in y), if $r=0$ there is no correlation between the two variables, if $r>0$ the correlation is positive (an increment of x leads to an increment of y).

The partial correlation coefficient is computed similarly to the simple coefficient but considering the effects of the other variables. This is useful, for example, if there is a strong correlation between two inputs. The correlation of the second input on the output may be adjusted after having considered the correlation between the first input and the output. Rank correlation coefficients use the ranked data instead of the actual ones. Ranks are obtained by ordering the data in ascending order and are more convenient to be used when inputs and outputs are characterized by sensible difference in magnitude. It is possible to understand if the input sample with the lower rank is associated to the output with the lower rank and so on [30,39]. To compute the rank correlation, DAKOTA uses the Spearman's rank correlation that is similar to Pearson's correlation but with the ranked data instead of the actual values. If two variables are monotonically related, without repetitions, the Spearman coefficient is -1 or +1 (depending upon whether the function is monotonically decreasing or increasing), since the ranked values are used. Moreover, Spearman's correlation is less sensitive to possible outlier values of the variables than Pearson's.

Table 5-5 and Table 5-17 show the response correlation reported in the automatically generated DAKOTA report for the Sample 1 and 2 respectively for a selected instant. For completeness, as example of time dependence computation of response correlation coefficient, the maximum cladding temperature Pearson and Spearman coefficient are reported based on a TRACE [21] analyses of a double ended guillotine break in a generic PWR-900 [26], Figure 4-1 and Figure 4-2.

On both graphs the values 0.2 and 0.5 (and -0.2 and -0.5) have been highlighted as measure of the correlation between the input parameter and the FOM. As indicated in [39], for the Spearman coefficient, if the coefficient is higher than 0.5 (or lower than -0.5) the correlation is significant, if it is between 0.2 and 0.5 (or -0.2 and -0.5) the correlation is moderate, otherwise it is low [40].

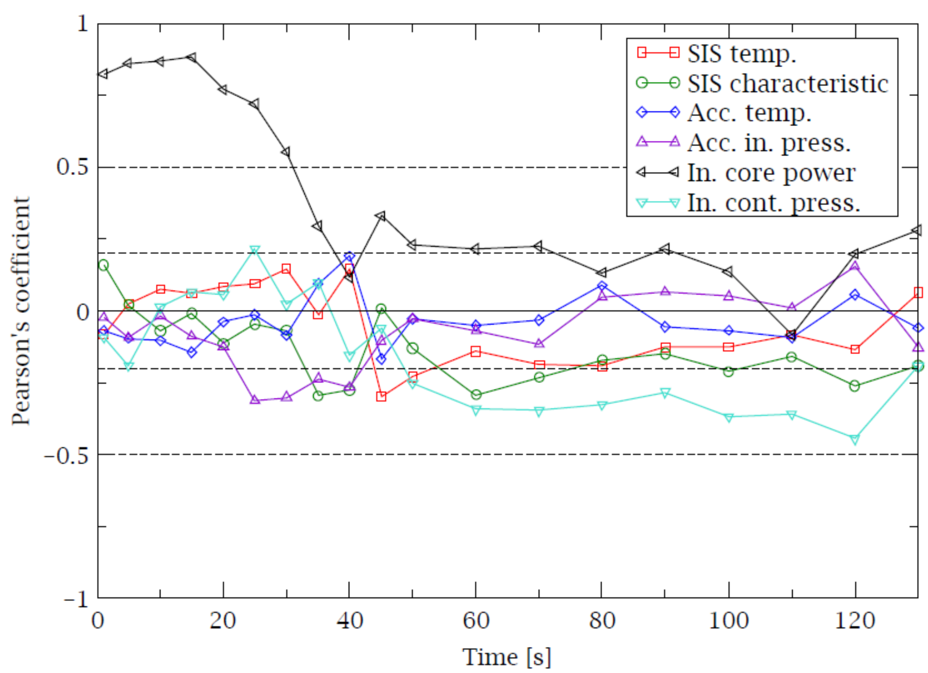

Figure 4-1 Maximum Cladding Temperature Pearson's Simple Correlation Coefficient (double-ended LBLOCA simulation with TRACE code coupled with DAKOTA for a generic PWR-900) [26]

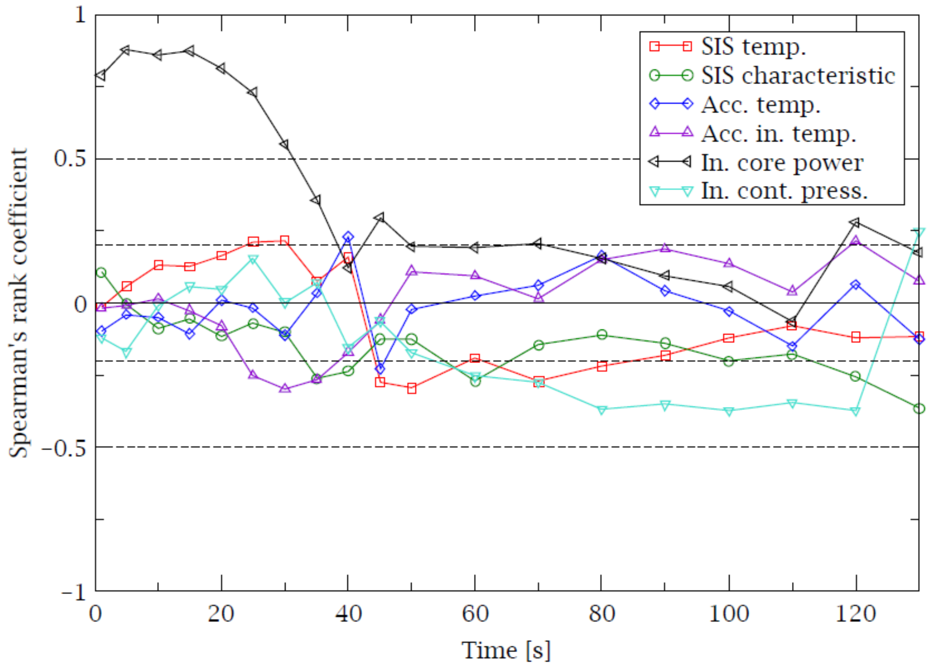

Figure 4-2 Maximum Cladding Temperature Spearman's Simple Correlation Coefficient (double-ended LBLOCA simulation with TRACE code coupled with DAKOTA for a generic PWR-900) [26]

5 MELCOR/DAKOTA COUPLING, IN A SNAP ENVIRONMENT/ARCHITECTURE, SAMPLES

MELCOR/DAKOTA uncertainty studies are reported here. These represent only the first 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 represent 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, to provide details on the capabilities provided by this methodology, and to show the great advantage to having a graphical user interface that allows:

- Development of input-decks from scratch,
- Importing 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 UA that automatically:
    - Run different random sampling tasks,
    - Develop requested dispersion plots, and
    - Generate statistical and response correlation analyses.
- Etc.

The base of these applications of MELCOR/DAKOTA in a SNAP environment/architecture has been presented by ENEA at the European MELCOR User Group (EMUG) 2019 [27].

5.1 SAMPLE 1: MELCOR/DAKOTA Coupling Against CSTF-AB1 Test

This activity was performed using the MELCOR input-model developed by ENEA for the EU-JASMIN project (Joint Advanced Severe Accidents Modelling and Integration for Sodium-Cooled Fast Neutron Reactors) coordinated by IRSN and funded in the 7th Framework Programme of the European Commission [41]. In that project ENEA was involved in the WP2.3 (ST) - Source term - coordinated by CIEMAT. A benchmark activity, coordinated by CIEMAT, was performed with the following codes: MELCOR, ASTEC-CPA, CONTAIN, FEUMIX, and ASTEC-CPA*(specific models for in-containment Na phenomena have been implemented). The tests selected for the benchmark were the CSTF-AB1 and AB2, FAUNA F2 and F3, and EMIS10b (Pool Fire Tests) [41,42]. ENEA used the MELCOR and ASTEC-CPA codes to simulate the selected tests in support of the benchmark for the CPA module in ASTEC-NA.

5.1.1 SAMPLE 1 CASE1

Following the completion of the JASMIM project, ENEA decided to perform their first application (CASE1) of the MELCOR/DAKOTA coupling within the SNAP environment/architecture to analyze the dispersion of the aerosol suspended mass (SUSP), aerosol mass median diameter (MMD), geometric standard deviation of the aerosol distribution (SSD), and total mass deposited (TOT_DEP) having as a base the CSTF-AB1 test [43].[11]. These variables constituted the list of FOMs. Aerosol constants associated with deposition and agglomeration phenomena were selected as uncertain input parameters for the study. Characteristics of the PDF for each identified uncertain input parameter were based on [44] and are provided in Table 5-2. For simplicity, the PDF are defined as uniform for all parameters.

Figure 5-1 shows the DAKOTA Properties Tab for the Case 1 (FOMs selected, selection of Latin hypercube sampling, and probability and confidence level of 98%). A model input set of 452 runs is computed such that (as a result of the previously described calculate samples bottom present in DAKOTA Property Tab) the four specified FOMs with a 98.0% probability and a 98.0% confidence level are satisfied. As an example for the following calculation, the data extracted to perform the UA are the values of the FOMs at the end of the pool fires.

A first DAKOTA run was performed using the specified uncertain input parameters, to generate a set of variates for each task. The individual tasks were then performed, and the FOMs were extracted from the completed calculations. A total of 452 tasks are required, 452 tasks were completed successfully. In Figure 5-2, the uncertain input parameters, CHI, GAMMA, FSLIP, STICK have been plotted against the iteration index. In Figure 5-3, the FOM-SUSP and FOM-MMD have been reported against the CHI and GAMMA uncertain input parameters. Figure 5-4 shows the dispersion band, created automatically by AptPlot, for the suspended mass along with the CDF and the PDF calculated by DAKOTA.

Figure 5-4, Figure 5-5, Figure 5-6, and Figure 5-7 respectively show the dispersion band, created automatically by AptPlot, for the FOMs along with the CDF and the PDF calculated by DAKOTA. Table 5-4, Table 5-6, Table 5-8, and Table 5-10 respectively show the statistical results, generated automatically by DAKOTA for the report, for the different FOMs. Table 5-5, Table 5-7, Table 5-9, Table 5-11 show the response correlation, reported in the automatically generated DAKOTA report, for the different FOMs.

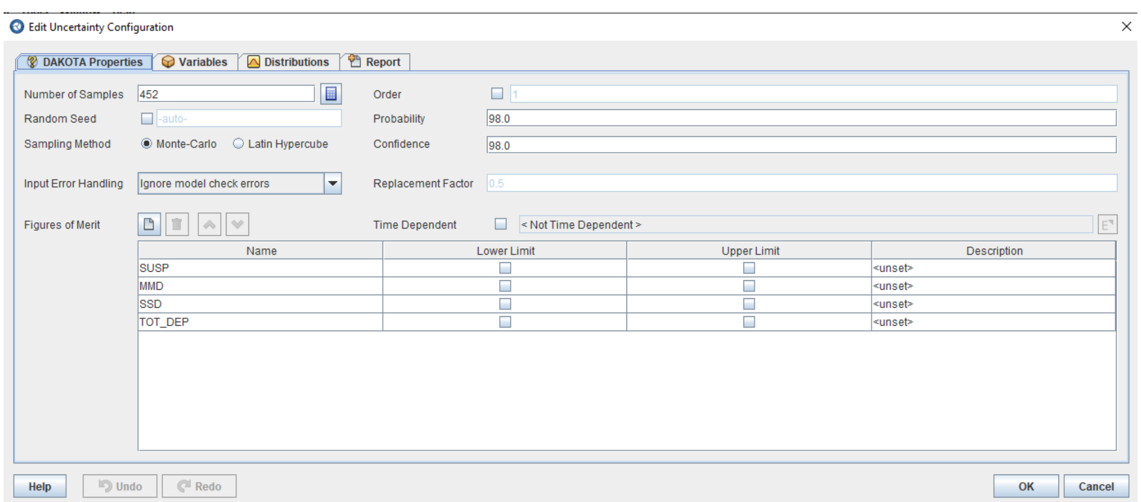

Figure 5-1 DAKOTA SNAP Property Tab for the CASE 1

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[11] Since the target of this report is not to do a representative UA of the MELCOR code but only to intend to demonstrate the MELCOR/DAKOTA coupling methodology and application, to simplify the analyses and the related description the CSTF AB1 experimental data are not reported in the dispersion plot.

Table 5-1 Uncertainty Quantification Input Options, Summary Table

SNAP Version	2.5.7
Uncertainty Plug-in Version	1.4.1
MELCOR v2.x Analysis Code	2.3.1
Model Name	unnamed
Model File	C:\Users\Fulvio Mascari\Desktop\LAVORO\NUREG\MELCOR_DAKOTA\CASE1\INPUT_PC_HP\NUREG\MELCOR_AB1_Q_ATM_Pool_REF_SS_BASE_UNC_prova_2_LH.med
Error Handling	Ignore model check errors
Random Seed	262754 (system-generated)
Sampling Method	Monte-Carlo
Order Statistics	disabled
Probability Level	98.0%
Confidence Level	98.0%
Number of Required Tasks	452
Number of Requested Tasks	452

Table 5-2 Uncertainty Input Parameters Range (CASE 1)

Distribution Name	Distribution Type	Application Rule	Distribution Parameters	Model Variables	Nominal
d1	Uniform	Scalar	a:1.0, b:5.0	CHI	Replacement
d2	Uniform	Scalar	a:1.0, b:5.0	GAMMA	Replacement
d3	Uniform	Scalar	a:1.14, b:1.257	FSLIP	Replacement
d4	Uniform	Scalar	a:0.5, b:1.0	STICK	Replacement
d5	Uniform	Scalar	a:1.0E-3, b:0.02	TURBDS	Replacement
d6	Uniform	Scalar	a:0.05, b:0.06	TKGOP	Replacement
d7	Uniform	Scalar	a:2.18, b:2.25	FTHERM	Replacement
d8	Uniform	Scalar	a:1.0E-5, b:1.0E-3	DELDIF	Replacement

Table 5-3 Application Information Table

Step	Application Info
MG_Step	Name: MELGEN_22_9607
	Description: The MELGEN severe accident analysis code.
	Location: C:\Codici\MELCOR\bin\Windows\bin\Melgen_RL_LIC_9607.exe
MC_Step	Name: MELCOR_22_9607
	Description: The MELCOR severe accident analysis code.
	Location: C:\Codici\MELCOR\bin\Windows\bin\Melcor_RL_LIC_9607.exe
GET_FOM	Name: Extract_Data
	Description: AptPlot Data Extraction
	Location: C:\Users\Fulvio Mascari\SNAP\APTPLOT\bin\AptBatch.exe

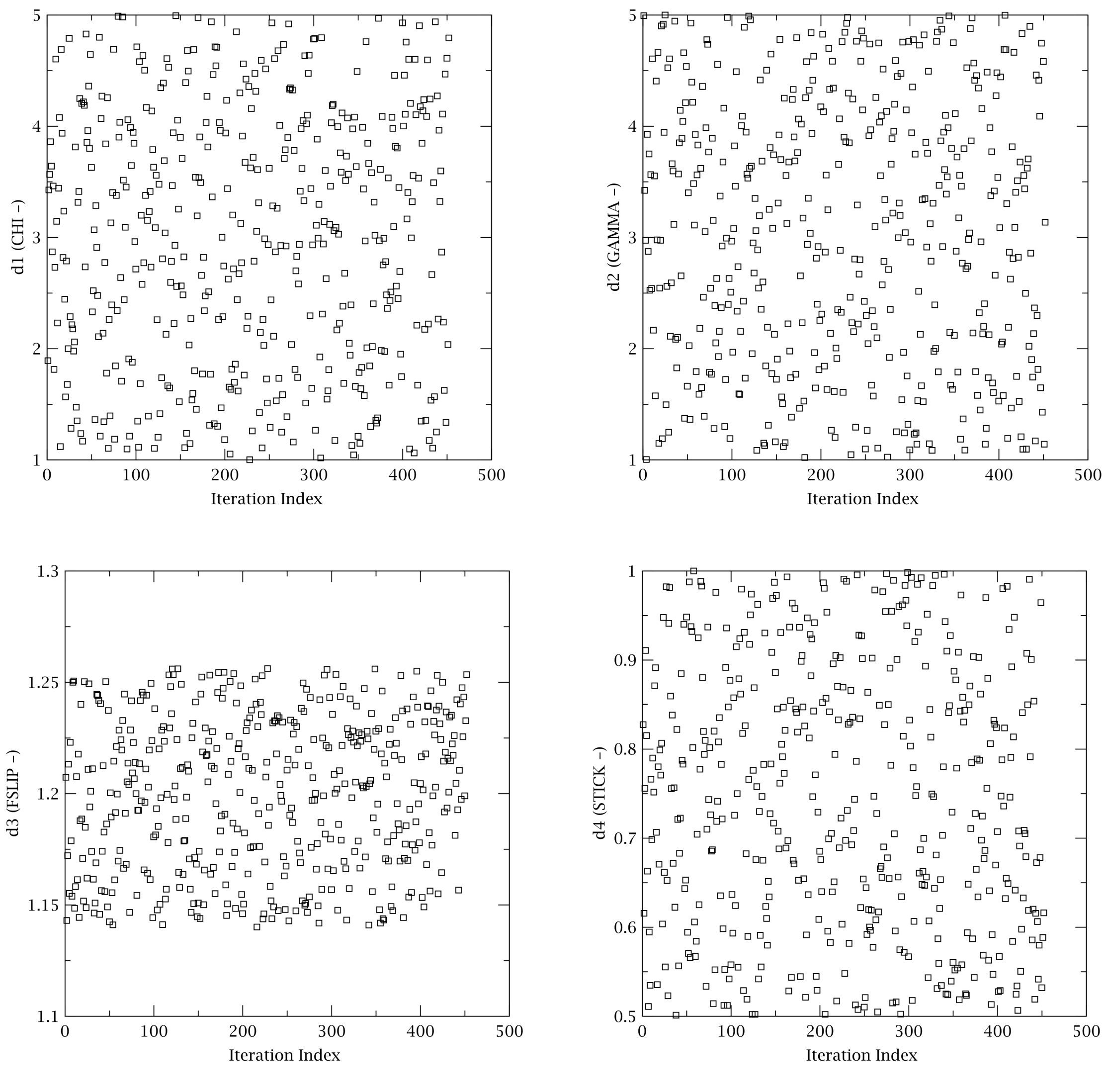


Figure 5-2 Variate and Response Data: Input Uncertain Parameter VS Iteration Index for the Case 1

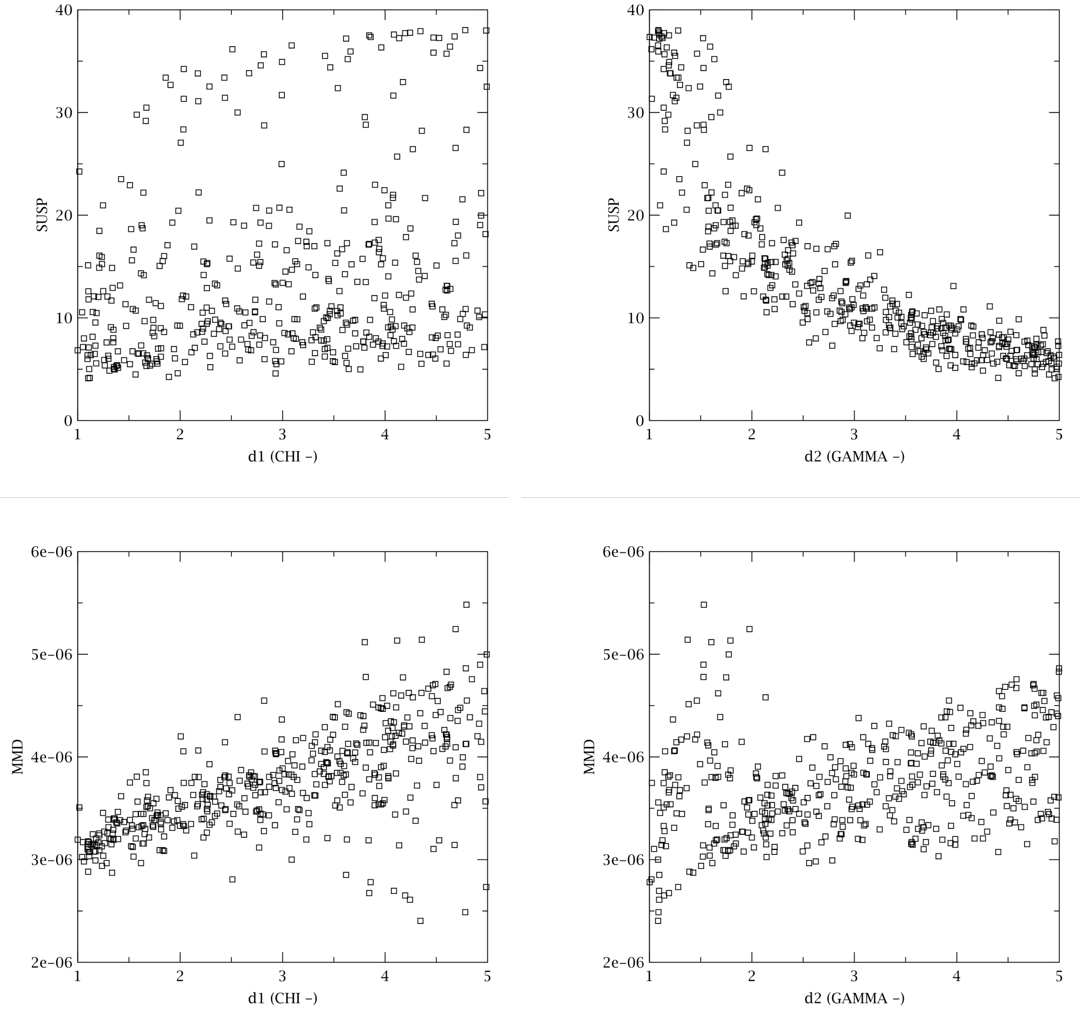


Figure 5-3 Variate and Response Data: FOM VS Input Uncertain Parameters: SUSP and MMD VS d1 (CHI) and d2 (GAMMA) for the Case 1

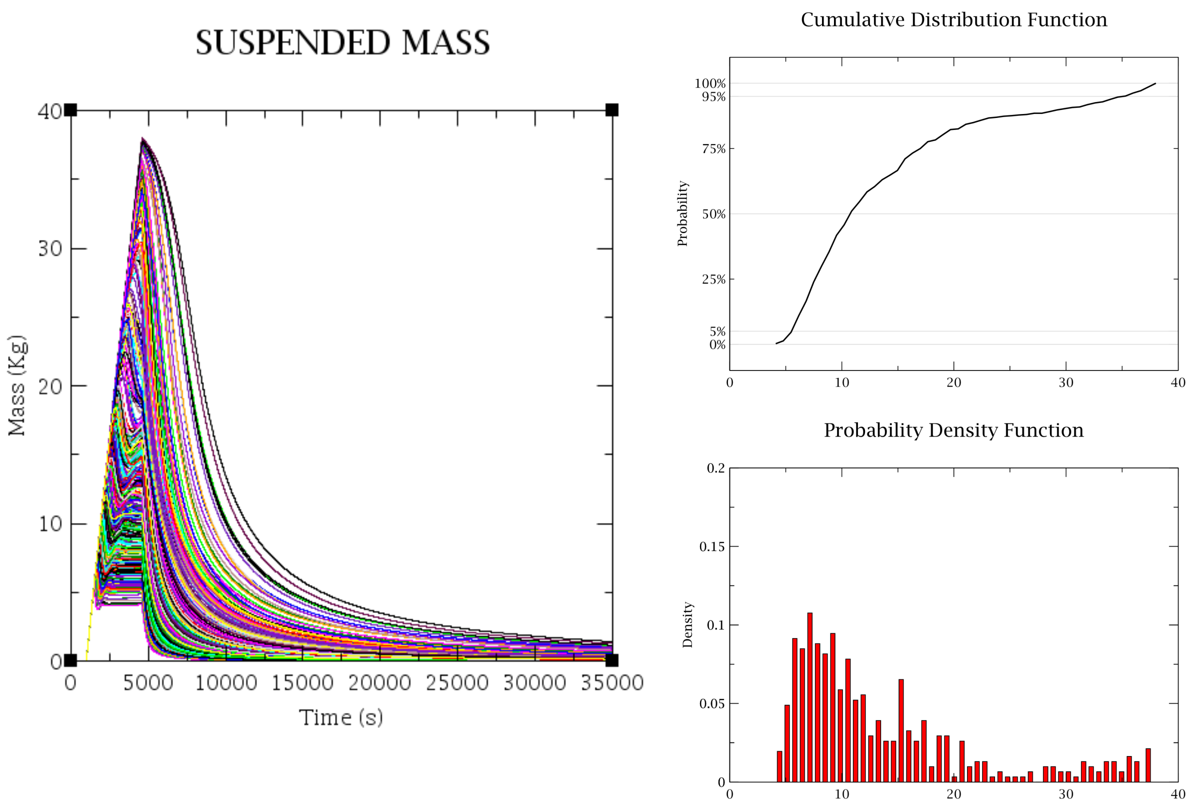


Figure 5-4 SUSP Dispersion of the Results, CDF, and PDF (CASE 1)

Table 5-4 Statistical Results, Reported in the Automatically Generated DAKOTA Report, for SUSP-FOM (CASE 1)

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	-

Table 5-5 Response Correlation, Reported in the Automatically Generated DAKOTA Report, for SUSP FOM (CASE 1)

	Simple	Partial	Simple Rank	Partial Rank
d1	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	-	-1.0	-

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

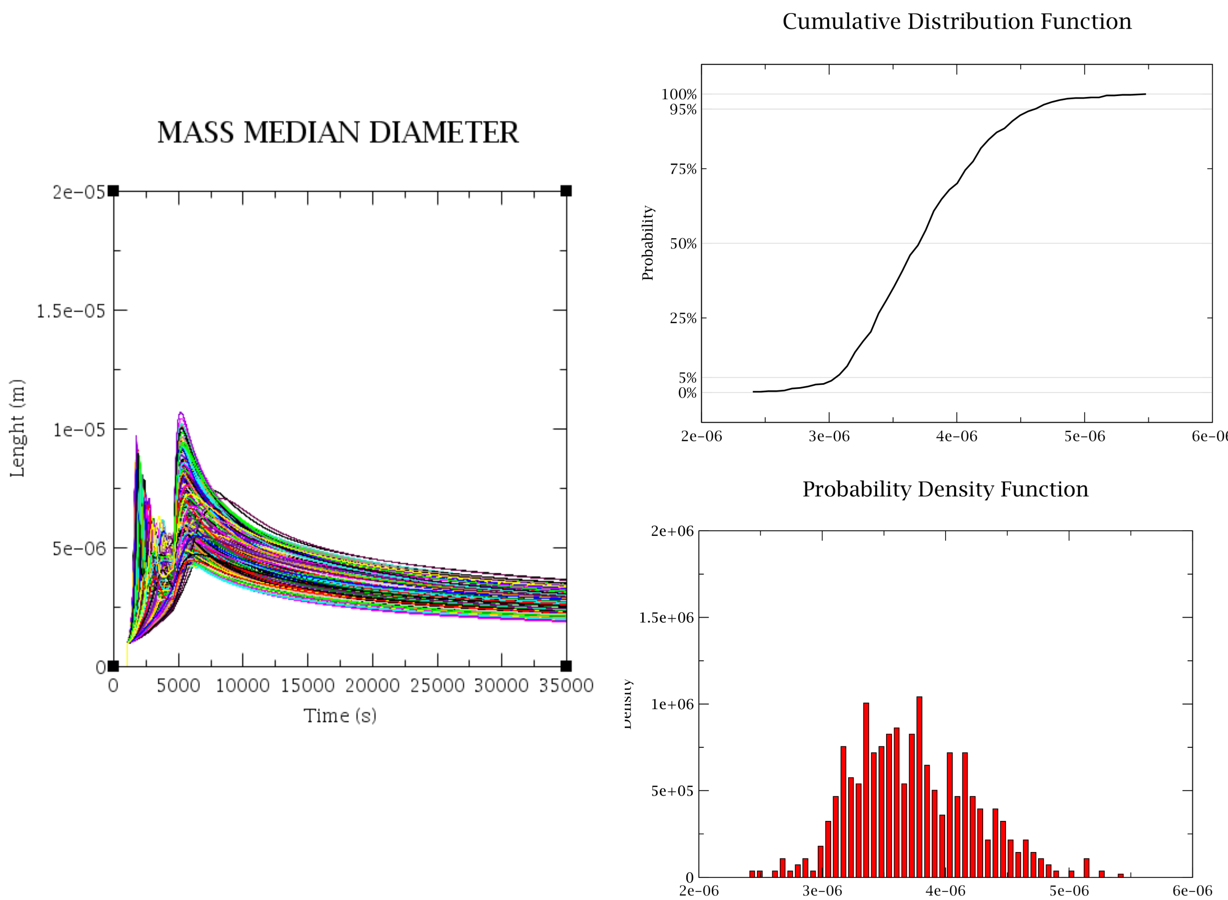


Figure 5-5 MMD Dispersion of the Results, CDF, and PDF (CASE 1)

Table 5-6 Statistical Results, Reported in the Automatically Generated DAKOTA Report, for MMD (CASE 1)

Summary	Value	Task #
Min Value	2.40206E-6	128
Max Value	5.48078E-6	309
Mean	3.7373E-6	-
Median	3.70472E-6	average of 185 and 223
Standard Deviation	4.93252E-7	-
Coefficient of Variance	0.38483	-

Table 5-7 Response Correlation, Reported in the Automatically Generated DAKOTA Report, for MMD (CASE 1)

	Simple	Partial	Simple Rank	Partial Rank
d1	0.643887	0.689261	0.684866	0.737895
d2	0.344623	0.450471	0.35905	0.494771
d3	-0.013526	-0.0124312	-0.00112314	0.0066317
d4	-0.107975	-0.153261	-0.112921	-0.172919
d5	0.0157974	0.0330014	-0.0103633	-0.00823132
d6	0.0643259	0.0873697	0.0527166	0.077581
d7	-0.0438612	-0.0267124	-0.0321103	-0.0123393
d8	0.00718814	-0.00368476	0.0145472	0.00554108
SUSP	-0.107979	-	-0.138996	-
SSD	0.613478	-	0.665808	-
TOT_DEP	0.107979	-	0.138996	-

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

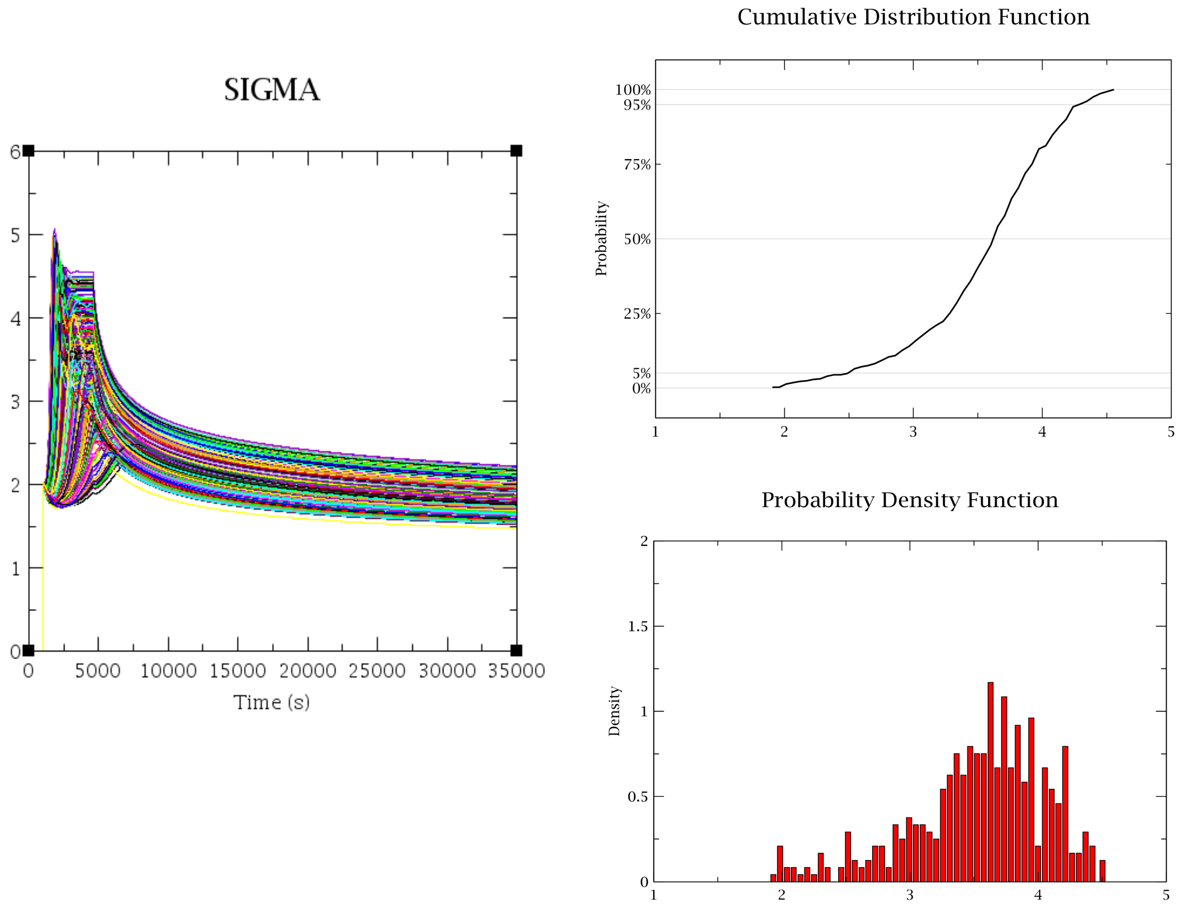


Figure 5-6 SSD Dispersion of the Results, CDF, and PDF (CASE 1)

Table 5-8 Statistical Results, Reported in the Automatically Generated DAKOTA Report, for SSD (CASE 1)

Summary	Value	Task #
Min Value	1.9065	128
Max Value	4.55593	407
Mean	3.54222	-
Median	3.61724	average of 309 and 194
Standard Deviation	0.53795	-
Coefficient of Variance	0.77371	-

Table 5-9 Response Correlation, Reported in the Automatically Generated DAKOTA Report, for SSDD (CASE 1)

	Simple	Partial	Simple Rank	Partial Rank
d1	0.342211	0.643424	0.440776	0.819195
d2	0.800288	0.894909	0.802827	0.934956
d3	-0.0153802	-0.0017017	0.003211	0.0591241
d4	0.183662	0.427701	0.158633	0.471277
d5	0.204668	0.477341	0.197187	0.563345
d6	-0.00369136	0.0158631	-0.013616	-0.00472948
d7	-0.0349918	0.00150876	-0.034065	-0.00662661
d8	-0.00958175	-0.0711485	0.0128401	-0.01947
SUSP	-0.797382	-	-0.716527	-
MMD	0.613478	-	0.665808	-
TOT_DEP	0.797382	-	0.716527	-

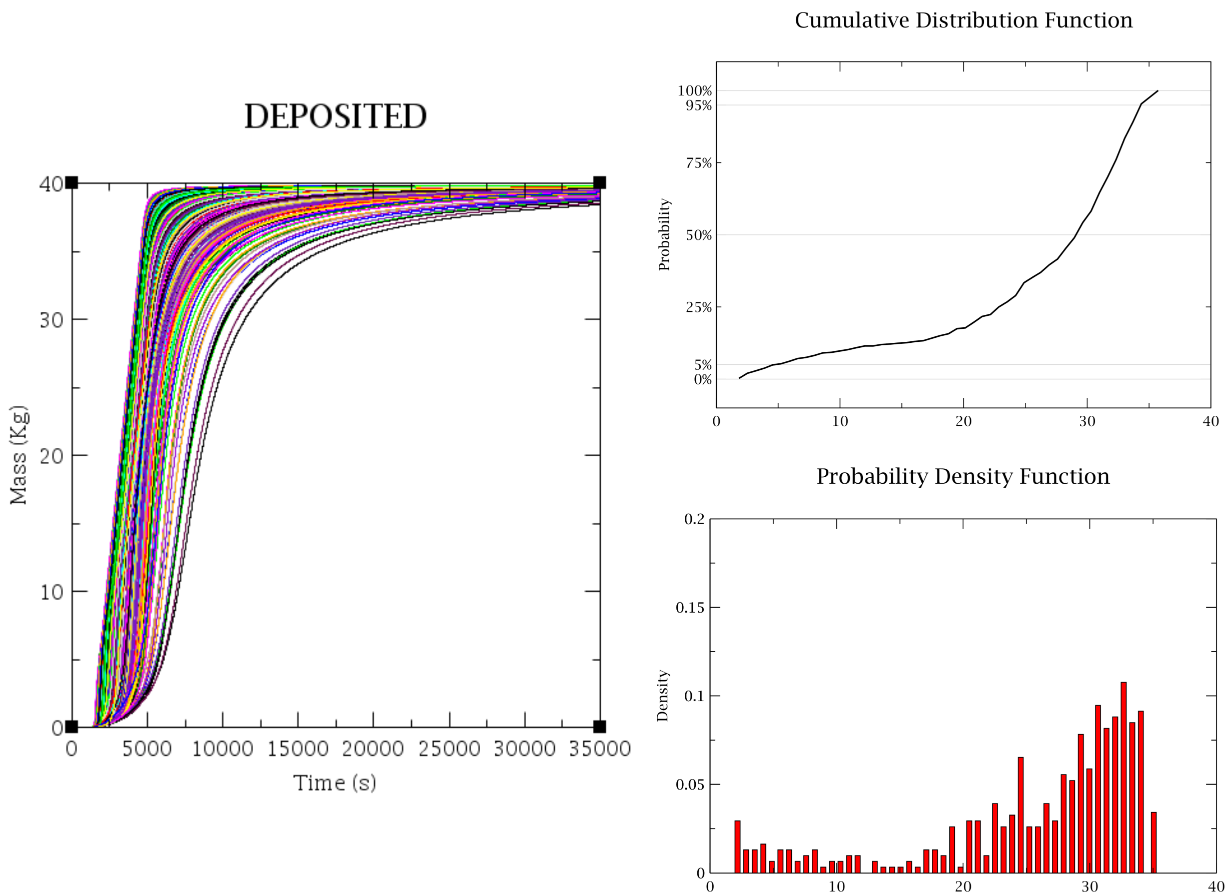


Figure 5-7 TOT_DEP Dispersion of the Results, CDF, and PDF (CASE 1)

Table 5-10 Statistical Results, Reported in the Automatically Generated DAKOTA Report, for TOT_DEP (CASE 1)

Summary	Value	Task #
Min Value	1.83064	300
Max Value	35.73402	121
Mean	25.95008	-
Median	29.14452	average of 436 and 419
Standard Deviation	8.68916	-
Coefficient of Variance	1.38387	-

Table 5-11 Response Correlation, Reported in the Automatically Generated DAKOTA Report, for TOT_DEP (CASE 1)

	Simple	Partial	Simple Rank	Partial Rank
d1	-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	-0.00950151	0.0383844	-0.0139928	0.0606922
d8	-0.019709	-0.0737938	0.0320248	0.134612
SUSP	-1.0	-	-1.0	-
MMD	0.107979	-	0.138996	-
SSD	0.797382	-	0.716527	-

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

5.1.2 SAMPLE 1 CASE1_SEN1

The determination of the uncertain input parameters and the related PDF is a very important and delicate task that influence the results of the UA. The code user must dedicate a lot of accuracy in this task and the PDF type and parameter range should be well posed and justified (e.g. use of coherent previous studies, justified engineering judgement, etc.). To show the influence of this parameter we decide to perform another analysis (CASE1_SEN1) by reducing the range of the CHI and GAMMA coefficient (from 1-5 to 1-2). Figure 5-8 shows the SUSP dispersion of the results, CDF, and PDF (CASE 1_SEN1). Table 5-13 shows the statistical results, reported in the automatically generated DAKOTA report, for SUSP (CASE 1_SEN1). Table 5-14 shows the response correlation, reported in the automatically generated DAKOTA report, for SUSP (CASE 1_SEN1).

Table 5-12 Uncertainty Input Parameters Range (CASE1)

Distribution Name	Distribution Type	Application Rule	Distribution Parameters	Model Variables	Nominal
d1	Uniform	Scalar	a:1.0, b:2.0	CHI	Replacement
d2	Uniform	Scalar	a:1.0, b:2.0	GAMMA	Replacement
d3	Uniform	Scalar	a:1.14, b:1.257	FSLIP	Replacement
d4	Uniform	Scalar	a:0.5, b:1.0	STICK	Replacement
d5	Uniform	Scalar	a:1.0E-3, b:0.02	TURBDS	Replacement
d6	Uniform	Scalar	a:0.05, b:0.06	TKGOP	Replacement
d7	Uniform	Scalar	a:2.18, b:2.25	FTHERM	Replacement
d8	Uniform	Scalar	a:1.0E-5, b:1.0E-3	DELDIF	Replacement

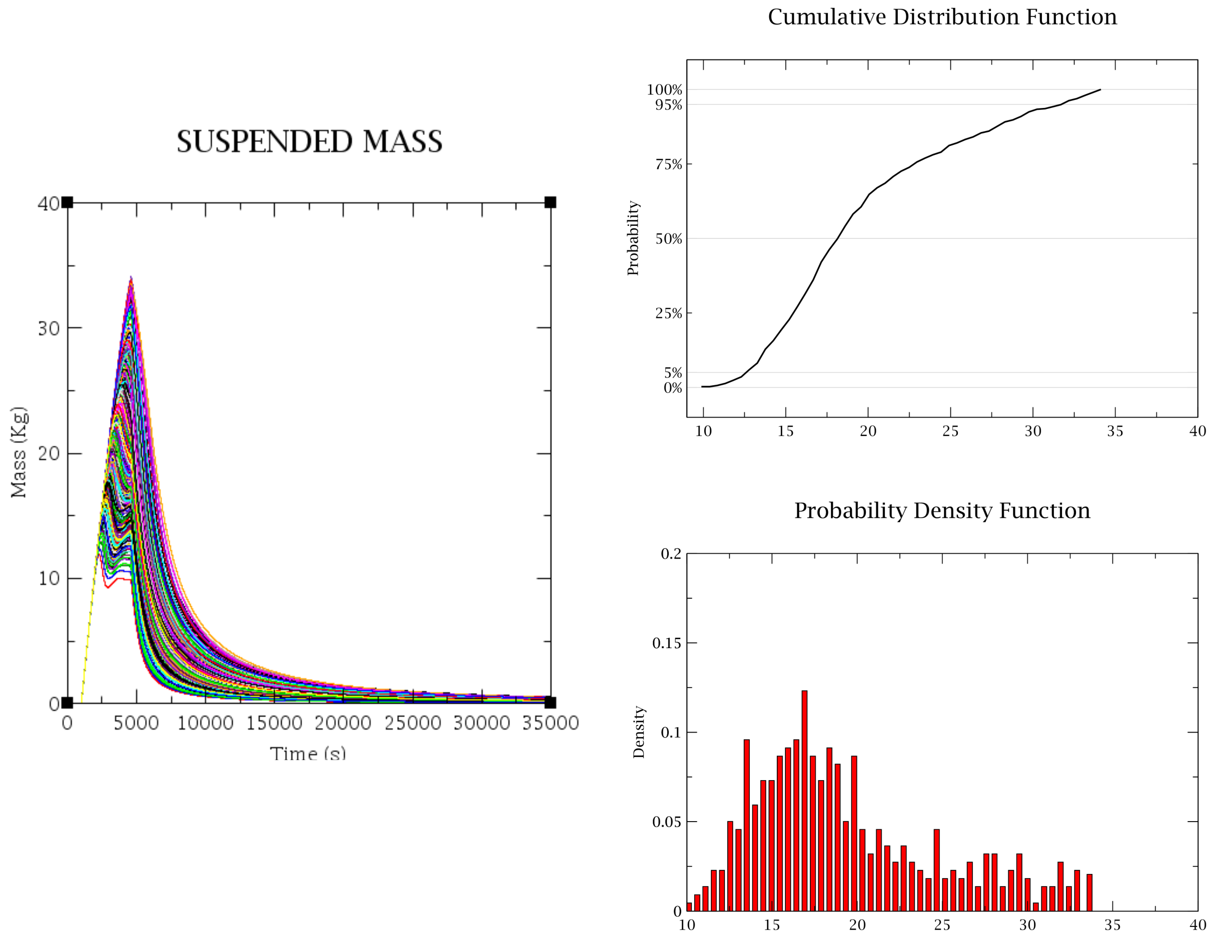


Figure 5-8 SUSP Dispersion of the Results, CDF, and PDF (CASE 1_SEN1)

Table 5-13 Statistical Results, Reported in the Automatically Generated DAKOTA Report, for SUSP (CASE 1_SEN1)

Summary	Value	Task#
Min Value	9.87732	241
Max Value	34.11971	139
Mean	19.59189	-
Median	18.13329	average of 3 and 80
Standard Deviation	5.68278	-
Coefficient of Variance	0.83962	-

Table 5-14 Response Correlation, Reported in the Automatically Generated DAKOTA Report, for SUSP (CASE 1_SEN1)

	Simple	Partial	Simple Rank	Partial Rank
d1	0.315522	0.74101	0.305205	0.83385
d2	-0.787962	-0.935602	-0.796141	-0.966736
d3	0.00534208	-0.0326338	0.00530394	-0.044095
d4	-0.309022	-0.714828	-0.327345	-0.836248
d5	-0.306533	-0.714604	-0.352758	-0.856024
d6	-0.0147849	-0.0384294	-0.0122616	-0.0453161
d7	0.00518501	0.0215833	-0.0138454	-0.0387434
d8	-0.0206283	-0.0630057	-0.00625165	-0.0177482
MMD	0.779187	-	0.819258	-
SSD	-0.723719	-	-0.560017	-
TOT_DEP	-1.0	-	-1.0	-

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

5.1.3 SAMPLE 1 CASE1 Time Dependent Analysis

CASE1 has also been adapted to show an example of a time dependent analysis, to perform the statistical analysis at various time instants selected by the user. This can be done by adding the token ${TIME} in the AptPlot Script for the data extraction (as shown in Figure 5-9) and setting the flag *Time Dependent* in the DAKOTA Properties Tab (Figure 3-17) with the addition of the desired time values for the data extraction.

The statistical analysis performed by DAKOTA for the four FOMs previously mentioned is shown from Figure 5-10 to Figure 5-13. The Pearson and Spearman correlation coefficients for the four FOMs are shown from Figure 5-14 to Figure 5-21. CHI and GAMMA are observed having the highest correlation with the FOMs, as expected. According to the results, the FOMs SUSP and TOT_DEP are inverse linearly correlated (Pearson coefficient -1).

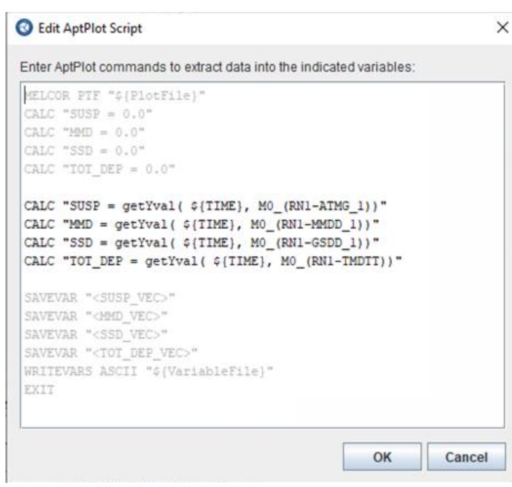


Figure 5-9 Time Dependent Analysis, Token in the AptPlot Script for the Data Extraction

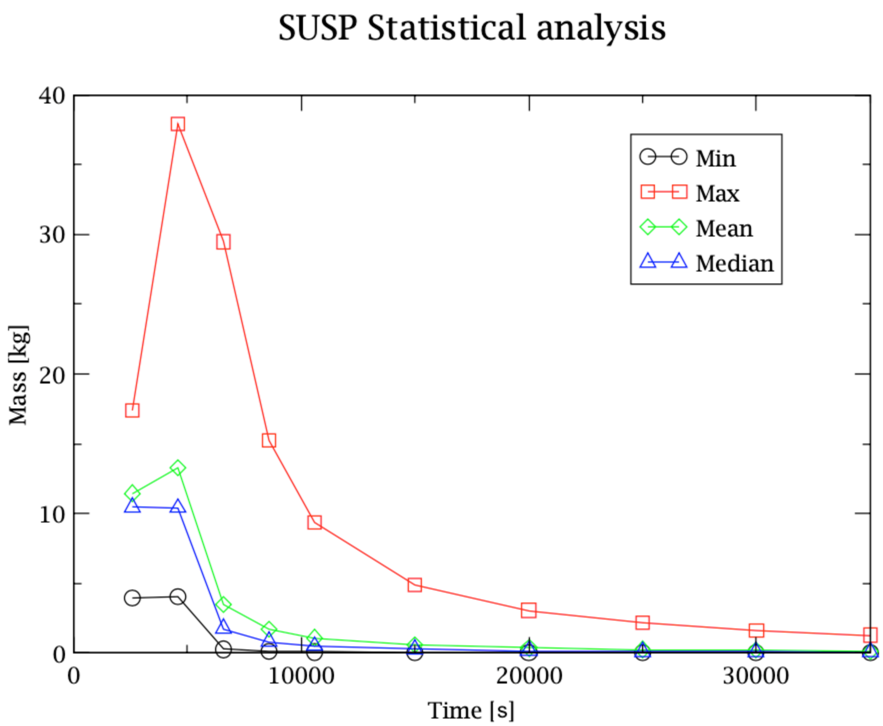


Figure 5-10 Time Dependent Analysis, SUSP Statistical Analysis

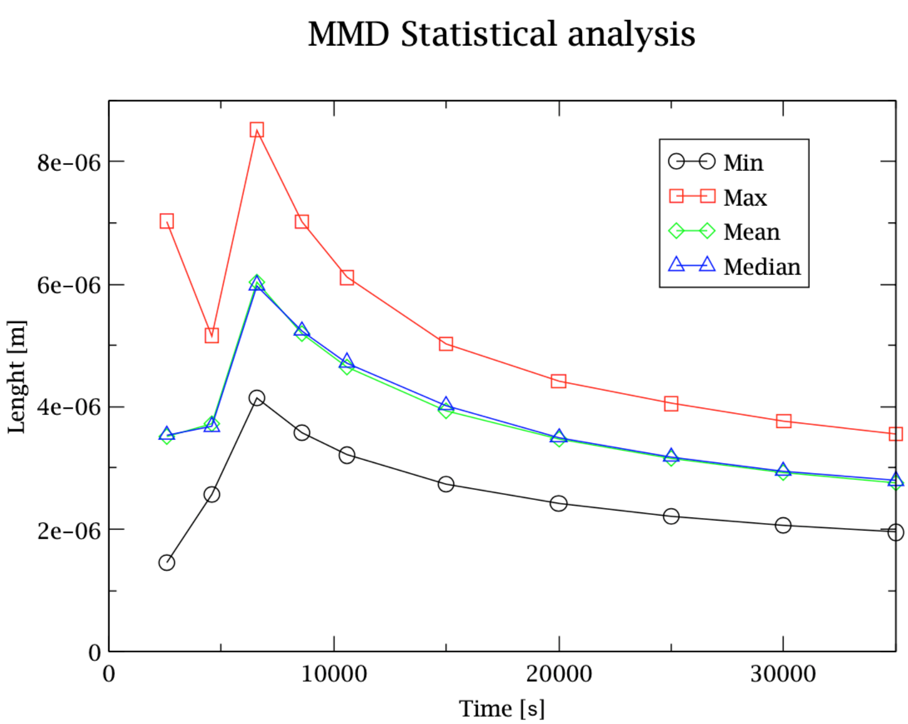


Figure 5-11 Time Dependent Analysis, MMD Statistical Analysis

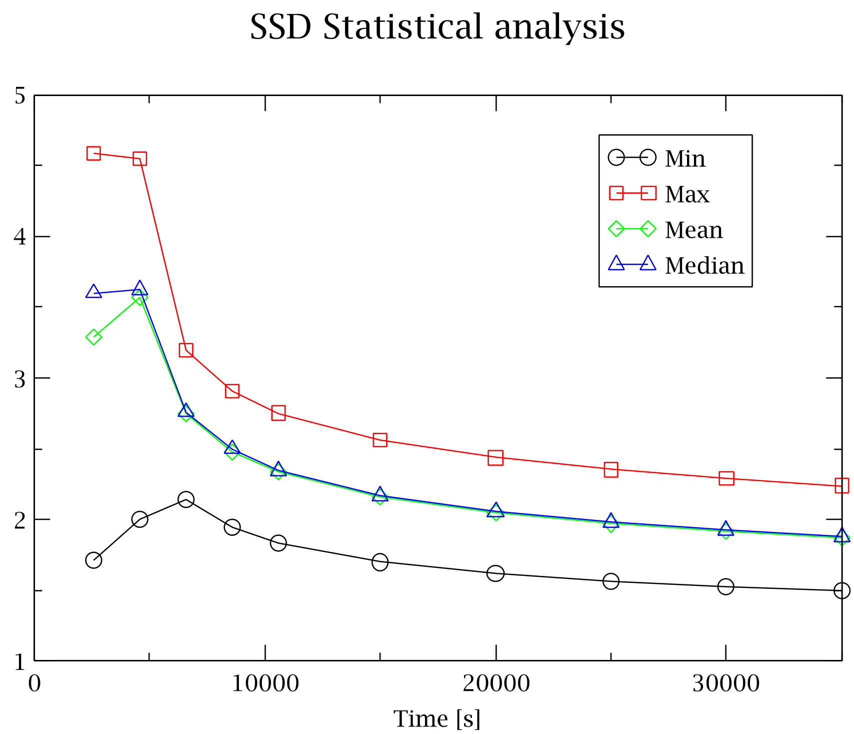


Figure 5-12 Time Dependent Analysis, SSD Statistical Analysis

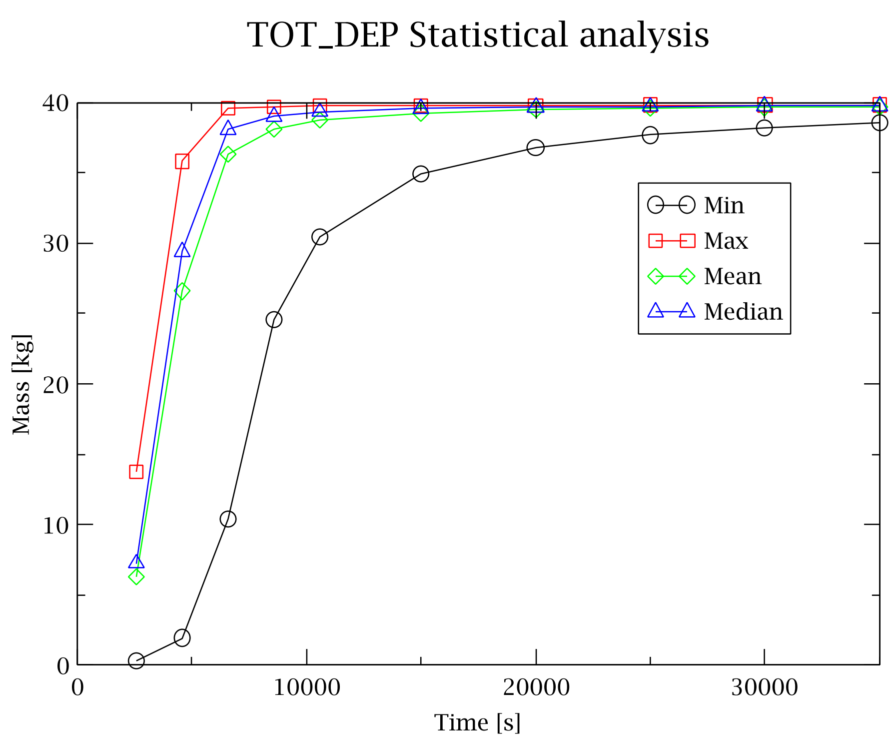


Figure 5-13 Time Dependent Analysis, TOT_DEP Statistical Analysis

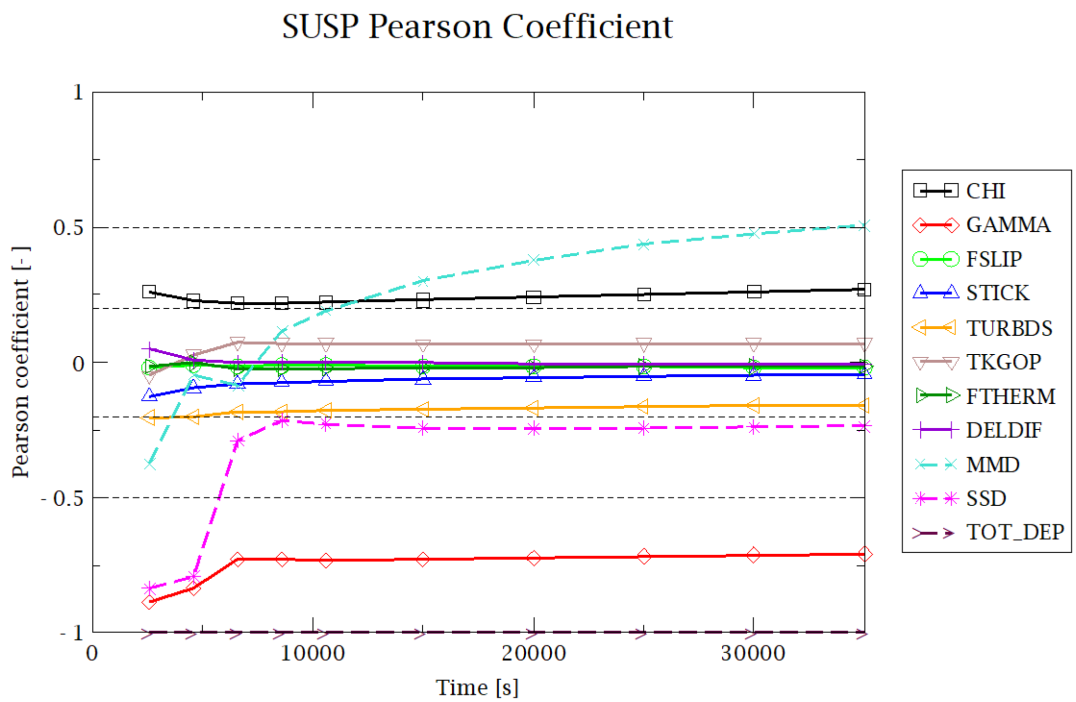


Figure 5-14 Time Dependent Analysis, SUSP Pearson Coefficient

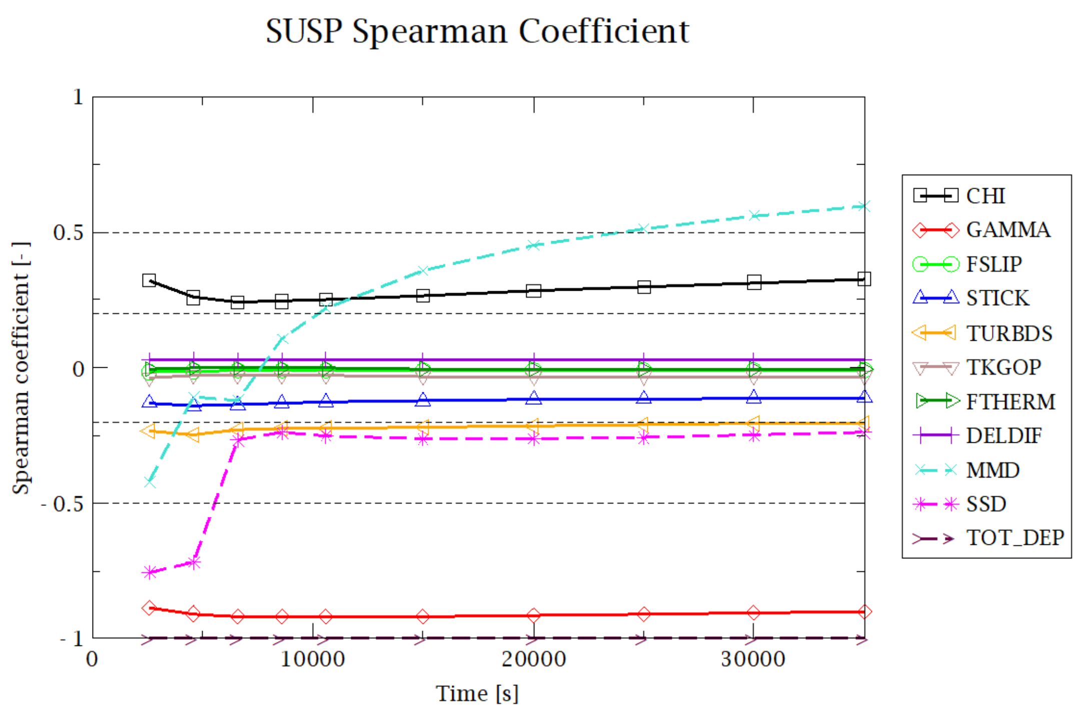


Figure 5-15 Time Dependent Analysis, SUSP Spearman Coefficient

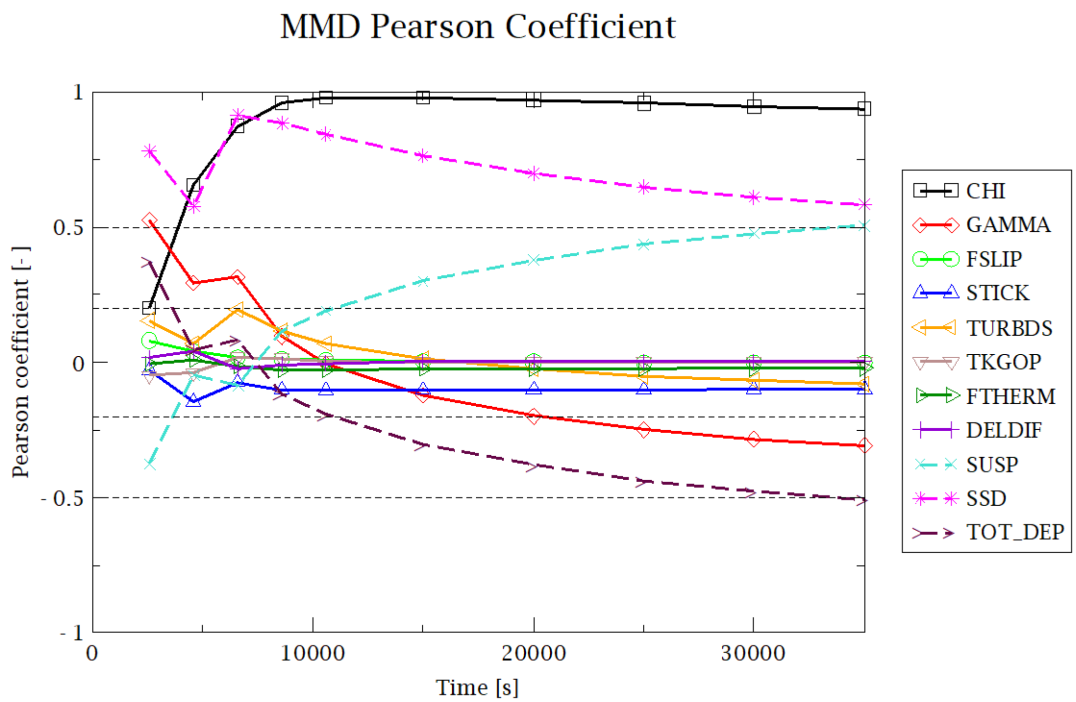


Figure 5-16 Time Dependent Analysis, MMD Pearson Coefficient

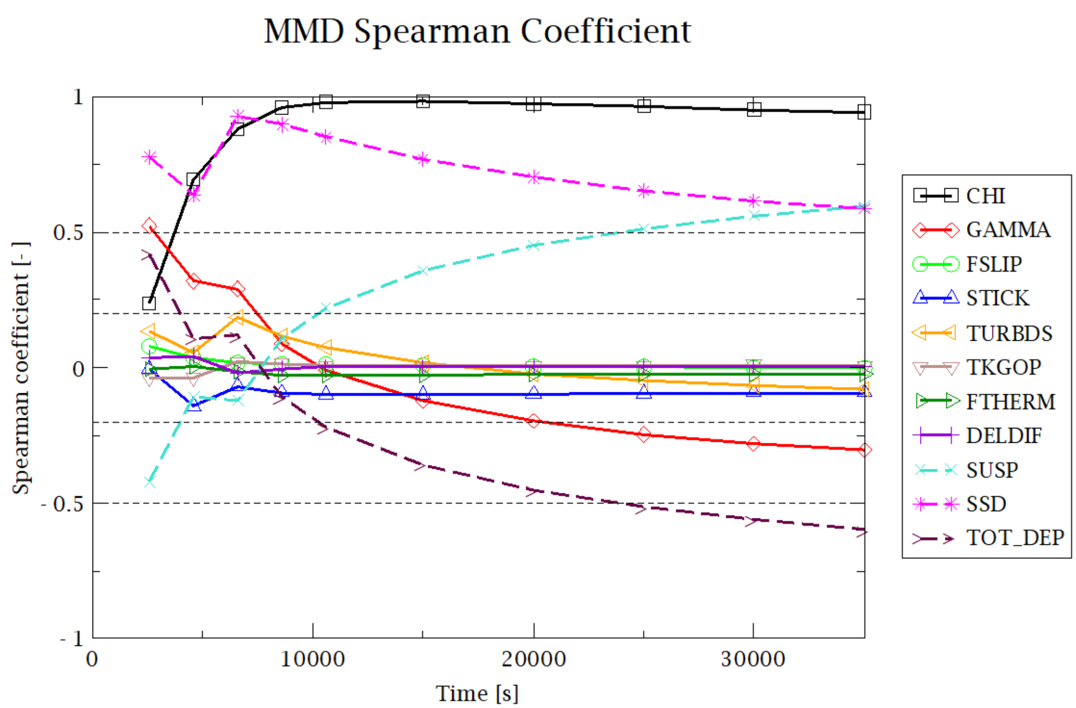


Figure 5-17 Time Dependent Analysis, MMD Spearman Coefficient

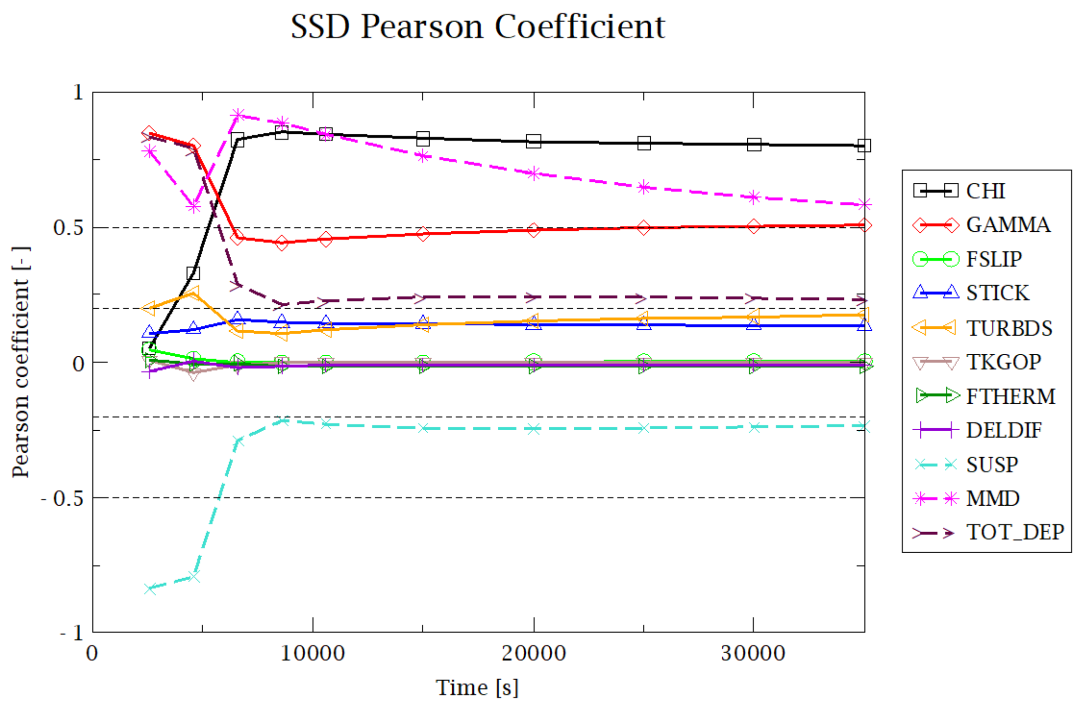


Figure 5-18 Time Dependent Analysis, SSD Pearson Coefficient

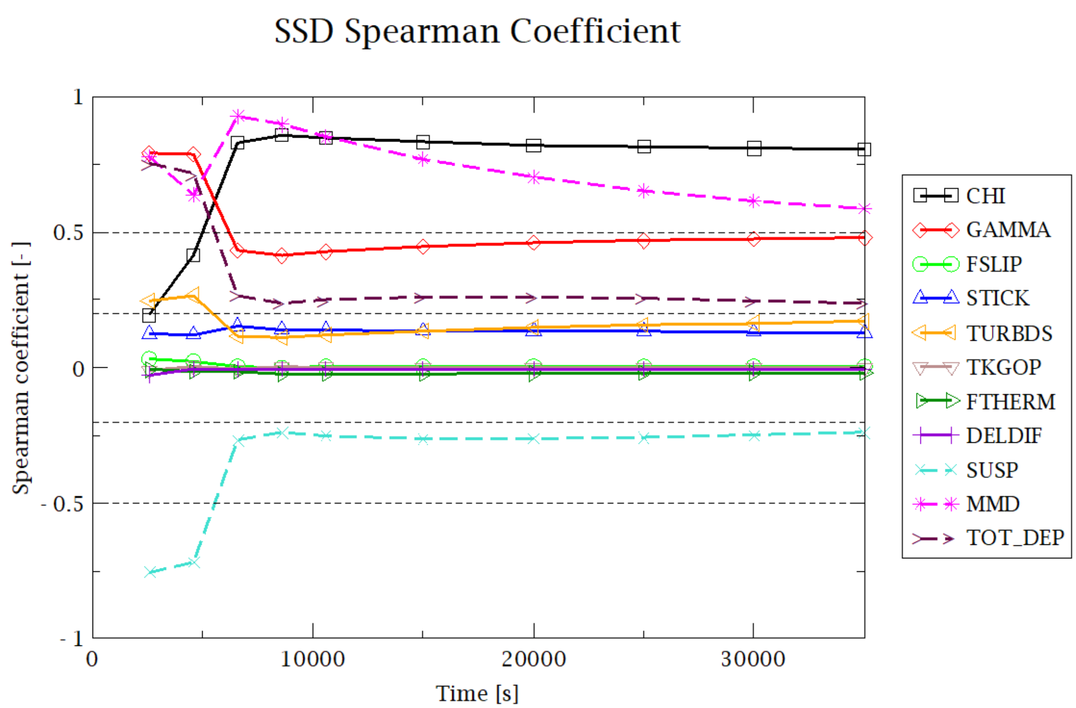


Figure 5-19 Time Dependent Analysis, SSD Spearman Coefficient

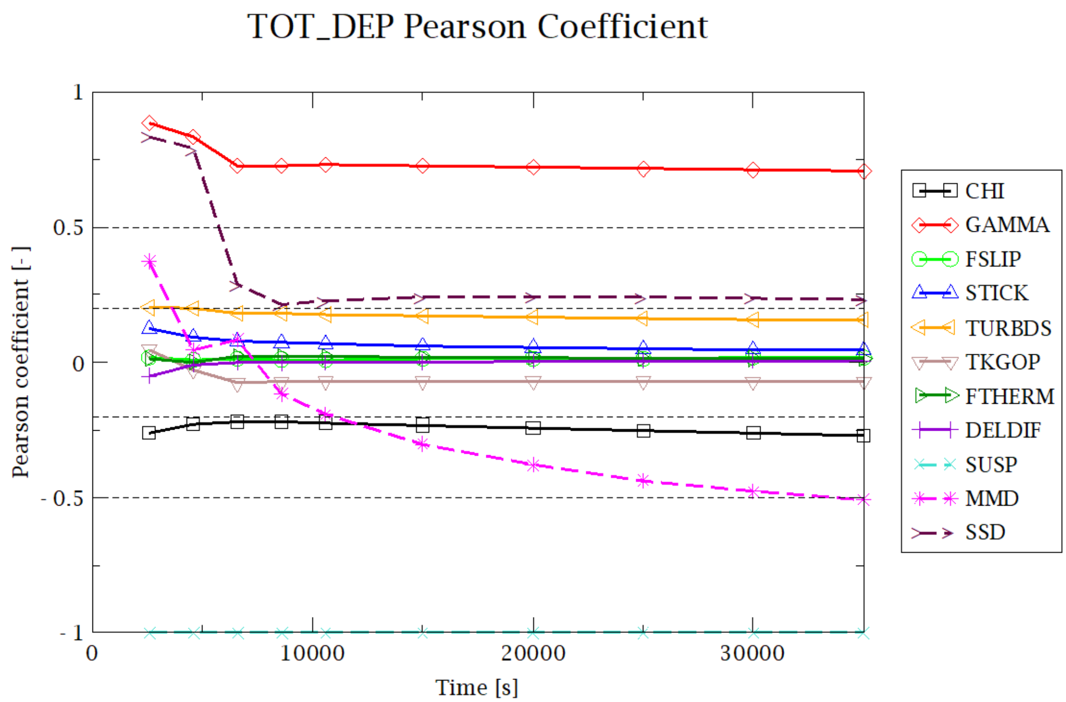


Figure 5-20 Time Dependent Analysis, TOT_DEP Pearson Coefficient

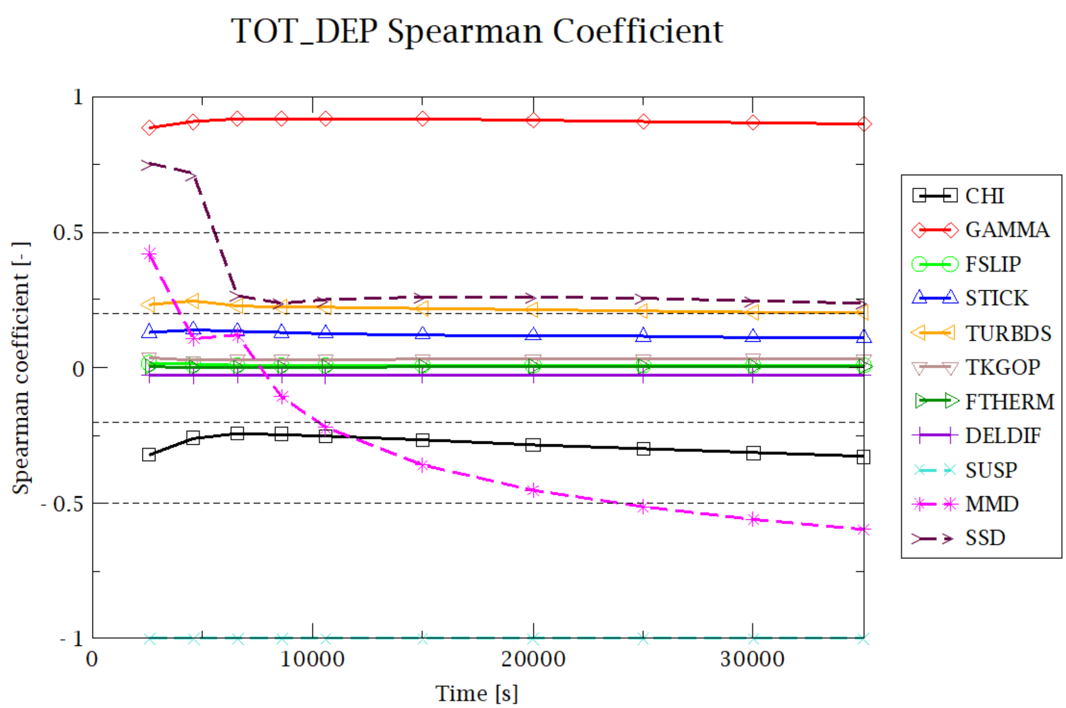


Figure 5-21 Time Dependent Analysis, TOT_DEP Spearman Coefficient

5.2 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.

The uncertain input parameters that have been selected for this example are:

- Vfall: Velocity of falling debris,
- Hdblh: Heat transfer coefficient from debris to the lower head,
- SC1132(1): Core Component Failure Parameters – Temperature at which oxidized fuel rods can stand in the absence of unoxidized Zr in the cladding,
- SC1131(2): Zircaloy melt breakout temperature,
- SC1141(2): Core Melt Breakthrough Candling Parameters – Maximum melt flow rate per unit width after breakthrough,
- SC1502(2): Minimum Component Masses – Minimum total mass of component subject to the maximum temperature change criterion for timestep control, and
- SC1250(1): Conduction Enhancement for Molten Components – Temperature above which enhancement is employed.

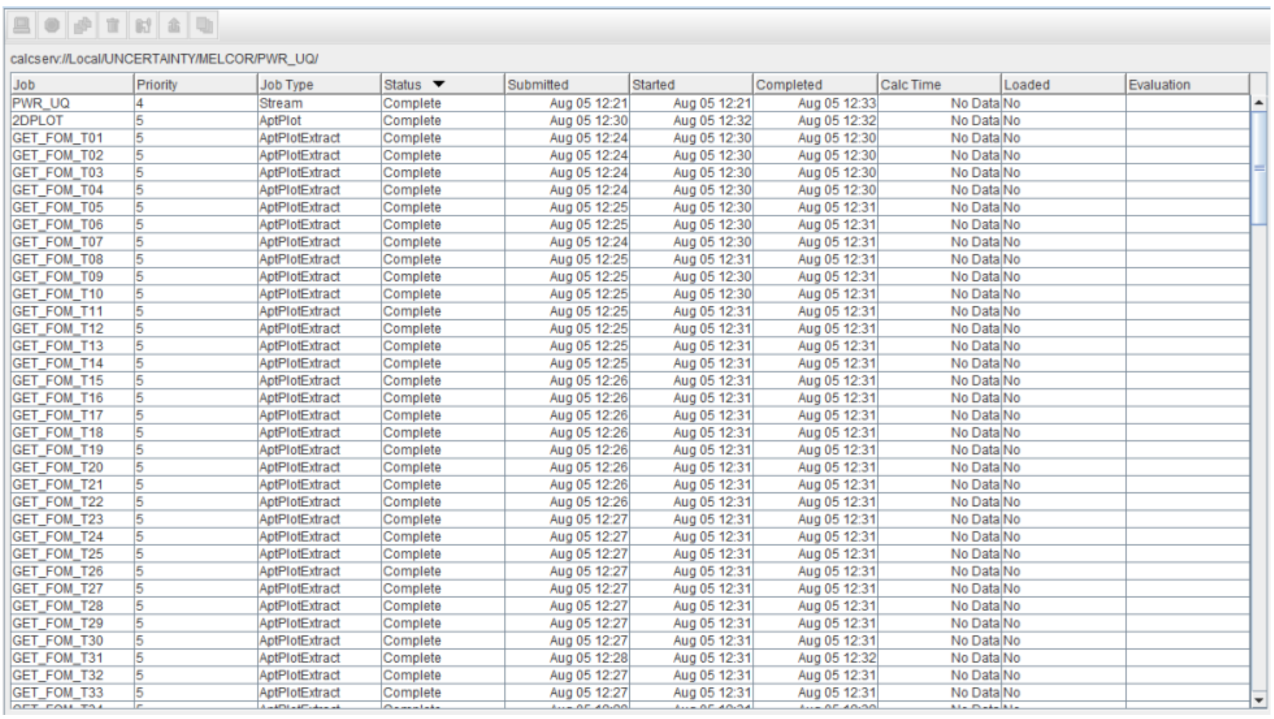
Only to show the methodology, the type of PDF and the range value of the input uncertain parameter are based on a first analyses reported in [15].[12]. Table 5-15 shows the model variables and distribution as summarized in the DAKOTA automatically generated report.

Figure 5-22 shows the SNAP Job-Status during the DAKOTA uncertainty application (providing a visual verification of the different extraction steps). Figure 5-23 shows the dispersion of the total hydrogen mass generated, CDF, and PDF (Case 2). Table 5-16 shows the statistical results based on the 59 samples, and Table 5-17 shows the response correlation reported in the automatically generated DAKOTA report based on the 59 samples (Case 2). The input file used in a -pre_run DAKOTA invocation to generate the random variates is reported in Figure 5-24.

[12] The characterization of the COR 1131-2 parameter, not present in [15], has been taken from the [45].

Table 5-15 Uncertainty Quantification Input Options - Model Variables and Distributions (SAMPLE 2)

Distribution Name	Distribution Type	Application Rule	Distribution Parameters	Model Variables	Nominal
d1	Triangular	Scalar	a:2098.0, m:2400.0, b:2550.0	COR 1131-2	Replacement
d2	Triangular	Scalar	a:0.01, m:0.083, b:1.0	COR 1141-2	Replacement
d3	Triangular	Scalar	a:0.05, m:0.1, b:1.2	VFALL	Replacement
d4	Triangular	Scalar	a:50.0, m:1000.0, b:1100.0	HDBLH	Replacement
d5	Normal	Scalar	μ:2700.0, σ:120.0, $[-\infty, \infty]$	COR 1132-1	Replacement
d6	Normal	Scalar	μ:5.0, σ:1.0, $[-\infty, \infty]$	COR 1502-2	Replacement
d7	Normal	Scalar	μ:2800.0, σ:150.0, $[-\infty, \infty]$	COR 1250-1	Replacement


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	
GET_FOM_T26	5	AptPlotExtract	Complete	Aug 05 12:27	Aug 05 12:31	Aug 05 12:31	No Data	No	
GET_FOM_T27	5	AptPlotExtract	Complete	Aug 05 12:27	Aug 05 12:31	Aug 05 12:31	No Data	No	
GET_FOM_T28	5	AptPlotExtract	Complete	Aug 05 12:27	Aug 05 12:31	Aug 05 12:31	No Data	No	
GET_FOM_T29	5	AptPlotExtract	Complete	Aug 05 12:27	Aug 05 12:31	Aug 05 12:31	No Data	No	
GET_FOM_T30	5	AptPlotExtract	Complete	Aug 05 12:27	Aug 05 12:31	Aug 05 12:31	No Data	No	
GET_FOM_T31	5	AptPlotExtract	Complete	Aug 05 12:28	Aug 05 12:31	Aug 05 12:32	No Data	No	
GET_FOM_T32	5	AptPlotExtract	Complete	Aug 05 12:27	Aug 05 12:31	Aug 05 12:31	No Data	No	
GET_FOM_T33	5	AptPlotExtract	Complete	Aug 05 12:27	Aug 05 12:31	Aug 05 12:31	No Data	No	

Figure 5-22 SNAP JOB-STATUS During the DAKOTA Uncertainty Application (SAMPLE 2)

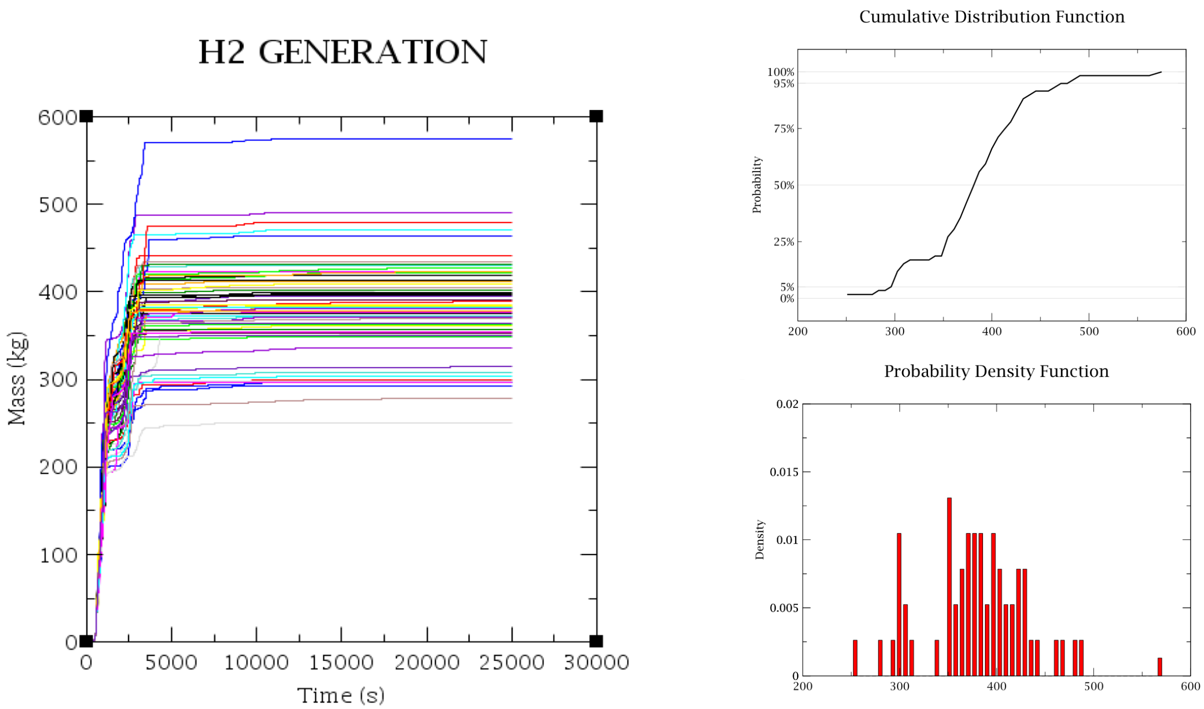


Figure 5-23 Tot Hydrogen Mass Generated Dispersion, CDF, and PDF (SAMPLE 2)

Table 5-16 Statistical Results Based on the 59 Samples (SAMPLE 2)

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	-

Table 5-17 Response Correlation Reported in the Automatically Generated DAKOTA Report Based on the 59 Samples (SAMPLE 2)

	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

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
```

Figure 5-24 DAKOTA Input Reported in the Automatically Generated Report.

5.3 Replacement Samples Option and Python Direct Job Stream

As previously described, the MELCOR/DAKOTA coupling can be done in SNAP. 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:

- 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” [48].
- Currently the “replacement samples” option is not available when using the SNAP/GUI. Therefore, if one calculation fails, it prevents UA finalization [49];
- The analysis of the MELCOR and DAKOTA coupling through SNAP PYTHON DIRECTED STREAM has been developed along the MUSA H2020 EURATOM project by UNIPI in collaboration with ENEA [50];
- Through this coupling approach, the management of failed code runs is possible by 3.1.6 SNAP version;
- This MELCOR/DAKOTA coupling is managed through a Python script, elaborated by SNAP, which permits to:
  - Run the MELGEN/MELCOR runs with the different sets of input uncertain parameters, created by the DAKOTA uncertainty plug-in;
  - Calculate the FOM values for each run;
  - Plot the dispersion of the FOMs through the module “PyPost”, developed by AptPlot;
  - Generate the UQ final report.
- Currently, the availability of PyPost to CSARP member is under discussion. In fact, the availability of the module PyPost is a fundamental requirement for the MELCOR/DAKOTA coupling in the SNAP environment/architecture with the Python Stream.

In Appendix A the new Python directed job-stream capability in SNAP is presented. This approach can be used to overcome the current limitations of the SNAP/GUI in the case of failed calculations.

6 CONCLUSION

In this report, the MELCOR/DAKOTA coupling for performing UAs is investigated considering two explorative applications (samples) previously conducted by ENEA. These analyses show the feasibility of using the MELCOR/DAKOTA coupling in the SNAP application for UAs for SA analysis using the probabilistic method to propagate input uncertainty.

The main steps necessary to couple DAKOTA and MELCOR within SNAP are presented in detail: the creation of the Job Stream, the setup of the analysis through the different Uncertainty Job Stream Tab, the plot definition, the data extraction and the execution of the UA. Moreover, the structure and content of the report automatically generated by DAKOTA at the end of the UA is also presented.

In addition, two explorative applications (samples) are also presented to show the potential of the MELCOR/DAKOTA coupling and the possible information that can be derived from the UA.

Currently the MUSA project, founded in Horizon 2020 EURATOM NFRP-2018-1- Safety assessments to improve accident management strategies for Generation II & III reactors, and the IAEA-CRP "Advancing the State-of-Practice in Uncertainty and Sensitivity Methodologies for Severe Accident Analysis in Water Cooled Reactors (I31033)" are in progress. In that framework representative uncertainty analyses are currently performed for plant application or against experimental data. These projects as well as the general MELCOR users, involved in other activities, can benefit from this guide and the provided examples.

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APPENDIX A PYTHON DIRECTED JOB STREAM

The set-up of the Python Directed Job Stream as an alternative way to perform an UA in SNAP will be presented in this appendix. The methodology is based on the use of SNAP as single platform to carry out the entire analysis, and on a user-specified Python script to guide it. Contrary to the previously presented approach, replacement samples are exploited in the case of code failures, allowing to successfully undertake the uncertainty analysis, as will be better explained below.

It should be highlighted that the following is an output of the activities done in the framework of the EURATOM MUSA project [46], coordinate by CIEMAT (Spain). In this regard, the Python script has been developed by University of Pisa, with a close interaction with ENEA, SNL and USNRC for the PHEBUS FPT1 [51] application developed in the WP4 (Application of UQ Methods against Integral Experiments – AUQMIE -) [52] of the MUSA project, coordinated by ENEA (Italy). In this report that script, have been updated applying to the sample 2.

A.1 General Approach

As the name suggests, the core of this approach is a user-specified Python script, which provides instructions to SNAP. The logic behind the script is shown in Figure A- 1.

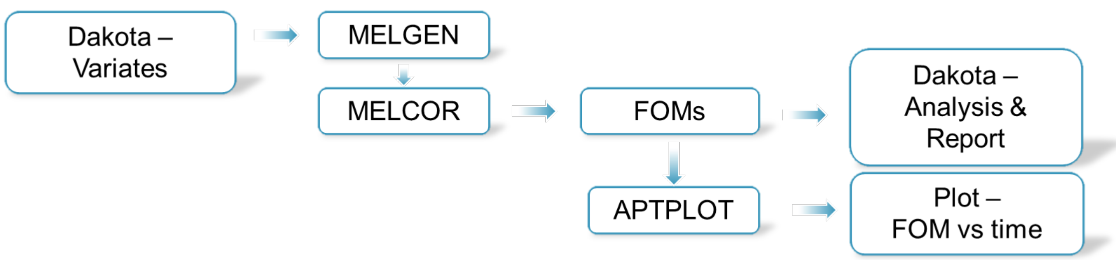

Figure A-1 Python Directed Job Stream Logic

DAKOTA, through the Uncertainty plugin embedded in SNAP, is employed to perform the sampling on the base of the user-selected input parameters and their distributions. Once the variates are created, several input decks are set up. The Python Job Stream manager handle the MELGEN/MELCOR runs, checking for their status. Additional calculations are run when one or more calculations fail, making use of the replacement samples. Afterwards, the selected FOM values are extracted and used by DAKOTA for the UA and the relative report. Finally, an extra step can be added for AptPlot to generate the required plots.

A step-by-step tutorial will be proposed in the next section.

A.2 Step-By-Step Tutorial

To proceed with the set-up of the Python Directed Job Stream, it is essential to have installed:

- SNAP 3.1.6 (or later versions);
- Updated SNAP uncertainty plugin;

- PyPost[13];
- MELGEN/MELCOR executables;
- Python 3 (3.6 or later) or Python 2.7 (optional).

The first step is the creation of a new Python Directed Job Stream (Figure A- 2):

- In the SNAP Model Editor, right-click on Job Streams;
- Select New;
- From the Job Stream list, select Python Directed.

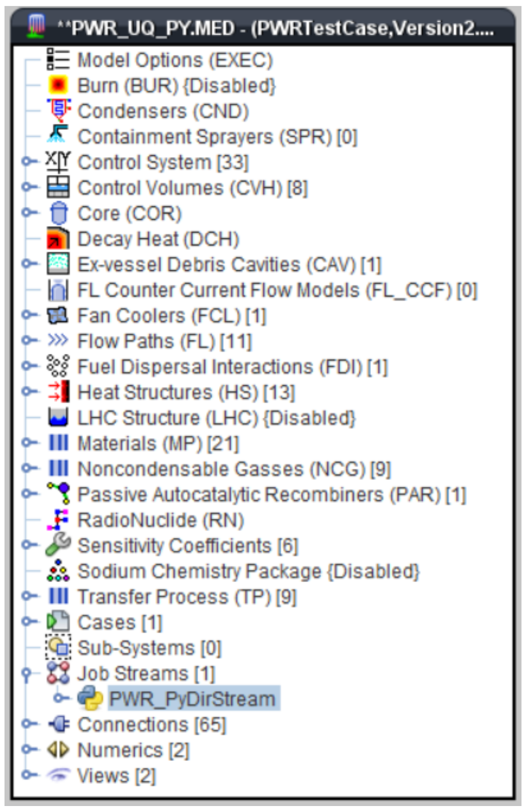

Figure A-2 New Job Stream

Once the Job Stream is created, the next step involves the configuration of the job properties (Figure A- 3):

- Name: the name for the job stream is imposed here;
- Root folder/relative location: the location of the folder in which the stream will be executed is chosen;

[13] PyPost is a Python Postprocessor for accessing and extracting variables plot data from several engineering analysis codes, such as MELCOR, RELAP5, TRACE, etc.

- Python application: possibility is given to select the Jython interpreter included in SNAP or Python, if installed on the computer;
- Python script: it is the core of the approach. Instructions are given to SNAP through this user-specified Python script. A basic example will be presented in the next section, complemented by a thorough description of each action;
- Uncertainty Quantification: the uncertainty configuration follows the same steps proposed in section 3.1.2. The only exception is the possibility to impose a number of additional variates to be created (namely Replacement Samples) to compensate for possible code failures (Figure A- 4).

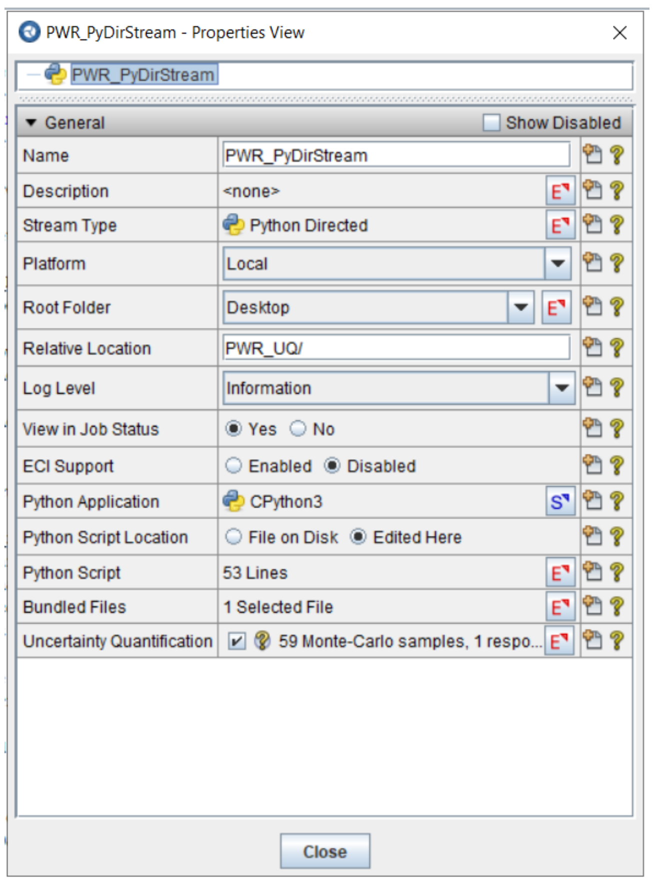

Figure A-3 Job Stream Properties

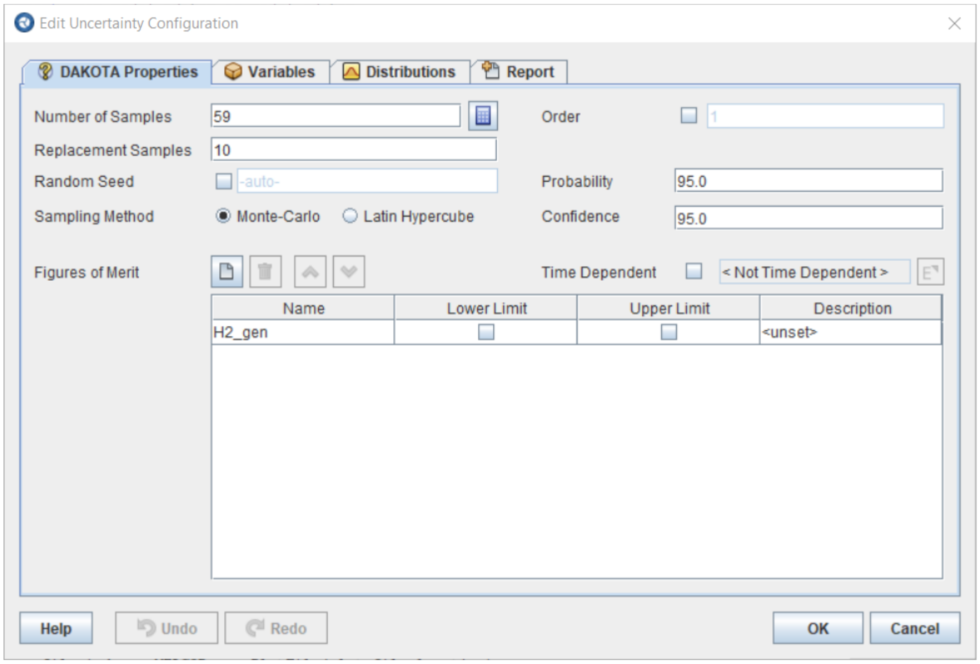

Figure A-4 Replacement Samples

Last step is the execution of the analysis:

- Right-click on the Python Directed Job Stream;
- Click on Check Stream;
- If no issues are found, right-click again on the Python Directed Stream;
- Click on Submit Stream to Local.

Once the steps have been completed, an “uncertainty report” folder is created, containing several files related to DAKOTA execution as well as the uncertainty report, as presented in Chapter 4.

A.2.1 Python Script

A basic Python script will be illustrated hereafter.

Python module ‘parametric’ is needed to retrieve the uncertainty configuration:

```
import parametric
```

SNAP streams and model editor, MELGEN and MELCOR jobs, and PyPost, are essential for the process to work. Therefore, the related modules are imported:

```
from snap import streams

import snap.model_editor as model_editor

from snap.codes.melcor import MelgenActor, MelcorActor
```

```
from pypost.codes.melcor import MELCOR
```

Reference is made to the current running stream:

```
stream = streams.get_stream()
```

The uncertainty table is here defined:

```
uq_table = parametric.get_table()
```

The base-case, to which variates will be applied to, is opened:

```
pwr_med = stream.get_bundled_file('PWR_UQ_PY.MED')

pwr = model_editor.open_model(pwr_med)
```

A function is added to the script for the generation of MELGEN and MELCOR jobs. The MELGEN and MELCOR jobs are created for each row of the uncertainty table (so considering each single of variates). Afterwards, they are added to the stream and launched:

```
def submit_jobs(table_row):
    melgen_run = MelgenActor(row.new_task_name("Melgen_Job"),
                             input=pwr)
    melcor_run = MelcorActor(row.new_task_name("Melcor_Job"),
                             input=pwr.case('MELCOR'),
                             restart_in=melgen_run.restart_out)
    stream.add([melgen_run, melcor_run])
```

A second function is added to the script to calculate the FOM (or FOMs) obtained in each run (i.e., for each UQ row). First, the plotfile associated with the MELCOR job is searched, with an error message shown in the case the plotfile does not exist. Afterwards, PyPost is employed to open the MELCOR plotfile and obtain the wanted data from it. And finally, the selected FOM value is stored in the UQ table:

```
def calculate_fom(table_row):
    plot_file = (row.search().label_eq("plot")
                 .task_name_contains("Melcor_Job")
                 .task_completed()
                 .result())
    if plot_file is None:
      stream.logger.error("Row {} failed or did not produce a plot file."
                          .format(table_row.row_index))
      table_row.failed = True
      return
```

```
        file_index = MELCOR.openPlotFile(plot_file.location)
        H2_gen = MELCOR.getData(file_index, 'COR-DMH2-TOT').maxYval()
        MELCOR.closeAll()

        print(H2_gen)
        row.set_fom_value('H2_gen', H2_gen)
```

A while-loop is employed to make use of the replacement samples in the case of runs' failures. New input decks are set up on the basis of the available additional variates, the new cases are launched and, once they all finished, the FOM is extracted and stored. Previously defined Python functions are employed:

```
    while uq_table.check_available():
        for row in uq_table.available():
            row.apply_values(pwr)
            submit_jobs(row)
        stream.wait()

        for row in uq_table.applied():
            calculate_fom(row)
```

Once the number of completed runs matches the number of runs defined during the uncertainty configuration, a job is created for the generation of the UQ report:

```
    parametric.get_table().generate_report()
```

As aforementioned, the script here presented is the most basic one. Additional features can be added to extract different type of data, as briefly explained in the PyPost documentation [47]. Moreover, instructions could be added in the script in order to obtain selected plots by means of AptPlot. The complete Python script is reported hereafter.

```
import parametric
from snap import streams
import snap.model_editor as model_editor
from snap.codes.melcor import MelgenActor, MelcorActor
from pypost.codes.melcor import MELCOR

stream = streams.get_stream()
uq_table = parametric.get_table()
pwr_med = stream.get_bundled_file('PWR_UQ_PY.MED')
pwr = model_editor.open_model(pwr_med)
```

```
def submit_jobs(table_row):
    melgen_run = MelgenActor(row.new_task_name("Melgen_Job"),
                             input=pwr)
    melcor_run = MelcorActor(row.new_task_name("Melcor_Job"),
                             input=pwr.case('MELCOR'),
                             restart_in=melgen_run.restart_out)
    stream.add([melgen_run, melcor_run])

def calculate_fom(table_row):
    plot_file = (row.search().label_eq("plot")
                 .task_name_contains("Melcor_Job")
                 .task_completed()
                 .result())

    if plot_file is None:
        stream.logger.error("Row {} failed or did not produce a plot file."
                            .format(table_row.row_index))
        table_row.failed = True
        return

    file_index = MELCOR.openPlotFile(plot_file.location)
    H2_gen = MELCOR.getData(file_index, 'COR-DMH2-TOT').maxYval()
    MELCOR.closeAll()

    print(H2_gen)
    row.set_fom_value('H2_gen', H2_gen)

while uq_table.check_available():
    for row in uq_table.available():
        row.apply_values(pwr)

        submit_jobs(row)

    stream.wait()

    for row in uq_table.applied():
        calculate_fom(row)

parametric.get_table().generate_report()
```

NRC FORM 335 (12-2010) NRCMD 3.7 U.S. NUCLEAR REGULATORY COMMISSION **BIBLIOGRAPHIC DATA SHEET** *(See instructions on the reverse)*	1. REPORT NUMBER (Assigned by NRC, Add Vol., Supp., Rev., and Addendum Numbers, if any.) **NUREG/IA-0532**
2. TITLE AND SUBTITLE **MELCOR – DAKOTA Coupling for Uncertainty Analyses, in a SNAP Environment/Architecture**	3. DATE REPORT PUBLISHED MONTH: **March** YEAR: **2023**
	4. FIN OR GRANT NUMBER
5. AUTHOR(S) F. Mascari(1, A. Bersano(1, G. Agnello(2, M. Angelucci(3, J. Phillips(4, D. Luxat(4	6. TYPE OF REPORT Technical
	7. PERIOD COVERED (Inclusive Dates)

8. PERFORMING ORGANIZATION - NAME AND ADDRESS (If NRC, provide Division, Office or Region, U. S. Nuclear Regulatory Commission, and mailing address; if contractor, provide name and mailing address.)

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9. SPONSORING ORGANIZATION - NAME AND ADDRESS (If NRC, type "Same as above", if contractor, provide NRC Division, Office or Region, U. S. Nuclear Regulatory Commission, and mailing address.)

Division of Systems Analysis
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555-0001

10. SUPPLEMENTARY NOTES

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11. ABSTRACT (200 words or less)

Uncertainty estimation to assess figure-of-merits characterizing evolution of a severe accident transient is a topic of current investigation in development of best-estimate plus uncertainty methodology. The probabilistic method to propagate input uncertainty is one of the methodologies used to develop Uncertainty Analyses (UAs). Using this methodology, UAs are performed by sampling probability distributions that describe the range of possible values that computer simulation model inputs can have. For each sample (or realization) of a set of uncertain input parameters, a computer simulation is performed. From the range of code simulation results obtained for each input realization, a distribution of code results is obtained. In this process, the distribution of input uncertainties is *propagated* to obtain a distribution of possible code results (i.e., the code output uncertainty). This probabilistic methodology is facilitated using Uncertainty Tools (UTs), which can be coupled with the accident analysis computer code to perform an UA. One of the UTs currently available is DAKOTA, developed by Sandia National Laboratories. DAKOTA is also provided as a SNAP plug-in. SNAP is a graphical user interface designed to support the use of USNRC codes. This report demonstrates the workflow within SNAP to assist other interested analysts with their applications given they are members of the USNRC Cooperative Severe Accident Research Program (CSARP). Two sample applications are shown.

12. KEY WORDS/DESCRIPTORS (List words or phrases that will assist researchers in locating the report.)	13. AVAILABILITY STATEMENT
Uncertainty Analyses, MELCOR, DAKOTA, SNAP	unlimited
	14. SECURITY CLASSIFICATION
	(This Page) unclassified
	(This Report) unclassified
	15. NUMBER OF PAGES
	16. PRICE

NUREG/IA-0532

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

April 2023