ICSBEP Benchmarking Workshop for DNCSH Project Teams

Section 3.0 – Benchmark Specifications
Section 4.0 – Results and Sample Calculations

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Section 3.0, Benchmark Specifications

- Document Content and Format Guide for the International Criticality Safety Benchmark Evaluation Project (Critical and Subcritical Measurements)
  - *In general, the benchmark specifications (Section 3.0) provide the information necessary to justify and construct calculational models that best represent the experiment.*

- Required subsections of Section 3.0
  - 3.1 Description of Model
  - 3.2 Dimensions
  - 3.3 Material Data
  - 3.4 Temperature Data
  - 3.5 Experimental and Benchmark-Model k_{eff} (and/or Subcritical Parameters)

- Model parameters should be given in SI units

Section 3.0, Benchmark Specifications

- Given the physical description and raw data from Section 1.0 and the evaluation of that data from Section 2.0, Section 3.0 describes the computational model of the experiment
  - Distilling the real-world into the virtual-world
  - Description should be code agnostic
- Major components include:
  - Simplifications and resulting biases (Section 3.1)
  - Benchmark-model specifications (Sections 3.2-3.4)
  - Benchmark-model k_{eff} (Section 3.5)
- From a benchmark user's perspective, Section 3.0 should give sufficient detail as to not need to refer to Sections 1.0 or 2.0 when constructing the model

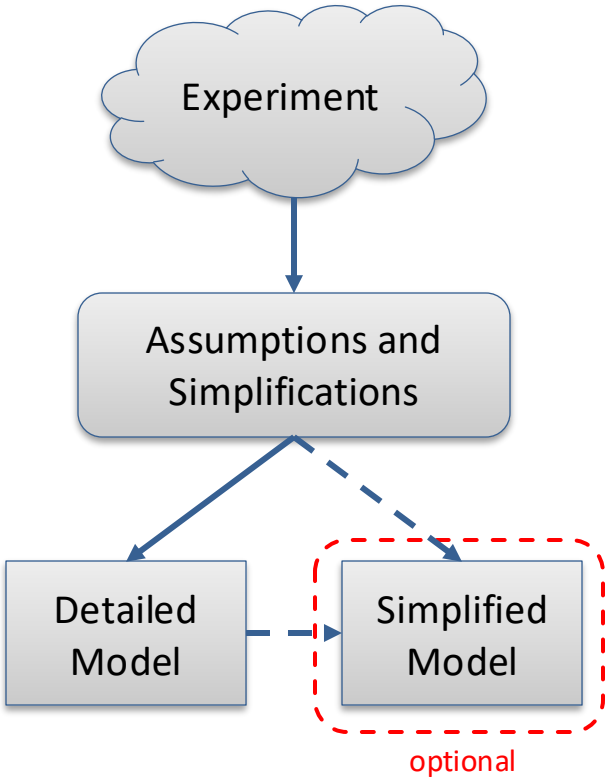
Comparison of Section 1.0 and Section 3.0

- The subsections of Section 3.0 mirror those of Section 1.0
  - Section 1.0 provides the physical description of the experiment
  - Section 3.0 describes the computational model of the experiment

Section 1.0	Section 3.0
1.1 Overview of Experiment	3.1 Description of Model
1.2 Description of Experimental Configuration	3.2 Dimensions
1.3 Description of Material Data	3.3 Material Data
1.4 Temperature Data	3.4 Temperature Data
1.5 Supplemental Experimental Measurements	3.5 Experimental and Benchmark-Model k_{eff}

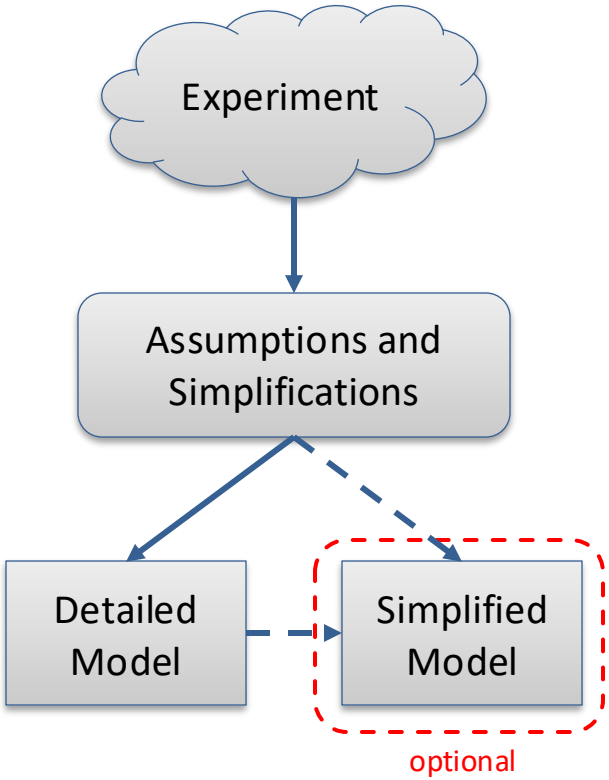
3.1 Description of Model

- Document Content and Formatting Guide on Section 3.1:
  - General description of main the physical features of the benchmark model(s)
  - Describe and justify simplifications and approximations made to geometric configurations or material specifications, including any resulting biases/uncertainties in k_{eff}
  - Explanation of all assumptions used in going from the real experimental configuration(s) to the benchmark-model configuration(s)



General Description

- Document Content and Formatting Guide on Section 3.1:
  - General description of main the physical features of the benchmark model(s)
  - Describe and justify simplifications and approximations made to geometric configurations or material specifications, including any resulting biases/uncertainties in k_{eff}
  - Explanation of all assumptions used in going from the real experimental configuration(s) to the benchmark-model configuration(s)



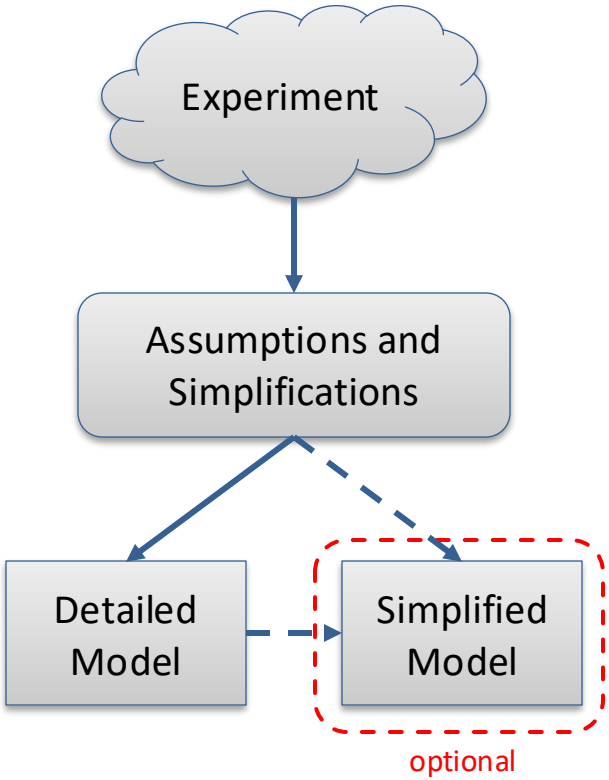
General Description

- Orient the benchmark user by providing a high-level description of the model of the experiment
  - Similar to Section 1.1, Overview of Experiment, now focusing on a description of the model
  - Describe the *main physical features*
  - State any significant differences between the model and experiment
- **TIP:** Provide a figure showing the overall model at the beginning of Section 3.0 to give the user an idea of what their model will look like. If there are multiple cases, include multiple figures or one representative model.

Typically describes the model in a few paragraphs, with a subsection for the detailed and simplified models (if included).

Simplifications

- Document Content and Formatting Guide on Section 3.1:
  - General description of main the physical features of the benchmark model(s)
  - Describe and justify simplifications and approximations made to geometric configurations or material specifications, including any resulting biases/uncertainties in k_{eff}
  - Explanation of all assumptions used in going from the real experimental configuration(s) to the benchmark-model configuration(s)



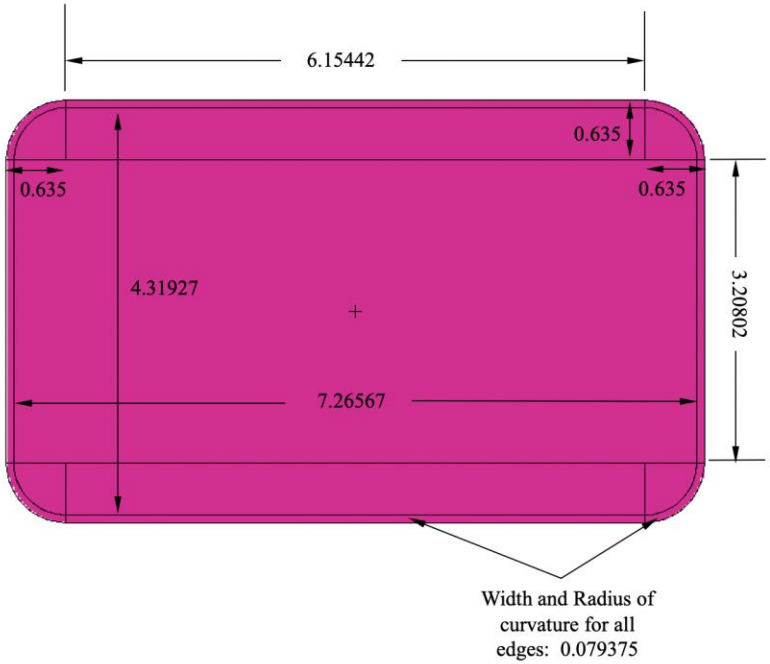
Simplifications

- Ease the modeling burden on the benchmark user while *retaining as much detail as necessary to preserve all important aspects of the actual experiment*
  - These important aspects are the benchmark quantity (e.g., k_{eff}), the neutron energy spectrum, and other characteristics of the experiment
- Common simplifications include:
  - Removal of the experiment room
  - Geometry and material simplifications
    - Removing minor details that have little to no effect in k_{eff} (screws/bolts, instrumentation, flaws, etc.)
    - Voiding of unimportant impurities
  - Averaging of similar part dimensions or materials
  - Temperature adjustment (nuclear data typically provided at 20°C)

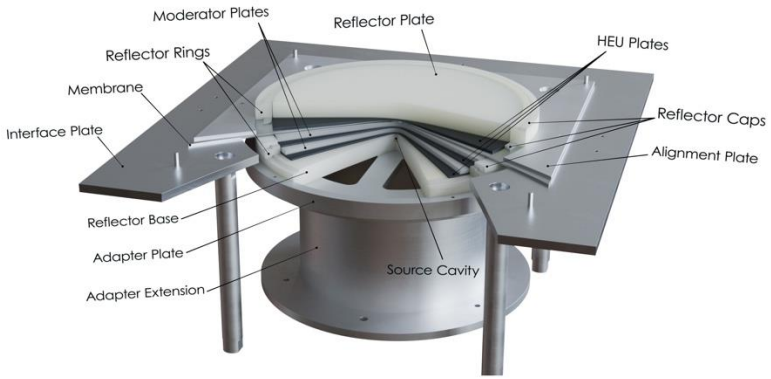
Typically includes a subsection with a paragraph describing each simplification and reports the effect on k_{eff} of the simplification.

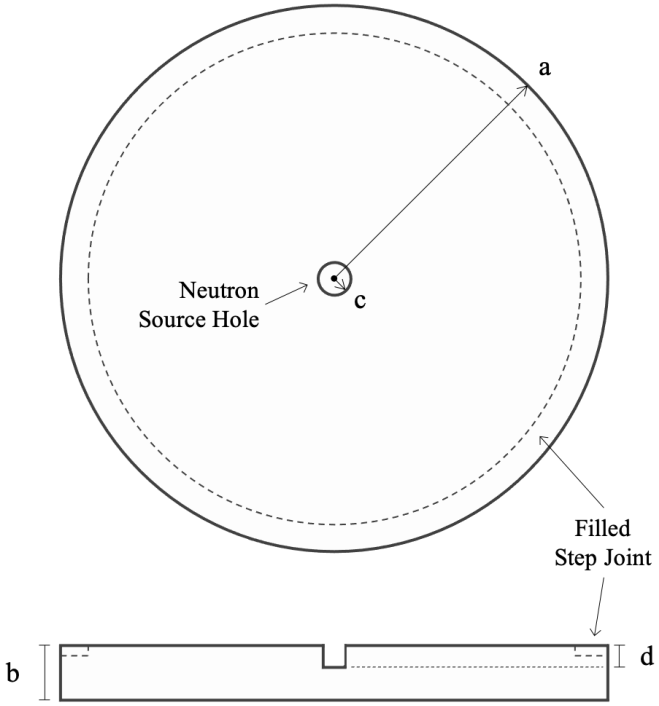
Example Simplification: PMM-002

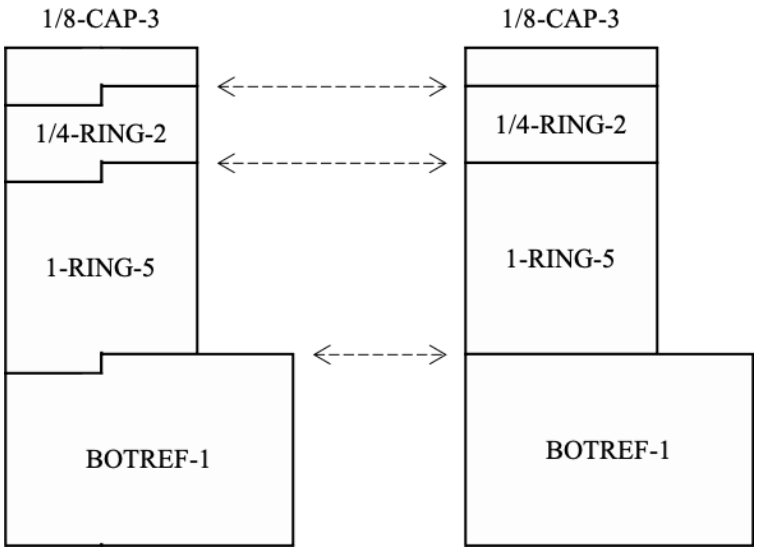
- Simplified the Pu core model by removed the curved edges of the plate
  - Reduced the Pu core model from 31 to 7 segments
- Conservation (mass, volume, etc.) is necessary when considering simplifications
  - *Straightening the curved edges requires adding additional material to the edges, and to maintain the same volume, the overall dimensions of the plate must be reduced*



Example Simplification: HMM-021







- Simplified the reflectors by removing the step joints
- Conserved total mass of the reflector by changing density

Simplification Bias

- Simplifications must *describe the transformation from the measured values to the benchmark-model values and include the effect of the transformation on k_{eff}*
- If the effect of this transformation on k_{eff} is small or negligible, this provides a strong justification for the simplification
  - However, expert judgement must be used to ensure *the basic nature of the configuration* is not changed (e.g., neutron spectrum)
- Calculated simplification biases (Section 3.1) are used to adjust the experimental k_{eff} (Section 2.0) to determine an expected benchmark-model k_{eff} (Section 3.5)
  - The benchmark-model k_{eff} is then compared to a sample calculation k_{eff} in Section 4.0, typically reporting the calculation-over-experiment (C/E)

Simplification Bias

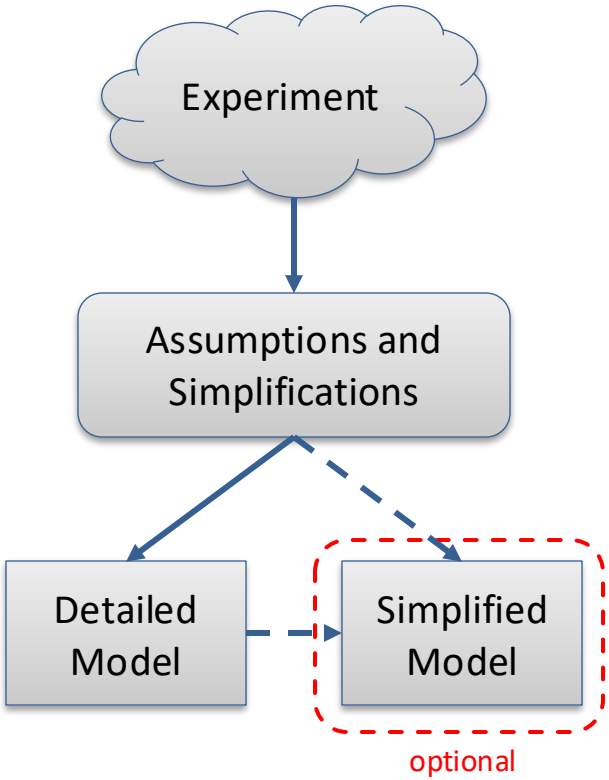
- Benchmarks must include the bias and uncertainty in the bias if model simplifications are made
  - However, not all benchmarks fully document the simplifications or assumptions used to build the benchmark-model
  - Some may include the simplification without a justification

- **TIP:** A useful tool for the benchmark user is a table summarizing the simplification biases, such as this table from PMM-002:

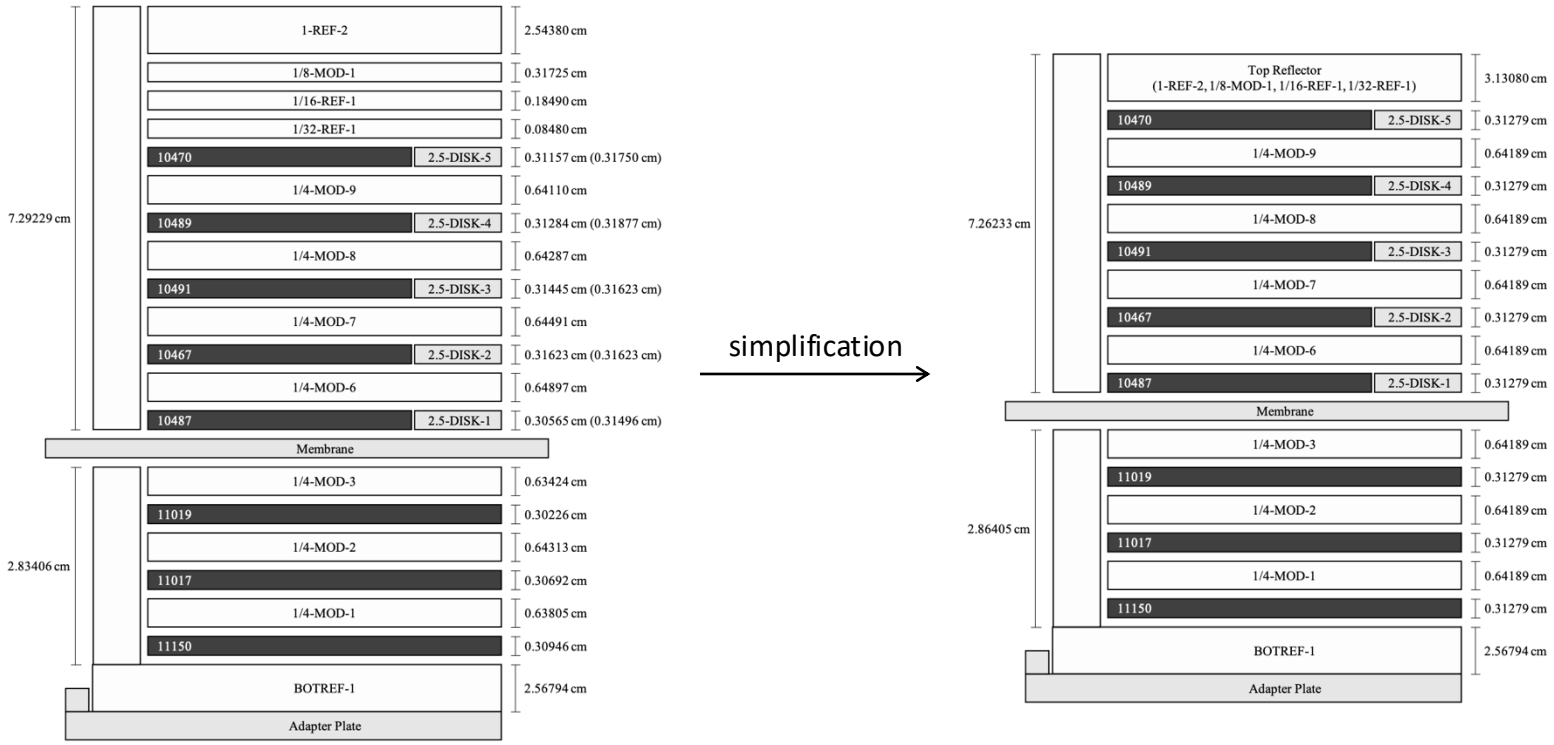
Bias Component	Case 1	Case 2	Case 3	Case 4	Case 5
Rivets, RTD, and PE impurities removal	+0.00005 ±0.00008	-0.00013 ±0.00009	-0.00001 ±0.00009	+0.00002 ±0.00009	-0.00016 ±0.00009
Temperature change to 20°C	+0.00002 ±0.00008	+0.00024 ±0.00009	+0.00091 ±0.00009	+0.00083 ±0.00009	-0.00019 ±0.00009
Room return (room removal)	-0.00070 ±0.00006	-0.00072 ±0.00005	-0.00061 ±0.00006	-0.00079 ±0.00006	-0.00048 ±0.00005
Total	**-0.00063 ±0.00013**	**-0.00061 ±0.00015**	**+0.00029 ±0.00015**	**+0.00006 ±0.00015**	**-0.00083 ±0.00015**

Detailed and Simplified Models

- Many benchmarks include only a single benchmark model, but some include both a detailed and simplified model
- Motivations for having a detailed and simplified model may include:
  - Desire to take advantage of software features such as latticing or repeating geometries typically requiring uniformity
  - Provide the user different model dimensionality (1D vs. 3D model)
  - Avoid limitations in the geometric representation of modeling software
- Having both a detailed and simplified model may increase the modeling burden on the benchmark evaluator



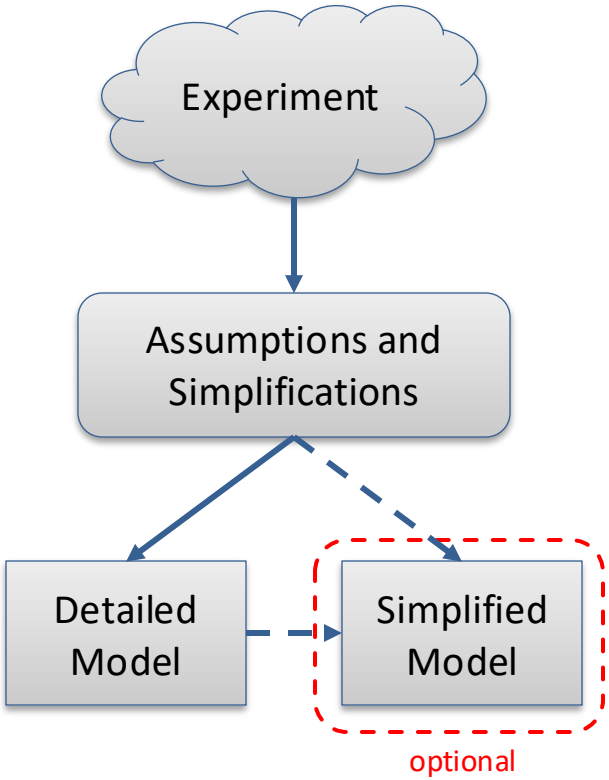
Example Detailed and Simplified Models: HMM-021



- Detailed model (left) includes all parts at their measured thickness while the simplified model (right) includes parts at an average thickness creating a repeatable geometry
- Both models include a simplified representation of the reflector (simplification bias)

Assumptions and Approximations

- Document Content and Formatting Guide on Section 3.1:
  - General description of main the physical features of the benchmark model(s)
  - Describe and justify simplifications and approximations made to geometric configurations or material specifications, including any resulting biases/uncertainties in k_{eff}
  - Explanation of all assumptions used in going from the real experimental configuration(s) to the benchmark-model configuration(s)



Assumptions and Approximations

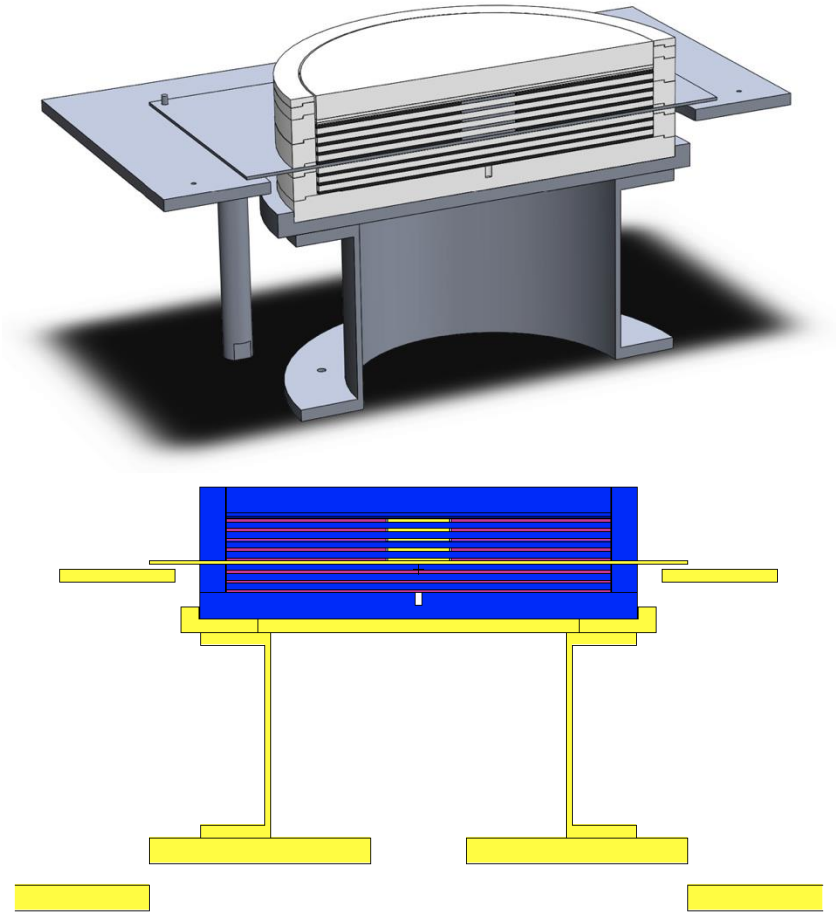
- Justification of simplifications, including the assumptions required to model the experiment given lacking or missing data (discussed and evaluated in Section 2.0)
  - Relevant to historical experiments benchmarked years later
- Make these assumptions clear to the benchmark user, allowing them to judge the potential impact on their use case
- Allow the TRG to easily judge the validity of the assumptions

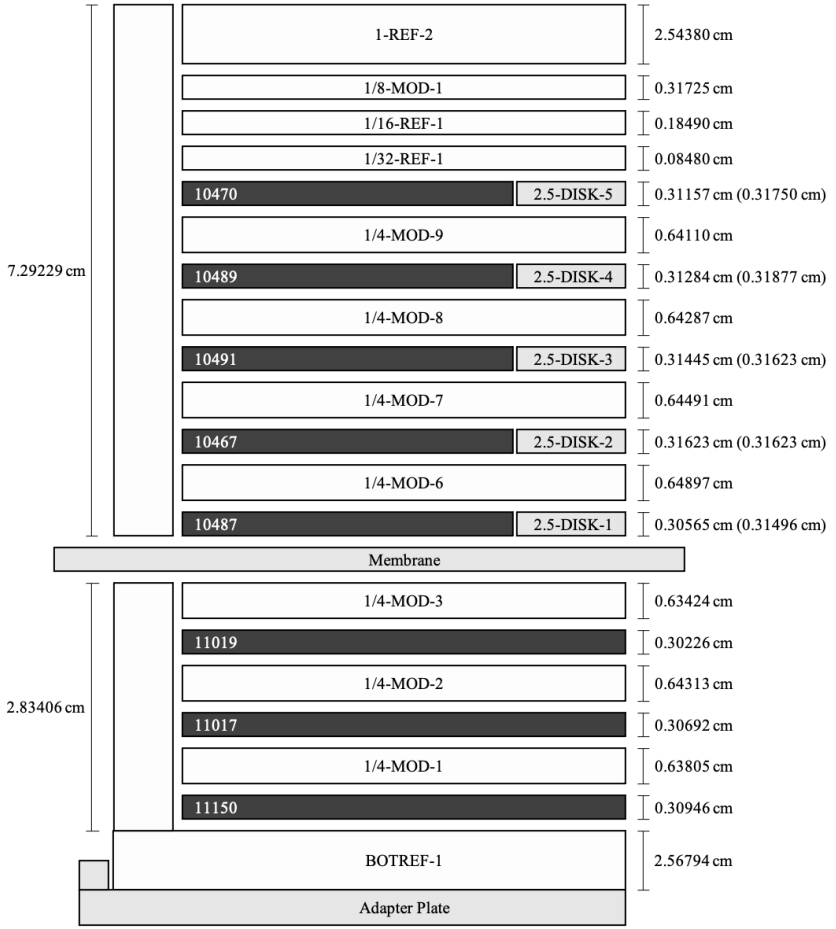
3.2 Dimensions

- Document Content and Formatting Guide on Section 3.2:
  - All required dimensions and information needed to completely describe the geometry of the benchmark model(s) are included in this section
  - Sketches, including dimensions and labels, of the benchmark model(s) should always be included
  - Report dimensions in SI units
- Provide the benchmark user detailed descriptions of part types and part dimensions, describing how the components fit together to model the experiment
  - All data evaluation completed in Section 2.0

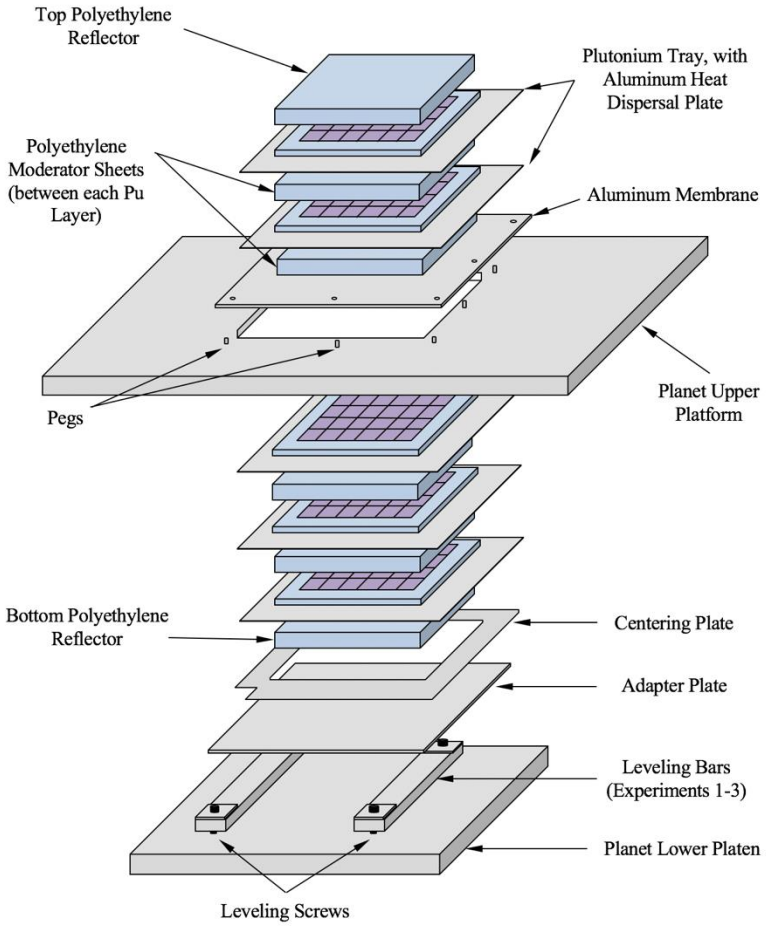
Typically, this subsection is the bulk of Section 3.0 (50%-75%) describing the model(s), including many figures with annotations and tables with dimensions.

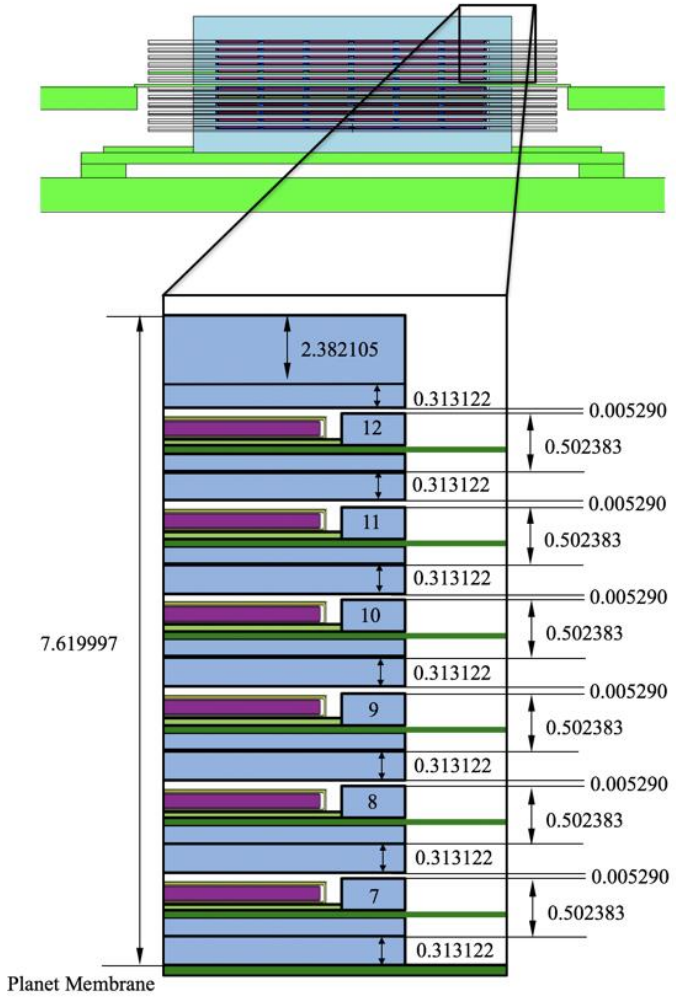
Example Model: HMM-021





Example Model: PMM-002





3.3 Material Data and 3.4 Temperature Data

- Document Content and Formatting Guide on Section 3.3:
  - Atom densities for all materials specified for the model(s) are derived from the reported compositions and masses or densities given in the previous sections and are concisely listed here

$$N = \frac{\rho N_A}{M}$$

  - The Document Content and Formatting Guide includes reference Nuclear Constants (Avogadro's Number and atomic weights)
    - If deviating from these, reference which contants are used
- Document Content and Formatting Guide on Section 3.4:
  - Temperature of the model is provided in this section

The text of both of these subsections is typically short, with Section 3.3 containing many tables listing the atom densities of all the materials in the benchmark model.

Atom Densities, Wt.%, and At.%

- The Document Content and Formatting Guide requires the benchmark evaluator to include atom densities (atoms-b/cm) for each material
- **TIP:** The evaluator may include other quantities, such as Wt.% and/or At.%, and report elemental and isotopic compositions
  - These values can be useful to the user and as inputs to various software, plus they're already typically required in the atom density calculation

Table 193: HEU elemental and isotopic composition used in all benchmark models.

Element	Wt.%	Isotope	Wt.%	At.%
U	1.00000E+02	^{234}U	1.03046E+00	1.03556E+00
		^{235}U	9.32324E+01	9.32940E+01
		^{236}U	2.32202E-01	2.31369E-01
		^{238}U	5.50498E+00	5.43904E+00

Table 195: HEU plate atom densities by case.

Isotope	Atom Density (atoms-b/cm)			
	Case 1	Case 2	Case 3	Case 4
^{234}U	4.84602E-04	4.84603E-04	4.83570E-04	4.84403E-04
^{235}U	4.36579E-02	4.36579E-02	4.35649E-02	4.36399E-02
^{236}U	1.08272E-04	1.08272E-04	1.08041E-04	1.08227E-04
^{238}U	2.54525E-03	2.54526E-03	2.53983E-03	2.54421E-03
Total	**4.67960E-02**	**4.67961E-02**	**4.66963E-02**	**4.67768E-02**

Isotope	Atom Density (atoms-b/cm)		
	Case 5	Case 6	Case 7
^{234}U	4.84177E-04	4.84347E-04	4.84728E-04
^{235}U	4.36195E-02	4.36349E-02	4.36692E-02
^{236}U	1.08176E-04	1.08215E-04	1.08300E-04
^{238}U	2.54302E-03	2.54391E-03	2.54591E-03
Total	**4.67549E-02**	**4.67714E-02**	**4.68081E-02**

3.5 Experimental and Benchmark-Model k_{eff} (and/or Subcritical Parameters)

- Document Content and Formatting Guide on Section 3.5:
  - Report the experimental k_{eff} and its uncertainty
  - If the experiment description is simplified, the effect on k_{eff} of this transformation, carefully quantified either from measurements or calculations, may result in an adjustment of the experimental k_{eff} to obtain k_{eff} of the benchmark model
- The benchmark-model k_{eff} represents the quantity that the evaluator is recommending be compared to calculations
  - Based on evaluated model simplifications

Typically contains a table detailing the benchmark-model k_{eff} calculation.

Benchmark-Model k_{eff}

- The experimental k_{eff} determined at the end of Section 2.0 is combined with the simplification bias (Section 3.1) and the Section 2.0 combined uncertainty to produce the benchmark-model k_{eff}
- Examples of these calculations from PMM-002 and HMM-021:

Case	Experimental $k_{eff} \pm 1\sigma$	Bias in $k_{eff} \pm 1\sigma$	Benchmark Model k_{eff}
1	1.00090 ± 0.00014	-0.00092 ± 0.00013	1.00073 ± 0.00260
2	1.00082 ± 0.00014	-0.00058 ± 0.00015	1.00024 ± 0.00236
3	1.00059 ± 0.00014	0.00013 ± 0.00015	1.00072 ± 0.00220
4	1.00067 ± 0.00013	0.00029 ± 0.00015	1.00083 ± 0.00287
5	1.00000 ± 0.00013	-0.000133 ± 0.00015	0.99940 ± 0.00193

Case	Experimental $k_{eff} \pm 1\sigma$	Bias in $k_{eff} \pm 1\sigma$	Benchmark Model k_{eff}
1	1.00026 ± 0.00132	0.00275 ± 0.00013	0.99751 ± 0.00133
2	1.00038 ± 0.00126	0.00300 ± 0.00013	0.99738 ± 0.00127
3	1.00067 ± 0.00129	0.00299 ± 0.00013	0.99768 ± 0.00130
4	1.00112 ± 0.00148	0.00282 ± 0.00013	0.99830 ± 0.00149
5	1.00094 ± 0.00119	-0.00068 ± 0.00013	1.00162 ± 0.00120

Section 4.0, Results of Sample Calculations

- Document Content and Formatting Guide on Section 4.0:
  - Calculated results obtained with the benchmark-model specification data given in Section 3 are tabulated in this section
  - Codes and cross section data sets used for the sample calculations are indicated in Section 4, but details about the calculations and input listings are given in Appendix A

- *Calculated results that differ from the benchmark-model values (Section 3.5) by more than 1% or 3σ (whichever is smaller) should be noted and may be explained if the reasons are thought to be known*

Table X. Sample Calculation Results

Code Name→ (Cross Section Set)→ Case Number ↓	Code Name (Cross Section Name)	Code Name (Cross Section Name)	Code Name (Cross Section Name)

Example Sample Calculation Results: HMI-013

- The uncertainty of the calculated k_{eff} represents the statistical uncertainty of the sample calculation(s)
- The uncertainty of the C/E results represent the Section 2.0 uncertainty combined with the statistical uncertainty of the sample calculation(s)

Table 205: Sample k_{eff} and C/E results with combined experimental and calculational uncertainties using MCNP® 6.2.2 with ENDF/B-VIII.0 (United States).

Case	MCNP® 6.2.2 (Continuous Energy ENDF/B-VIII.0)	
	Calculated k_{eff}	C/E
1	1.00097 ± 0.00003	1.00194 ± 0.00147
2	1.00135 ± 0.00003	1.00227 ± 0.00158
3	0.99854 ± 0.00004	0.99918 ± 0.00154
4	0.99574 ± 0.00004	0.99731 ± 0.00124
5	0.99947 ± 0.00004	0.99770 ± 0.00147
6	0.99850 ± 0.00004	0.99907 ± 0.00142
7	0.99605 ± 0.00003	0.99662 ± 0.00137

Final Notes

- The most detailed model is still a simplification of reality
- Figures should be clear, do not necessarily need to be to scale if doing so improves clarity
  - Provide identifying information as to what material a part is in the figure, if useful to the user
- Note the relationships between parts, report the dimensions between parts that go together (e.g., gaps or parts that are stacked)
- Pay attention to the sign (+/-) of the bias(es) in Section 3.1 and how the benchmark-model k_{eff} is corrected in Section 3.5

Conclusion

- Section 3.0 fully describes the model used to represent the physical benchmark experiment
  - Including desired (or necessary) simplifications
  - *Retaining as much detail as necessary to preserve all important aspects of the actual experiment*
- Section 4.0 provides the benchmark user sample calculation results based on the Section 3.0 model
  - Up to the user to reproduce based on applicable codes and/or use cases
- Possible shortcomings:
  - Unjustified use of nominal dimensions
  - Unreported assumptions or simplifications
  - Lacking/missing data or use of simplifications that have too large an effect on k_{eff}

Resources

- ICSBEP Handbook
  - Request through the OECD/NEA: oecd-nea.org/jcms/pl_24498/
- Included with the ICSBEP Handbook:
  - 600+ Accepted Evaluations
  - Document Content and Formatting Guide (Critical and Subcritical Measurements)
  - ICSBEP Guide to Expression of Uncertainties (for Section 2.0)
  - ICSBEP Review Check List
    - Used by reviewers of the ICSBEP Technical Review Group, providing a high-level checklist of what is required in each section and subsection
- **TIP:** Review a selection of past evaluations from various institutions and authors to become familiar with their organization and content.



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