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Mixed Uranium-Plutonium Solution Validation of KENO V.a and KENO-VI in SCALE 6.1.2 and 6.2b3 Using Multigroup and Continuous-Energy ENDF/B-VII.0 Libraries

Elizabeth Jones, B.J. Marshall,

and Ivan Maldonado

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Outline

- Introduction
- Code Description
- Description of MST Experiments
- Method for Comparison
- Results
- Conclusions
- Future Work

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Introduction

- SCALE 6.1 was assessed at ORNL for hundreds of critical benchmarks from a range of different types of systems
- Benchmarks are from IHECSBE and included in the VALID library maintained at ORNL
- The purposes of this study:
  - Quantify KENO performance for MSTs
  - Compare SCALE 6.1.2 and SCALE 6.2b3 for MSTs
- Study parameters:
  - MST-002, MST-004, MST-005
  - KENO V.a and KENO-VI codes and ENDF/B-VII.0 data
  - Continuous-energy libraries
  - 238-group for SCALE 6.1.2, 252-group for SCALE 6.2b3

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Code Description

- SCALE 6.1 has two 3D Monte Carlo transport codes for calculation of k_{eff}
- KENO V.a
  - Simple descriptions of complex systems using repeating Cartesian arrays and holes
  - No intersections and all objects parallel to a major axis
- KENO-VI
  - Contains SCALE Generalized Geometry Package
  - Uses mostly pre-defined geometry objects to define regions
  - Allows Cartesian, hexagonal, and dodecahedral arrays as well as holes
  - Supports intersections and rotation

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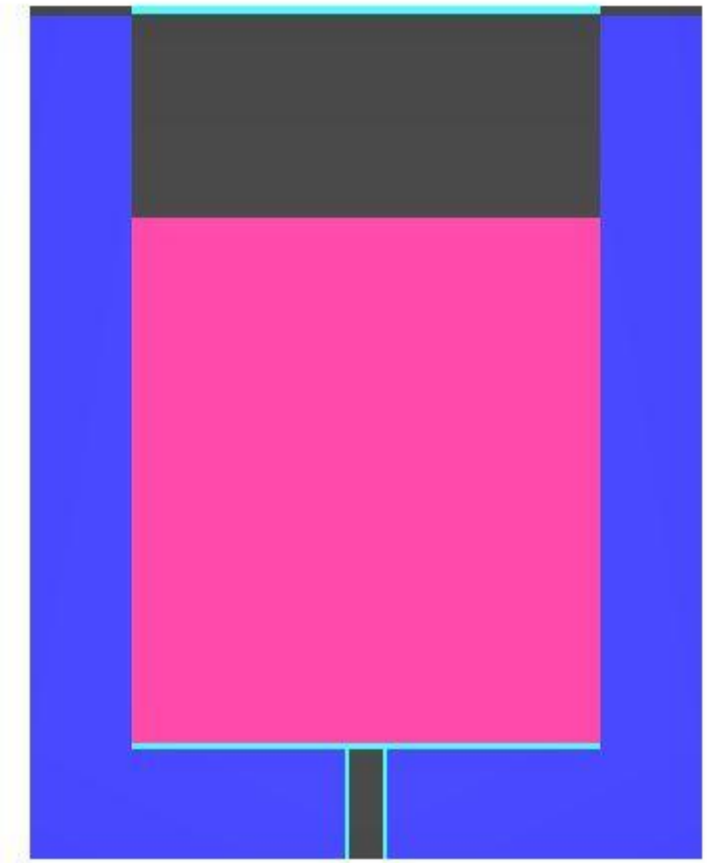
Description of MST-002

Vertical plan view for the model geometry of MST-002



- 3 critical experiments
- Plutonium fraction of 0.2 and 0.5 in a large cylindrical tank with water reflection
- Consists of a cylindrical reaction vessel with a 68.68 cm ID
- Height of the reaction vessel is ~108.5 cm
- Model did not include the concrete room
- Cases differ due to varying fissile solution compositions, critical solution heights and reflector temperatures
- Calculations performed in KENO V.a

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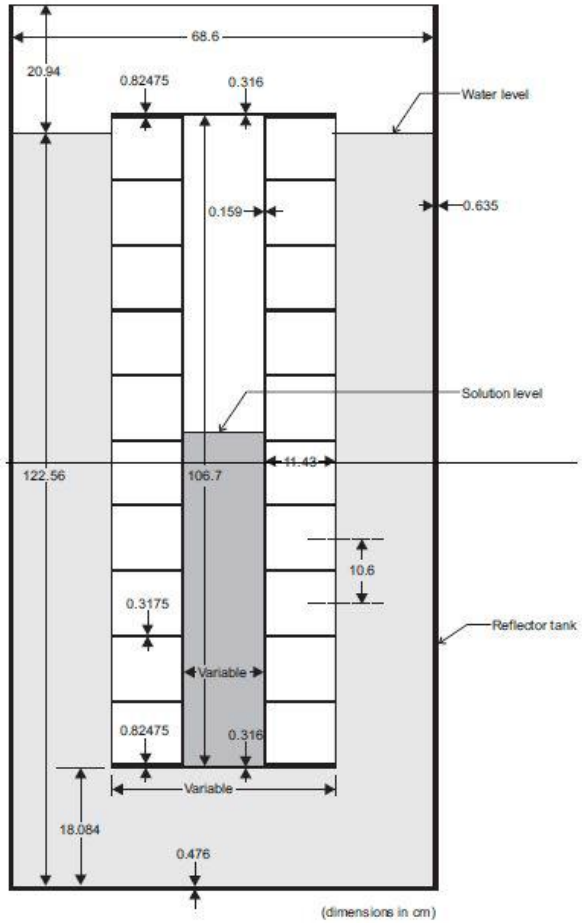
Description of MST-005

Elevation view for part of the model geometry of MST-005



- 7 critical experiments
- Plutonium fraction of 0.4 in slab geometry
- Slab tank has square stainless steel walls ~107.3 cm in height and width
- A support grid reinforces the faces of the tank
- Cases differ due to varying solution compositions, critical solution heights and widths
- Three experiments are bare, four cases are water reflected
- Water-reflected cases are modeled with only the tank, the support grid, and the reflector tank
- Bare cases include room to capture room return
- Calculations performed in KENO V.a

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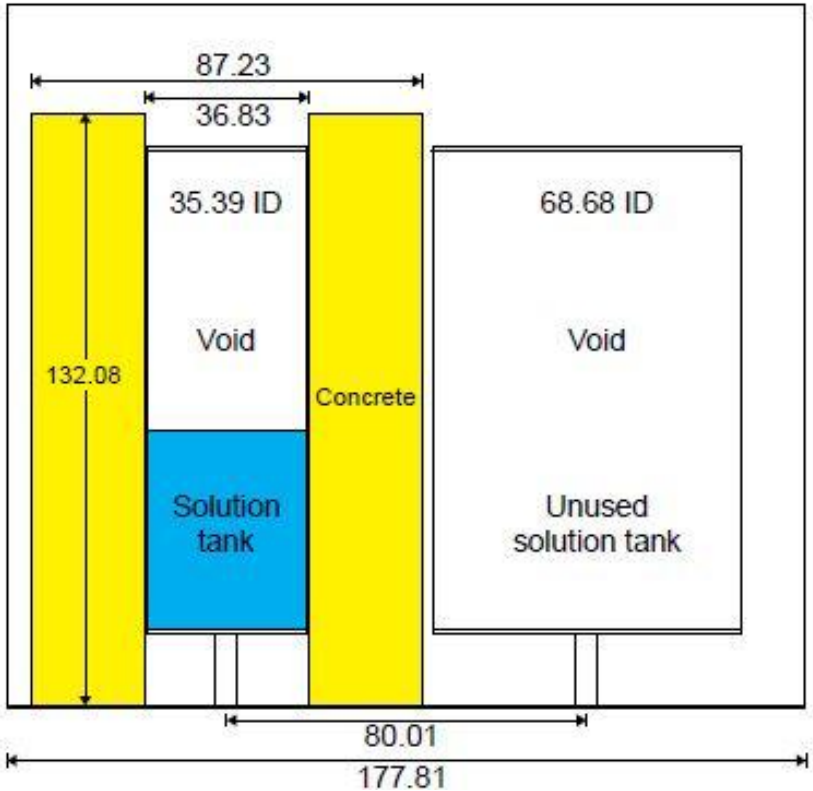
Description of MST-004

Elevation view for part of the model geometry of MST-004



- 9 critical experiments
- Plutonium fraction of 0.4 in a small cylindrical tank with three different reflectors
- Model consists of a cylindrical reaction vessel with a 35.39 cm ID
- Reaction vessel is ~108.5 cm tall
- Bare and concrete-reflected models include the auxiliary empty cylinder, water reflector tank, and the room
- Cases differ due to varying solution compositions, reflectors, and critical solution heights
- 3 bare, 3 water-reflected, and 3 concrete-reflected experiments
- Calculations performed in KENO-VI

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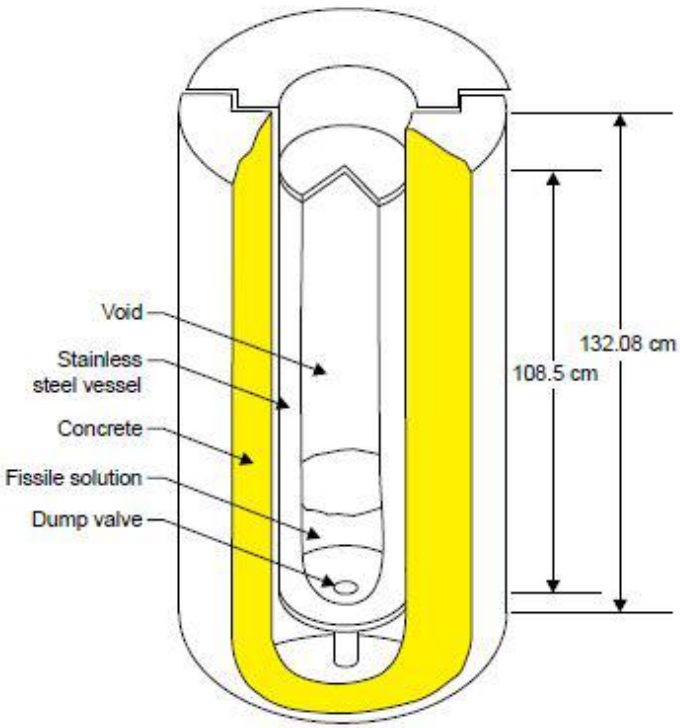
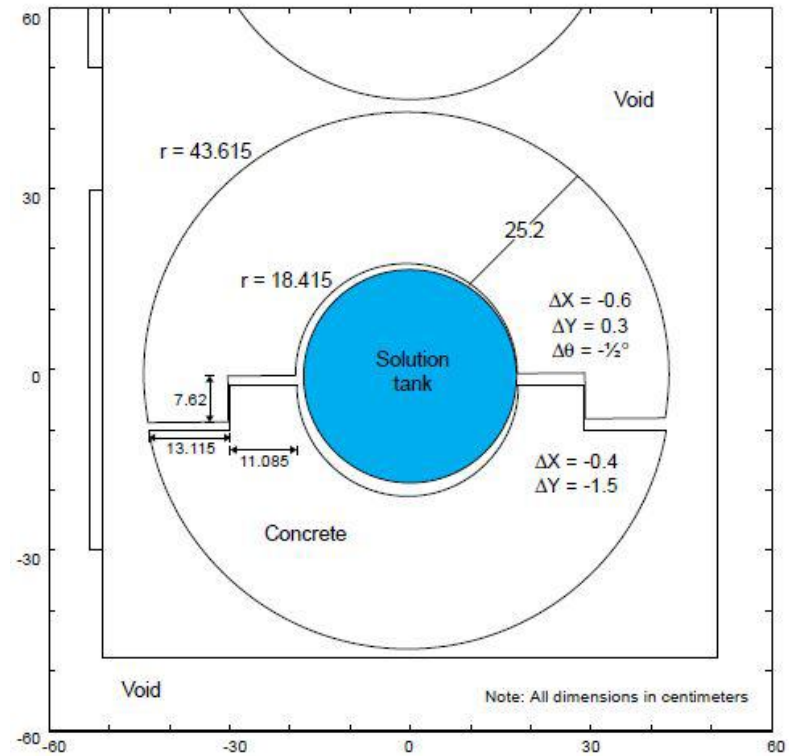
Description of MST-004 Cont.





Elevation view and plan view of the more complicated, concrete reflected cases

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Method for Comparison

- Performance reported in terms of calculated-to-experiment ratio (C/E)
- Average C/E values are determined for each version of KENO for both SCALE 6.1.2 and 6.2b3
- Propagation of uncertainty in C/E: $$\sigma_{\frac{C}{E}} = \left(\sqrt{\left(\frac{\sigma_{exp}}{k_{exp}}\right)^2 + \left(\frac{\sigma_{KENO}}{k_{KENO}}\right)^2}\right) \times \frac{C}{E}$$
  - Uncertainty in benchmark model k_{eff} is 20 to 80 times larger than KENO k_{eff} uncertainty
- The results are generated and reported for each nuclear data library
  - Allows comparison of multigroup and continuous-energy performance

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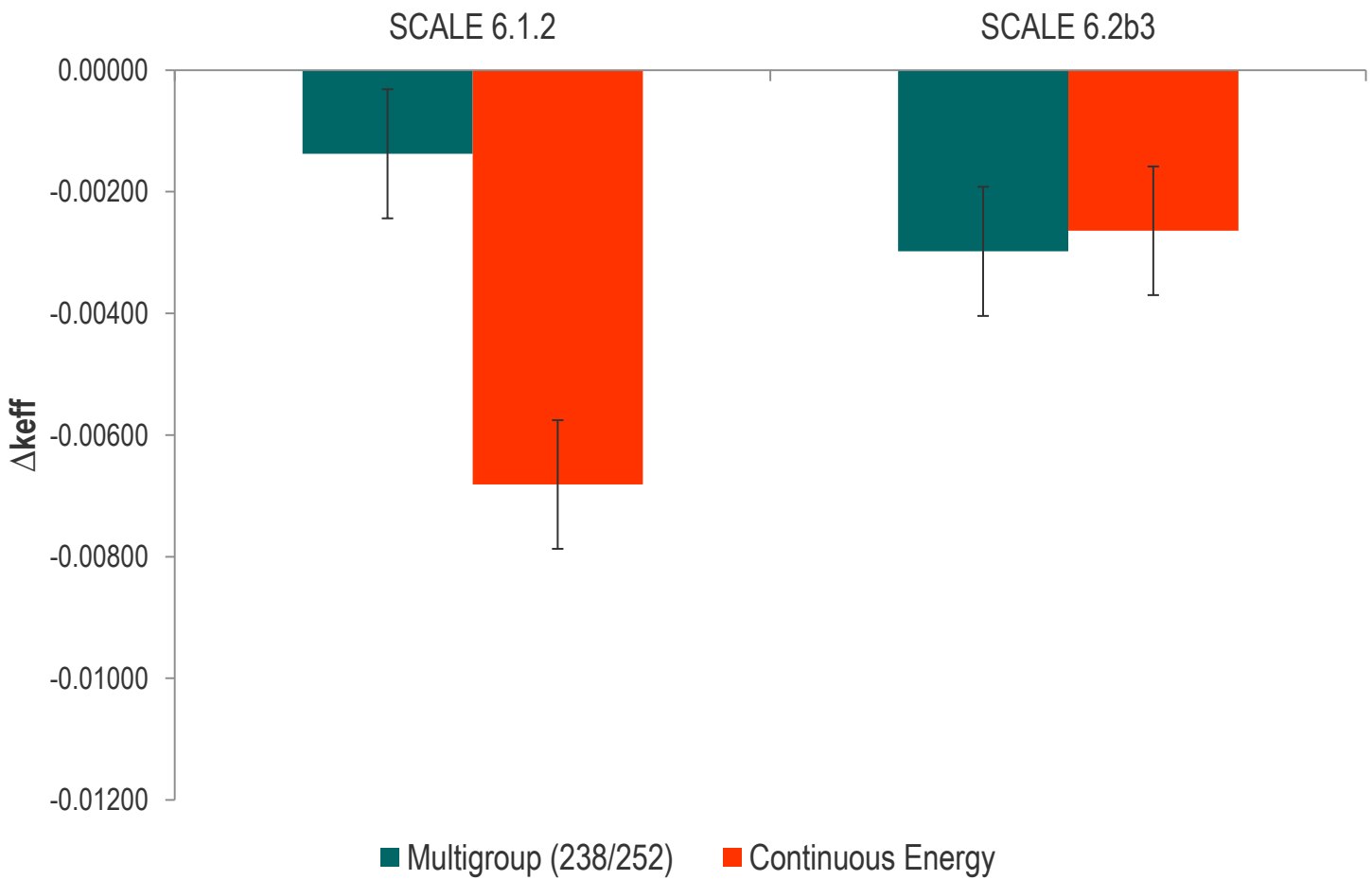
Results



Difference from unity of average C/E values by SCALE version for KENO V.a (Δk_{eff})

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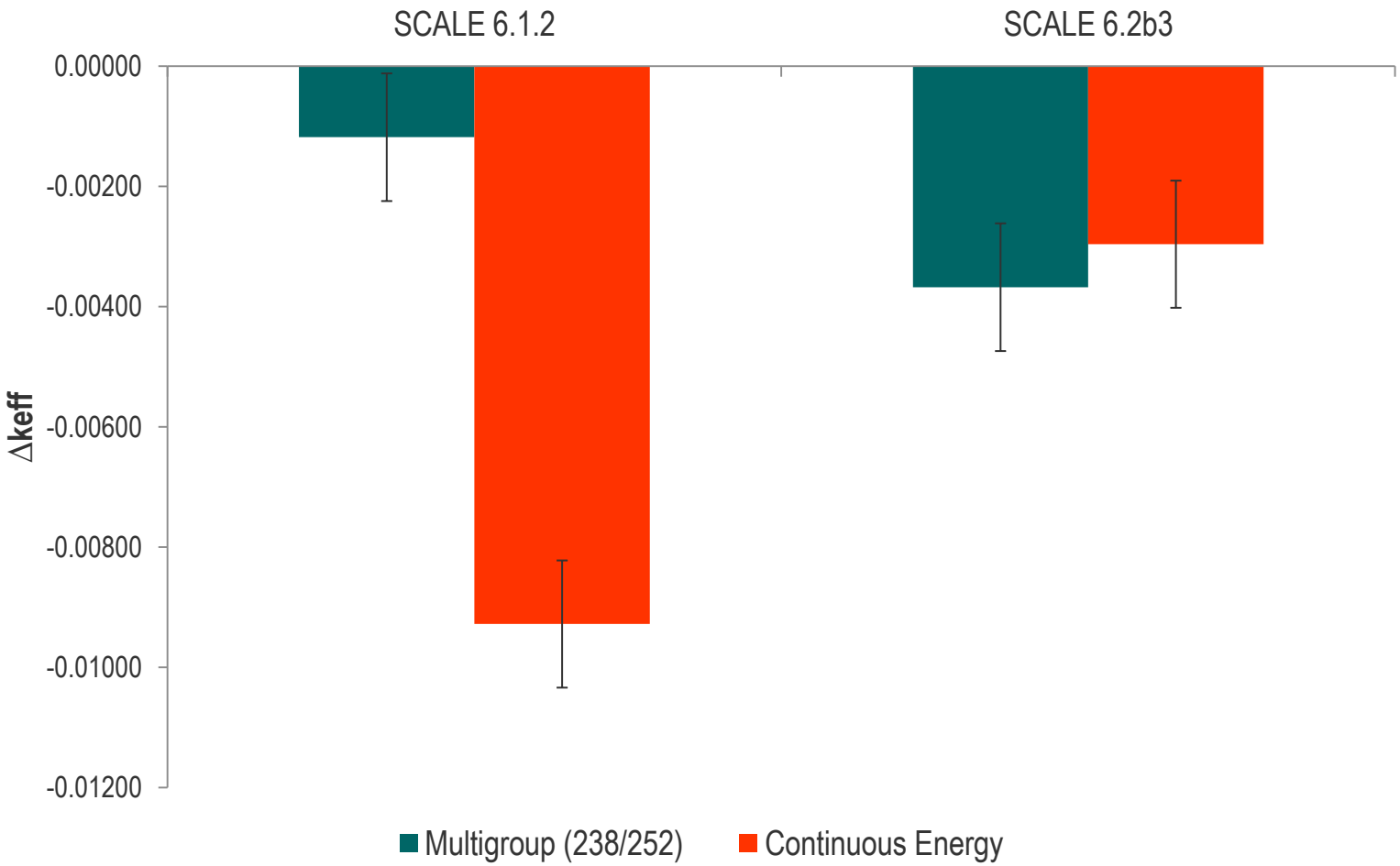
Results



Difference from unity of average C/E values by SCALE version for KENO-VI (Δk_{eff})

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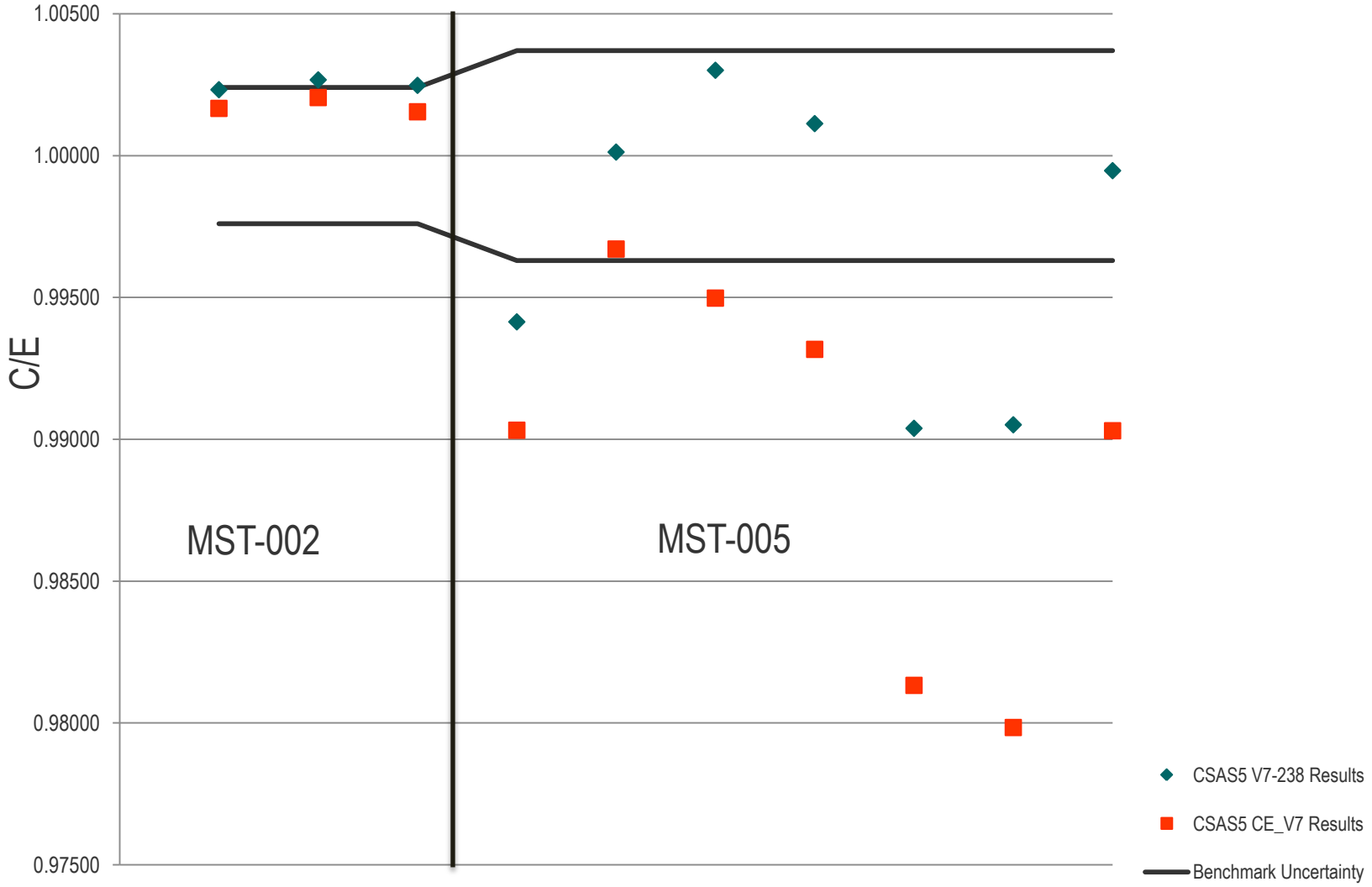
C/E CSAS5 Results for SCALE 6.1.2



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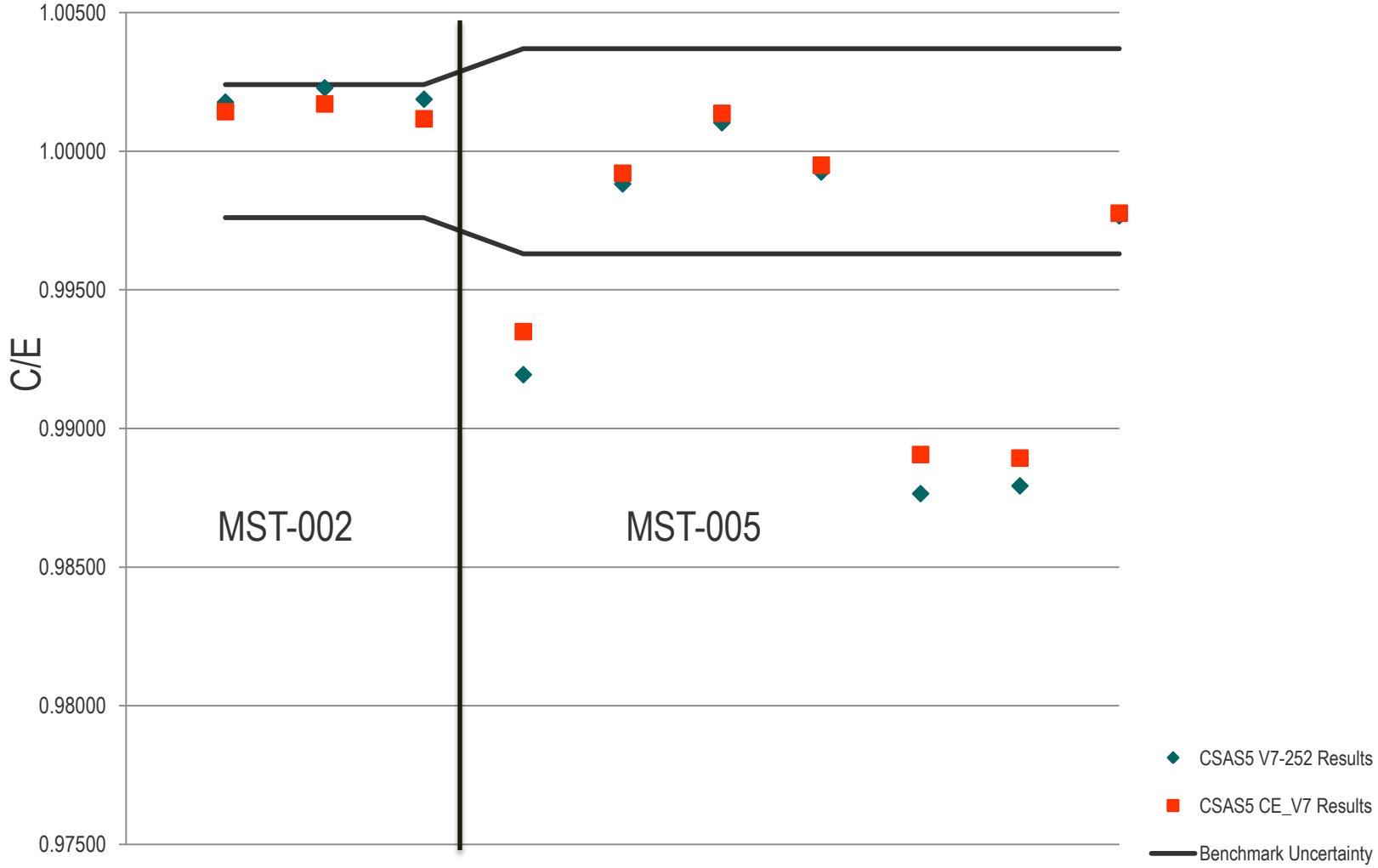
C/E CSAS5 Results for SCALE 6.2b3



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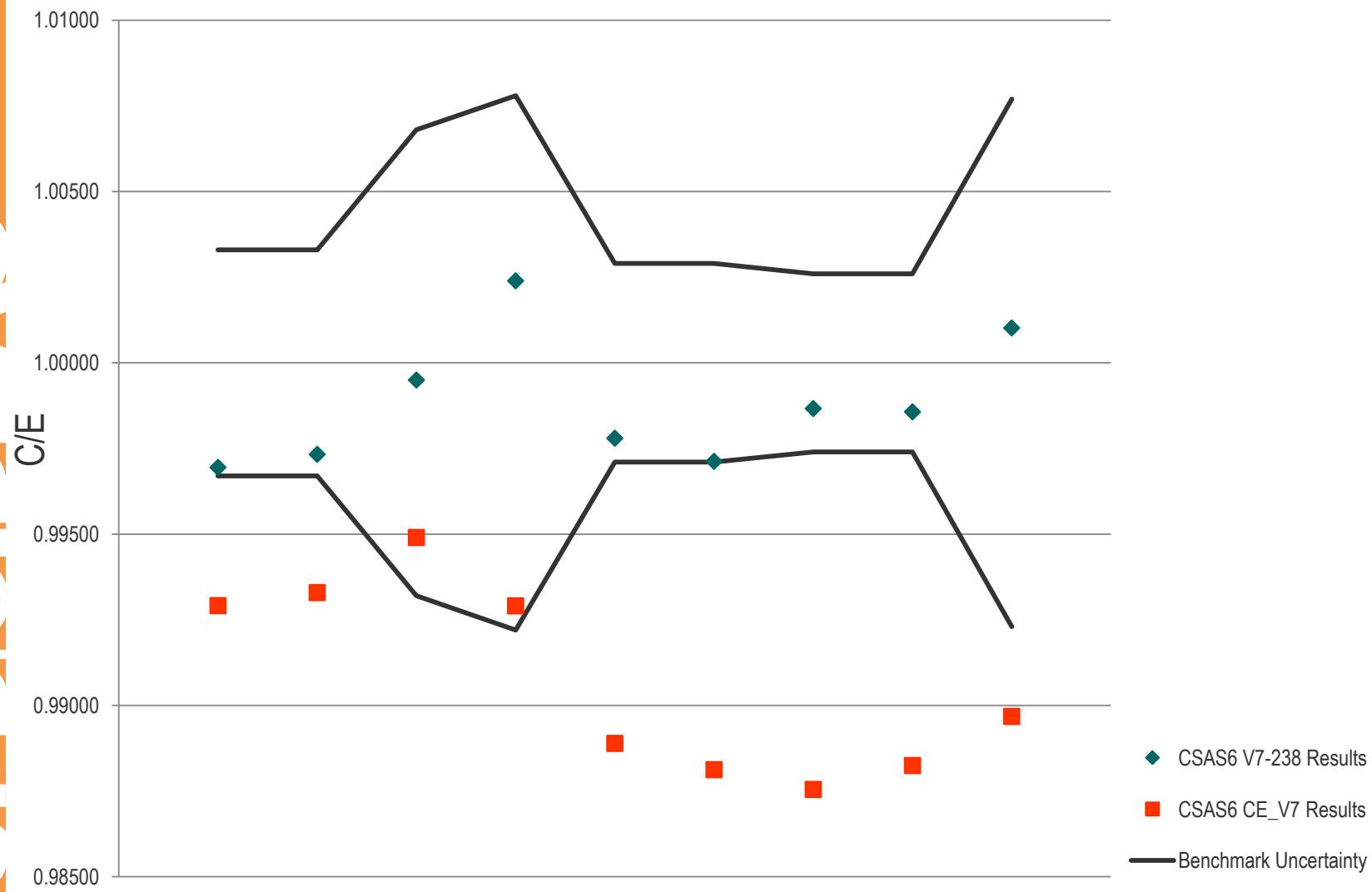
C/E CSAS6 Results for SCALE 6.1.2



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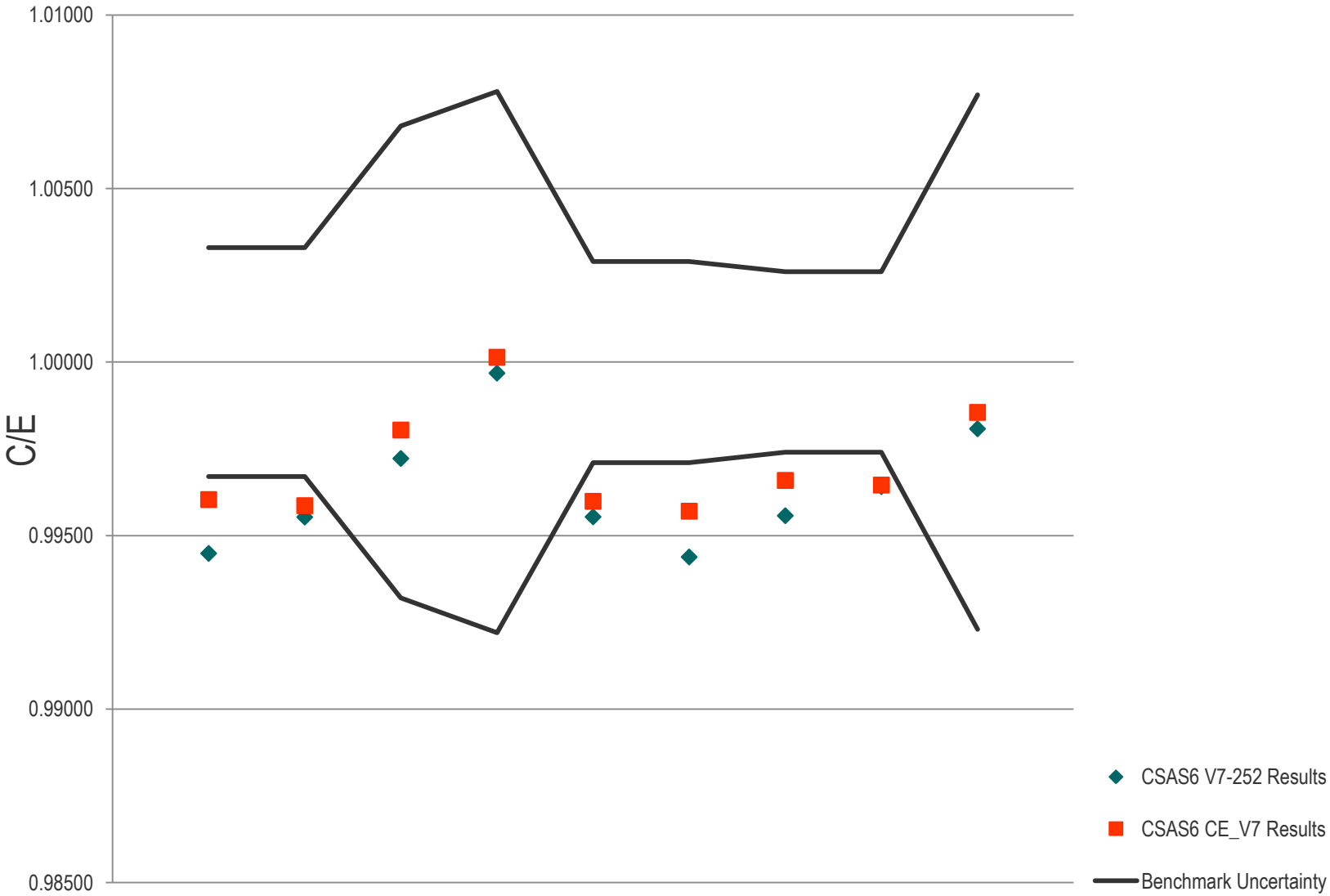
C/E CSAS6 Results for SCALE 6.2b3



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Conclusions

- KENO Monte Carlo codes perform well predicting k_{eff} for MST systems in SCALE 6.1.2 and 6.2b3 with ENDF/B-VII.0 cross sections
- The C/E values indicate that the code bias for MST systems is fairly small when using multigroup libraries
- SCALE 6.2b3 provides C/E values closer to unity with continuous-energy physics due to corrections in thermal scattering data

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Future Work

- Additional IHECSBE benchmark evaluations
  - MST-007, MST-010
  - LCT-008, HMF-052, HMM-017, MMT-001
- Generate and verify the sensitivity data files (SDFs) for MST-002, -004 and -005
- Perform review on SDFs then add evaluations to the VALID library
  - SDF for each case in VALID distributed with IHECSBE

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Acknowledgements

This work was supported by the Department of Energy (DOE) Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration.

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Questions?

Results

Table I: SCALE 6.1.2 V7-238 and CE_V7 Results

KENO V.a Evaluations						
	Benchmark Model Values		CSAS5 V7-238 Results		CSAS5 CE_V7 Results	
Case	k_{eff}	σ	C/E	σ	C/E	σ
MST-002-001	1.000	0.0024	1.00232	0.00241	1.00167	0.00241
002	1.000	0.0024	1.00267	0.00241	1.00205	0.00241
003	1.000	0.0024	1.00248	0.00241	1.00155	0.00241
MST-005-001	1.000	0.0037	0.99414	0.00368	0.99032	0.00367
002	1.000	0.0037	1.00013	0.00370	0.99671	0.00369
003	1.000	0.0037	1.00301	0.00371	0.99498	0.00368
004	1.000	0.0037	1.00113	0.00371	0.99317	0.00368
005	1.000	0.0037	0.99039	0.00367	0.98133	0.00363
006	1.000	0.0037	0.99051	0.00367	0.97984	0.00363
007	1.000	0.0037	0.99947	0.00370	0.99030	0.00367
Average:			0.99862	0.00106	0.99319	0.00105
KENO-VI Evaluations						
	Benchmark Model Values		CSAS6 V7-238 Results		CSAS6 CE_V7 Results	
Case	k_{eff}	σ	C/E	σ	C/E	σ
MST-004-001	1.000	0.0033	0.99695	0.00329	0.99291	0.00328
002	1.000	0.0033	0.99733	0.00329	0.99329	0.00328
003	1.000	0.0068	0.99950	0.00680	0.99490	0.00677
004	1.000	0.0078	1.00239	0.00782	0.99291	0.00775
005	1.000	0.0029	0.99780	0.00290	0.98889	0.00287
006	1.000	0.0029	0.99713	0.00289	0.98813	0.00287
007	1.000	0.0026	0.99867	0.00260	0.98755	0.00257
008	1.000	0.0026	0.99857	0.00260	0.98825	0.00257
009	1.000	0.0077	1.00102	0.00771	0.98968	0.00762
Average:			0.99882	0.00164	0.99072	0.00163

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Results

Table II: SCALE 6.2b3 V7-252 and CE_V7 Results

KENO V.a Evaluations						
	Benchmark Model Values		CSAS5 V7-252 Results		CSAS5 CE_V7 Results	
Case	k_{eff}	σ	C/E	σ	C/E	σ
MST-002-001	1.000	0.0024	1.00177	0.00241	1.00143	0.00241
002	1.000	0.0024	1.00228	0.00241	1.00170	0.00241
003	1.000	0.0024	1.00187	0.00241	1.00117	0.00240
MST-005-001	1.000	0.0037	0.99194	0.00367	0.99349	0.00368
002	1.000	0.0037	0.99882	0.00370	0.99921	0.00370
003	1.000	0.0037	1.00103	0.00371	1.00136	0.00371
004	1.000	0.0037	0.99925	0.00370	0.99950	0.00370
005	1.000	0.0037	0.98765	0.00366	0.98906	0.00366
006	1.000	0.0037	0.98793	0.00366	0.98893	0.00366
007	1.000	0.0037	0.99767	0.00369	0.99777	0.00369
Average:			0.99702	0.00106	0.99736	0.00106

KENO-VI Evaluations						
	Benchmark Model Values		CSAS6 V7-252 Results		CSAS6 CE_V7 Results	
Case	k_{eff}	σ	C/E	σ	C/E	σ
MST-004-001	1.000	0.0033	0.99449	0.00328	0.99604	0.00329
002	1.000	0.0033	0.99553	0.00329	0.99586	0.00329
003	1.000	0.0068	0.99722	0.00678	0.99804	0.00679
004	1.000	0.0078	0.99968	0.00780	1.00014	0.00780
005	1.000	0.0029	0.99554	0.00289	0.99599	0.00289
006	1.000	0.0029	0.99438	0.00289	0.99570	0.00289
007	1.000	0.0026	0.99557	0.00259	0.99659	0.00259
008	1.000	0.0026	0.99641	0.00259	0.99646	0.00259
009	1.000	0.0077	0.99808	0.00769	0.99855	0.00769
Average:			0.99632	0.00164	0.99704	0.00164

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SCALE 6.1.2 Results Compared to IHECSBE Section 4 Results

Table III: SCALE 6.1.2 V7-238 and CE_V7 Results Compared to Section 4

KENO V.a Evaluations

Case	Benchmark Model Values		CSAS5 V7-238		CSAS5 CE_V7		KENO (Hansen-Roach)		KENO (27-Group ENDF/B-IV)		MCNP (Continuous Energy ENDF/B-V)	
	k_{eff}	σ	k_{eff}	σ	k_{eff}	σ	k_{eff}	σ	k_{eff}	σ	k_{eff}	σ
MST-002-001	1.000	0.0024	1.00232	0.00010	1.00167	0.00010	1.01890	0.00100	1.00960	0.00090	1.00820	0.00020
002	1.000	0.0024	1.00267	0.00010	1.00205	0.00010	1.02030	0.00090	1.01150	0.00090	1.00740	0.00050
003	1.000	0.0024	1.00248	0.00010	1.00155	0.00010	1.02020	0.00090	1.01160	0.00100	1.00790	0.00040
MST-005-001	1.000	0.0037	0.99414	0.00010	0.99032	0.00010	0.99910	0.00040	1.00290	0.00040	1.00150	0.00080
002	1.000	0.0037	1.00013	0.00010	0.99671	0.00010	1.00480	0.00150	1.00530	0.00150	1.00340	0.00070
003	1.000	0.0037	1.00301	0.00010	0.99498	0.00010	1.01090	0.00140	1.01020	0.00150	1.00190	0.00080
004	1.000	0.0037	1.00113	0.00010	0.99317	0.00010	1.01210	0.00150	1.00680	0.00160	1.00000	0.00080
005	1.000	0.0037	0.99039	0.00010	0.98133	0.00010	0.99970	0.00040	0.99790	0.00040	0.99340	0.00090
006	1.000	0.0037	0.99051	0.00010	0.97984	0.00010	1.00580	0.00040	0.99720	0.00040	0.99020	0.00080
007	1.000	0.0037	0.99947	0.00010	0.99030	0.00010	1.01600	0.00150	1.00390	0.00160	0.99900	0.00080

KENO-VI Evaluations

Case	Benchmark Model Values		CSAS6 V7-238		CSAS6 CE_V7		KENO (Hansen-Roach)		KENO (27-Group ENDF/B-IV)		MCNP (Continuous Energy ENDF/B-V)	
	k_{eff}	σ	k_{eff}	σ	k_{eff}	σ	k_{eff}	σ	k_{eff}	σ	k_{eff}	σ
MST-004-001	1.000	0.0033	0.99695	0.00010	0.99291	0.00010	1.00380	0.00040	1.00630	0.00040	1.00250	0.00130
002	1.000	0.0033	0.99733	0.00010	0.99329	0.00010	1.00270	0.00150	1.00390	0.00140	1.00150	0.00110
003	1.000	0.0068	0.99950	0.00010	0.99490	0.00010	1.00410	0.00040	1.00800	0.00040	1.00660	0.00120
004	1.000	0.0078	1.00239	0.00010	0.99291	0.00010	1.01260	0.00040	1.00830	0.00040	1.00400	0.00110
005	1.000	0.0029	0.99780	0.00010	0.98889	0.00010	1.00730	0.00150	0.99840	0.00160	0.99940	0.00120
006	1.000	0.0029	0.99713	0.00009	0.98813	0.00009	1.00970	0.00040	1.00440	0.00040	0.99660	0.00130
007	1.000	0.0026	0.99867	0.00009	0.98755	0.00009	1.01790	0.00040	1.00560	0.00040	0.99720	0.00130
008	1.000	0.0026	0.99857	0.00010	0.98825	0.00010	1.01570	0.00150	1.00600	0.00150	0.99880	0.00120
009	1.000	0.0077	1.00102	0.00010	0.98968	0.00010	1.01520	0.00040	1.00580	0.00040	1.00200	0.00120

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SCALE 6.2b3 Results Compared to IHECSBE Section 4 Results

Table IV: SCALE 6.2b3 V7-252 and CE_V7 Results Compared to Section 4

KENO V.a Evaluations

Case	Benchmark Model Values		CSAS5 V7-252		CSAS5 CE_V7		KENO (Hansen-Roach)		KENO (27-Group ENDF/B-IV)		MCNP (Continuous Energy ENDF/B-V)	
	k_{eff}	σ	k_{eff}	σ	k_{eff}	σ	k_{eff}	σ	k_{eff}	σ	k_{eff}	σ
MST-002-001	1.000	0.0024	1.00177	0.00010	1.00143	0.00010	1.01890	0.00100	1.00960	0.00090	1.00820	0.00020
002	1.000	0.0024	1.00228	0.00010	1.00170	0.00010	1.02030	0.00090	1.01150	0.00090	1.00740	0.00050
003	1.000	0.0024	1.00187	0.00010	1.00117	0.00010	1.02020	0.00090	1.01160	0.00100	1.00790	0.00040
MST-005-001	1.000	0.0037	0.99194	0.00010	0.99349	0.00010	0.99910	0.00040	1.00290	0.00040	1.00150	0.00080
002	1.000	0.0037	0.99882	0.00010	0.99921	0.00010	1.00480	0.00150	1.00530	0.00150	1.00340	0.00070
003	1.000	0.0037	1.00103	0.00010	1.00136	0.00010	1.01090	0.00140	1.01020	0.00150	1.00190	0.00080
004	1.000	0.0037	0.99925	0.00010	0.99950	0.00010	1.01210	0.00150	1.00680	0.00160	1.00000	0.00080
005	1.000	0.0037	0.98765	0.00010	0.98906	0.00010	0.99970	0.00040	0.99790	0.00040	0.99340	0.00090
006	1.000	0.0037	0.98793	0.00010	0.98893	0.00010	1.00580	0.00040	0.99720	0.00040	0.99020	0.00080
007	1.000	0.0037	0.99767	0.00010	0.99777	0.00010	1.01600	0.00150	1.00390	0.00160	0.99900	0.00080

KENO-VI Evaluations

Case	Benchmark Model Values		CSAS6 V7-252		CSAS6 CE_V7		KENO (Hansen-Roach)		KENO (27-Group ENDF/B-IV)		MCNP (Continuous Energy ENDF/B-V)	
	k_{eff}	σ	k_{eff}	σ	k_{eff}	σ	k_{eff}	σ	k_{eff}	σ	k_{eff}	σ
MST-004-001	1.000	0.0033	0.99449	0.00010	0.99604	0.00010	1.00380	0.00040	1.00630	0.00040	1.00250	0.00130
002	1.000	0.0033	0.99553	0.00010	0.99586	0.00010	1.00270	0.00150	1.00390	0.00140	1.00150	0.00110
003	1.000	0.0068	0.99722	0.00010	0.99804	0.00010	1.00410	0.00040	1.00800	0.00040	1.00660	0.00120
004	1.000	0.0078	0.99968	0.00010	1.00014	0.00010	1.01260	0.00040	1.00830	0.00040	1.00400	0.00110
005	1.000	0.0029	0.99554	0.00010	0.99599	0.00010	1.00730	0.00150	0.99840	0.00160	0.99940	0.00120
006	1.000	0.0029	0.99438	0.00009	0.99570	0.00009	1.00970	0.00040	1.00440	0.00040	0.99660	0.00130
007	1.000	0.0026	0.99557	0.00009	0.99659	0.00009	1.01790	0.00040	1.00560	0.00040	0.99720	0.00130
008	1.000	0.0026	0.99641	0.00010	0.99646	0.00010	1.01570	0.00150	1.00600	0.00150	0.99880	0.00120
009	1.000	0.0077	0.99808	0.00010	0.99855	0.00010	1.01520	0.00040	1.00580	0.00040	1.00200	0.00120

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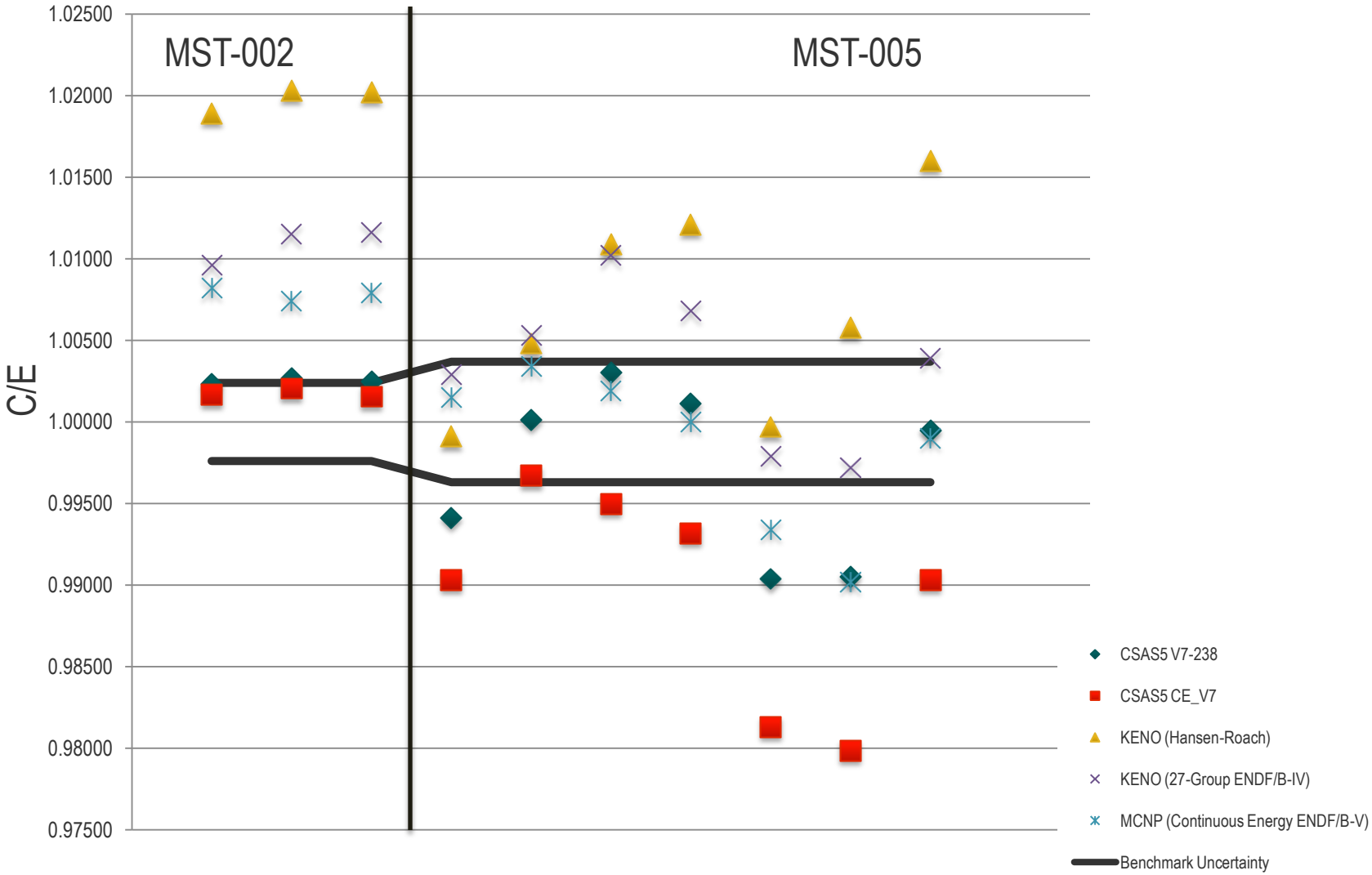
C/E CSAS5 Results for SCALE 6.1.2 Compared to IHECSBE Section 4 Results



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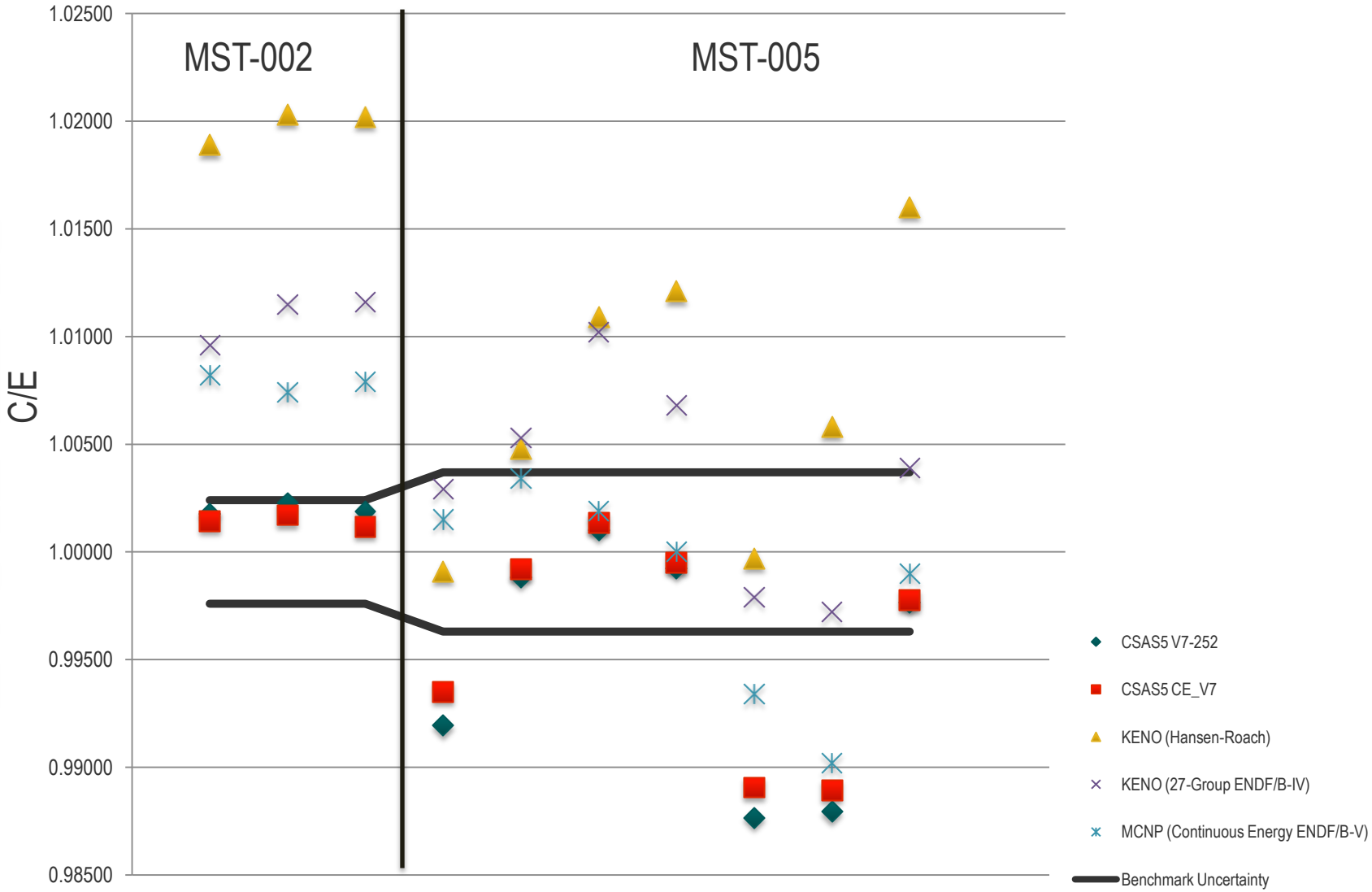
C/E CSAS5 Results for SCALE 6.2b3 Compared to IHECSBE Section 4 Results



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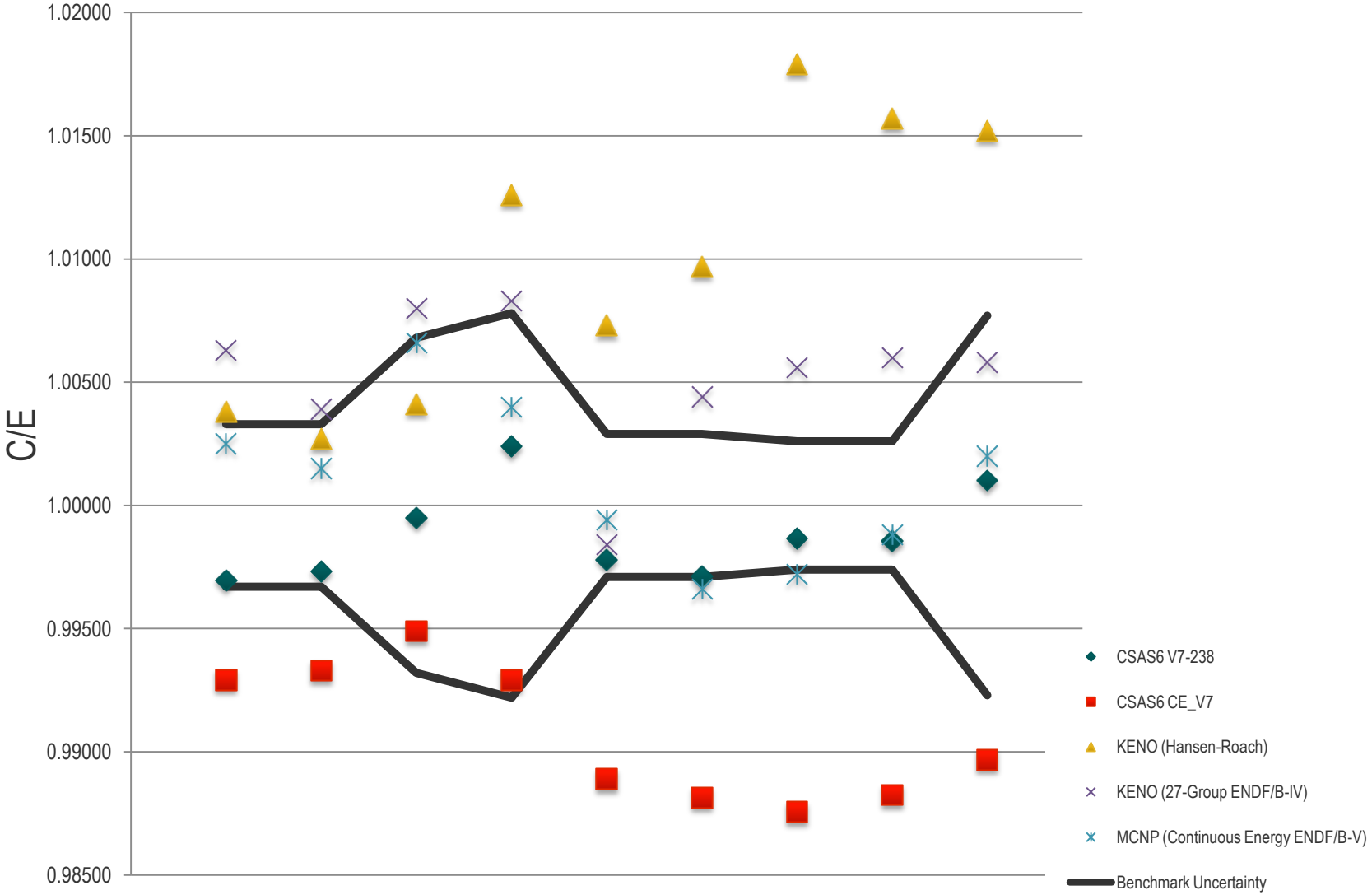
C/E CSAS6 Results for SCALE 6.1.2 Compared to IHECSBE Section 4 Results



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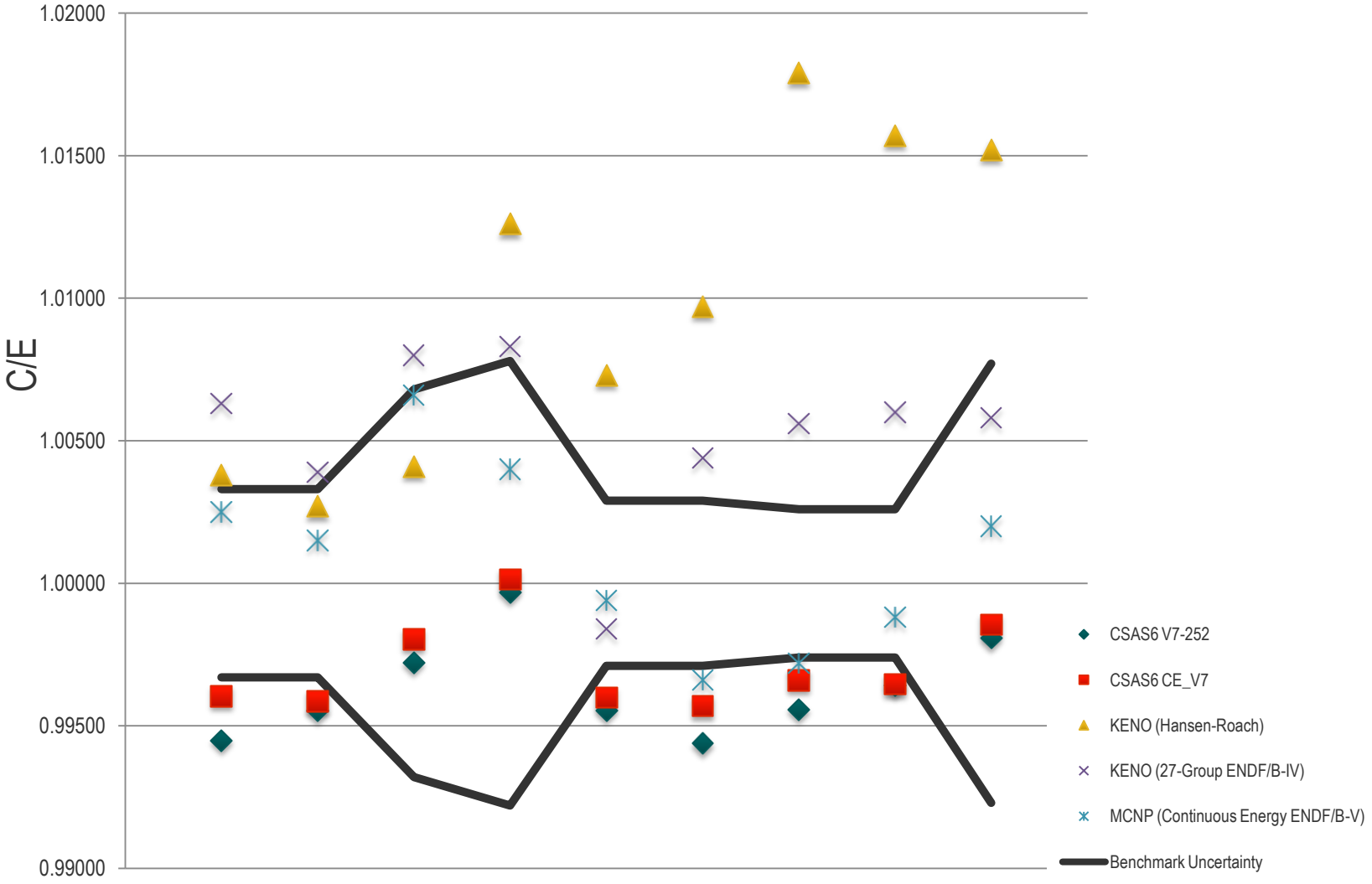
C/E CSAS6 Results for SCALE 6.2b3 Compared to IHECSBE Section 4 Results



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