Comparison of Validation Results for GEMER, MCNP and SCALE6.1/ KENO-VI

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NCSD 2013 Topical Meeting
Sep 29 – Oct 3, 2013
Wilmington, North Carolina

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Overview

- Introduction
- Heterogeneous System Modeling
- Statistical Methodology
- Benchmark Selection
- Validation Results
- Conclusions

Introduction

- Global Nuclear Fuel - Americas (GNF-A) fuel fabrication facility is involved in production, processing, handling, and storage of uranium oxides enriched to $\leq$ 5 wt.% ^{235}U.
- Monte Carlo codes are routinely used at GEH/GNF-A for criticality safety calculations.
- Monte Carlo simulation of heterogeneous systems challenges code capability and computation efficiency.
- Validation results of three Monte Carlo codes: GEMER, MCNP and SCALE are compared for homogenous and heterogeneous low enriched uranium (LEU) systems.

Introduction (cont.)

- GEMER 1.2 is a GEH proprietary code and uses190 energy group cross sections from ENDF/B-IV library.
- MCNP-05P is a GEH modified LANL MCNP5 (1.3) code and uses continuous energy cross sections from ENDF/B-VII.0 library.
- SCALE6.1 is an ORNL code and uses both 238 group and continuous energy cross sections from ENDF/B-VII.0 library.

Heterogeneous System Modeling

- **Virtual Fill Option (VFO) in GEMER**
  - Allows easy creation of heterogeneous models
  - Triangular-pitched arrays are easily created using geometry constructs (INTERS, SPINTERS, TRITERS).
  - Results in faster run time
- **Lattice cell in MCNP**
- **Dodecahedral array in SCALE**

Statistical Methodology

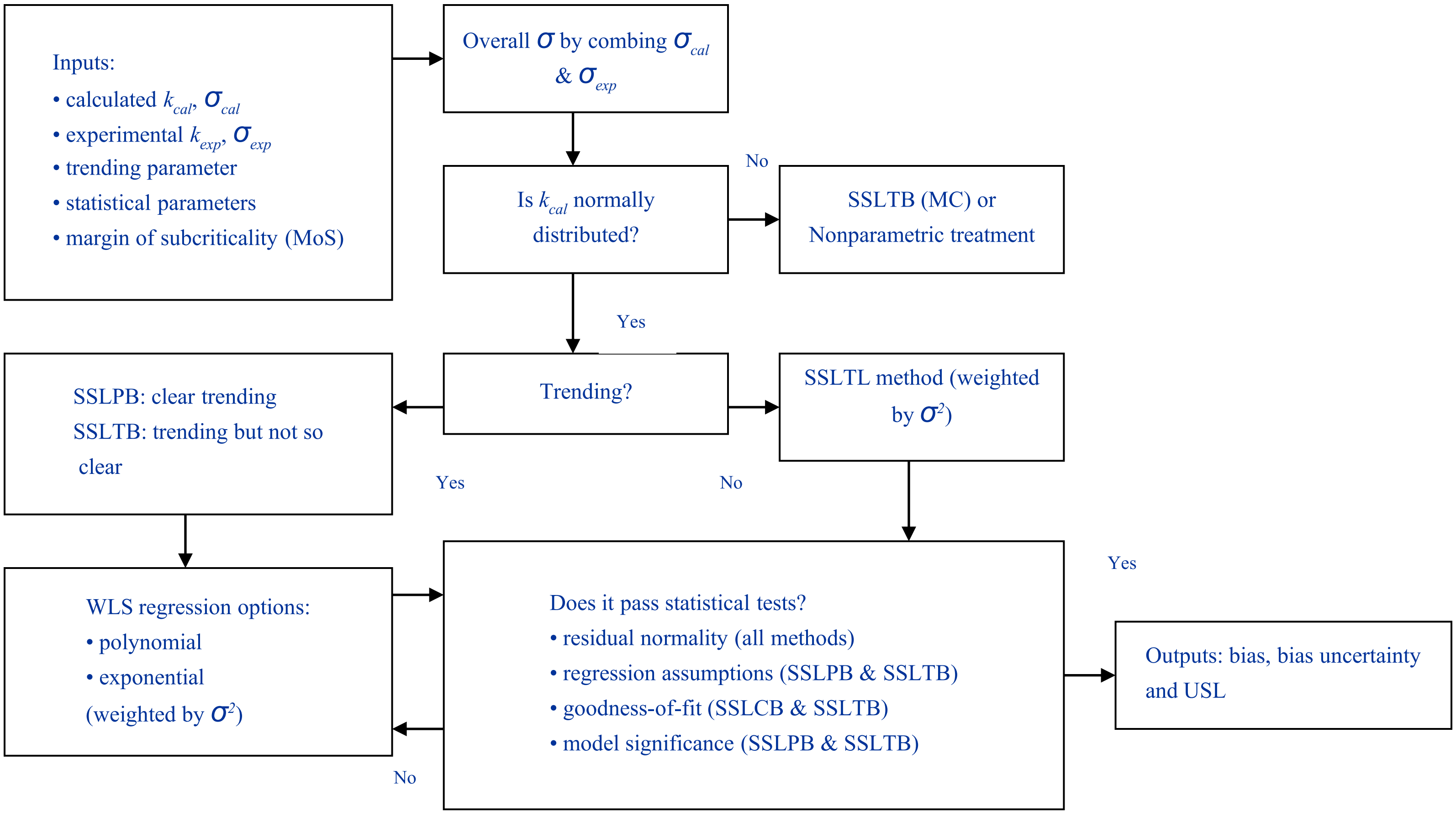
USLSA (Upper Subcriticality Limit Statistical Analysis) is a statistical tool developed for criticality safety analysis code validation.

USLSA provides:

- A bias trend for benchmark experiments versus selected parameters by trending analysis, and then interpolates or extrapolates it to applications
- Bias and bias uncertainty for benchmark experiments versus system parameters
- Upper Subcriticality Limit (USL) for an application
- Statistical justification of validity in USL, bias and bias uncertainty

Statistical Methodology

USLSA Flowchart



Statistical Methodology - Bias Determination

USL	$$USL(x) = \bar{k}_e - b(x) - \Delta b - \Delta k_m$$	Where, x = independent trending variable $\bar{k}_e$ = weighted mean of all k_{exp} values b(x) = regression fit of bias Δb = bias uncertainty Δk_m = minimum margin of subcriticality (MMS) k_{calc} = calculated k_{eff} value of benchmark experiment k_{exp} = experimental k_{eff} value of benchmark $k_{calc}(\beta; x)$ = regression fit of calculated k_{eff} values of benchmark experiments β = regression model parameters σ_i = overall uncertainty: $$\sigma_i = \sqrt{\sigma_{exp,i}^2 + \sigma_{calc,i}^2}$$ σ_{calc} = calculational uncertainty σ_{exp} = experimental uncertainty
Bias	$$b = k_{calc} - k_{exp}$$	
WLS Regression	$$Min: Q = \sum_{i=1}^{n} \frac{1}{\sigma_i^2}[k_{calc,i} - k_{calc}(\beta; x_i)]^2$$	
Statistical Tests	<u>Regression Tests (residual assumptions):</u> • Normality • Equal variance • Independence • Zero Mean <u>Model Tests:</u> • Goodness-of-fit (χ^2 and reduced χ^2 tests) • Magnitude of model effect (R^2 and R_{adj}^2) • Model significance (F test)	

Statistical Methodology - Bias Uncertainty Estimation

Method	Bias Uncertainty	Notation	Applicability
SSLPB Single-Sided Lower Prediction Band	$\Delta b = \max[t_{1-\alpha,\nu} s_p \sqrt{1 + L(x)' S^{-1} L(x)}]$ L(x) = coefficient partial derivative vector evaluated at x S = design matrix	$s_p^2 = s_f^2 + s_c^2$ $s_f^2 = \frac{1}{n-m}\sum_{i=1}^{n}\frac{1}{\sigma_i^2}[k_i - k_c(x_i)]^2$ $s_c^2 = \frac{1}{n}\sum_{i=1}^{n}\sigma_i^2$	Trend with high goodness-of-fit explained by physics
SSLTB Single-Sided Lower Tolerance Band	$\Delta b = C_{(1-\alpha)/P} \cdot s_p$ Tolerance factor, $C_{(1-\alpha)/P} = \max\left\{\frac{\bar{k}_i - z_{P,i}}{s_i}\right\}_{i=1,n}$ estimated by Monte Carlo	$t_{1-\alpha,\nu}$ = 100(1-α)% of inverse of central t cdf with ν degrees of freedom $t'_{1-\alpha,\nu}(\delta)$ = 100(1- α)% of the inverse of noncentral t cdf with noncentrality parameters δ and ν degrees of freedom	Trend with any type of linear/nonlinear regression model for normal/non-normal data
SSLTL Single-Sided Lower Tolerance Limit	$\Delta b = \frac{1}{\sqrt{n}} t'_{1-\alpha,n-1}(z_P \cdot \sqrt{n}) \cdot s_p$	z_P = 100P% of the inverse of standard normal cdf	Non-trend and normal data

Benchmark Selection

Benchmark Experiment Parameters

Parameters	Homogeneous	Heterogeneous
Material	Uranium	Uranium
Chemical Form	UF_4,UO_2,UO_2F_2, $UO_2(NO_3)_2$	UO_2
Enrichment (wt% ^{235}U)	2-10	2-5
Physical Form	Solution, Solid	Solid
Moderator (in fuel region)	H_2O, Paraffin,	H_2O
Physical Form	Solution, Solid	Solution
Moderation Ratio ($H/^{235}U$)	16 -1438	50 - 450
Reflector (in fuel region)	Bare, H_2O, Paraffin, Polyethylene	H_2O
Physical Form	Solution, Solid	Solution
Absorber (in fuel region)	None	None
Neutron Energy Spectrum	Thermal	Thermal
Number of Experiments	7	12
Number of Configurations	49	48

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Benchmark Selection

**Homogenous System Benchmarks - ** 49 LEU compound experiments

Benchmark	Form	Wt% ^{235}U	$H/^{235}U$	Reflector/Geometry	Description
LCT33 (14)	UF_4	2 - 3	133 - 973	Paraffin/Polyethylene - reflected & unreflected cuboids	Solid blocks of UF_4 dispersed in paraffin moderator
ICT01 (6)	UF_4-CF_2	29.83	16 - 64	Plexiglas - reflected cuboids	Stacked arrays of 1"x1"x1" UF_4-CF_2 and polyethylene blocks
LCT45 (7)	U_3O_8	4.46	38 - 98	Concrete and Plexiglas - reflected cuboids	Large U_3O_8 powder systems with low moderation content
LCT49 (4)	UO_2	5	40 - 60	Polyethylene - reflected array of cuboids	Large UO_2 powder systems with low moderation content
LST02 (2)	UO_2F_2	4.9	1001 - 1098	Unreflected and water reflected spheres	174 L sphere containing UO_2F_2 Solution
LST03 (9)	UNH	10.07	770 - 1438	Unreflected Spheres	Full and truncated spheres containing uanyl nitrate solution
LST04 (7)	UNH	9.97	719 - 1018	Water reflected cylinders	Cylindrical 60 cm diameter tank containing uranyl nitrate solution

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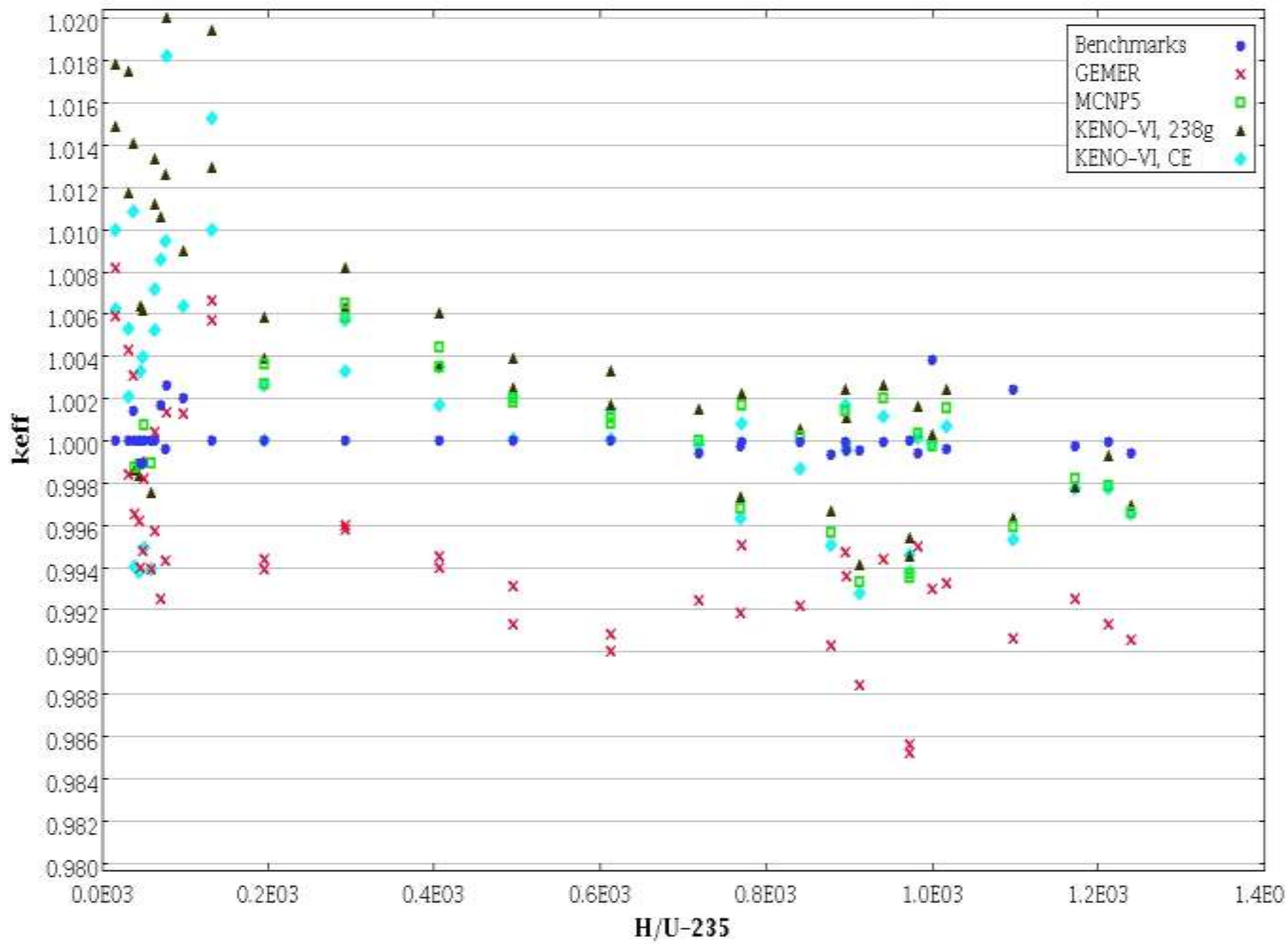
Benchmark Selection

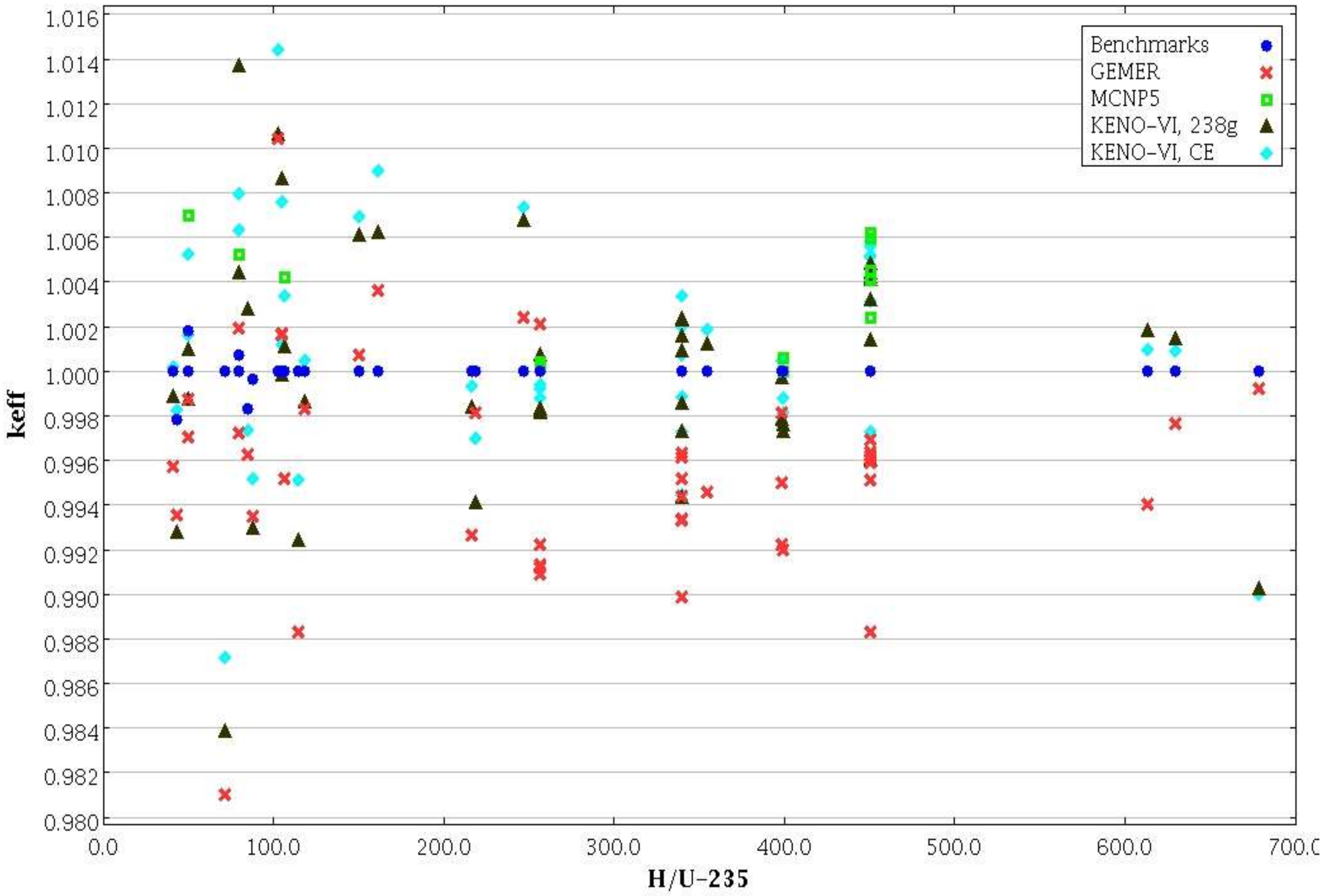
Heterogeneous System Benchmarks - 48 LEU compound experiments

Benchmark	Form	Wt% ^{235}U	$H/^{235}U$	Reflector/Geometry	Description
LCT09 (3)	UO_2	4.306	257	Water reflected array of fuel rods	Square lattice of water moderated fuel rods
ICT10 (3)	UO_2	4.306	107 - 257	Depleted Uranium or steel reflected array of fuel rods	Square lattices of water moderated fuel rods
LCT16 (2)	UO_2	2.35	399	Water reflected array of fuel rods	Square lattices of water moderated fuel rods
LCT17 (4)	UO_2	2.35	219 - 399	Lead, depleted uranium or steel - reflected array of fuel rods	Square lattices of water moderated fuel rods
LCT18 (1)	UO_2	7	118	Water reflected array of fuel rods	Square lattices of water moderated fuel rods
LCT19 (3)	UO_2	5	103 - 162	Water reflected array of fuel rods	Hexagonal lattices of water moderated fuel rods
LCT20 (7)	UO_2	5	451	Water reflected array of fuel rods	Hexagonal lattices of water moderated fuel rods
LCT22 (7)	UO_2	9.83	50 - 629	Water reflected array of fuel rods	Hexagonal lattices of water moderated fuel rods
LCT23 (6)	UO_2	9.83	340	Water reflected array of fuel rods	Hexagonal lattices of water moderated fuel rods
LCT24 (2)	UO_2	9.83	41 - 105	Water reflected array of fuel rods	Square or hexagonal lattices of water moderated fuel rods
LCT25 (4)	UO_2	7.41	72 - 355	Water reflected array of fuel rods	Hexagonal lattices of water moderated fuel rods
LCT26 (6)	UO_2	4.92	43 - 107	Water reflected array of fuel rods	Hexagonal lattices of water moderated fuel rods

Validation Results - Homogenous Systems



Validation Results - Heterogeneous Systems



Validation Results - Upper Safety Limits

Code	Homogeneity	USL Method	USL ($H/^{235}U$)
GEMER	Homogeneous	SSLTB	$0.9582-3.3201E\text{-}5X+5.1004E\text{-}8X^2-2.2784E\text{-}11X^3$
MCNP		SSLTL	0.9614
SCALE6.1-KENO-VI		SSLTB (238-group)	0.9567 for X<=1175 0.9632-5.5873E-6X for X> 11.75
		SSLTL (CE)	0.9571
GEMER	Heterogeneous	SSLTL	0.9524
MCNP		SSLTL	0.9569
SCALE6.1-KENO-VI		SSLTB (238-group)	0.9554
		SSLTB (CE)	0.9565

Conclusions

- Validation results for GEMER1.2, MCNP-05P and SCALE6.1-KENO-VI agree well for the systems evaluated.
- GEMER calculated k_{eff} values are generally lower than those calculated by MCNP or SCALE6.1-KENO-VI.