CSCT Minutes for March 28, 2023

Meeting Attendance		
Attendee		**Present**
M	Arm, Cheryl	**x**
M	Berg, Larry	
EM	Bowen, Doug	**x**
EM	Brady, Mikey	
M	Brooks, Franklin	**x**
M	Bunde, Kermit	**x**
M	Chambers, Angela	**x**
M	Collens, Jake	
M	Damba, Darwin	**x**
M	Dyke, Jimmy	
M	Eberle, Cris	**x**
EM	Erickson, David	**x**
M	Fischahs, Christopher	**x**
M	Gilbertson, Sarah	
M	Hahn, Kevin	**x**
EM	Hayes, David	
S	Henley, Marsha	**x**
M	Hines, Tom	
M	Janson, Stephen	
M	Levine, Michael	
M	Ly, Gary	**x**
M	Marenchin, Thomas	**x**
M	Moore, Josiah	
M	Moss, Patrick	
M	Murphy, Katie	
M	Perry, Christopher	**x**
M	Petraglia, Jeffrey	**x**
M	Russell, Paige	
M	Sandgren, Kevin	
M	Thrasher, David	
M	Udenta, Gladys	
M	Vickers, Linda	
M	Wallace, George	**x**
M	Washburn, Peter	
M	Wilson, Robert	**x**
M	Wise, Tammy	**x**

M – Member
EM – Ex-Officio
S – Scribe

Virtual Roll call – please acknowledge your presences in Teams chat.

- Joining us from LANL – Kelly Aldrich, Jennifer Alwin, Riley Bulso, Norann Calhoun, Noline Clark, Theresa Cutler, Jessica Hartman, Robert Sanchez, Ray Sartor, Robert Vrooman
- Christopher Perfetti, Tara Robertson, UNM, joined the meeting
- Alex Lang, ORNL, joined the meeting

Previous items update:

- No open items to update

Items for discussion:

- Eberle - Administrative reminder about CSCT discussions
- LANL Chlorine in-situ experiments – slide presentation (full hour agenda)

Open discussion:

-

Topics for future meetings?

- NDA measurement issues that affect process analysis for the criticality safety analysis.
- Site fire department personnel taking CS training.

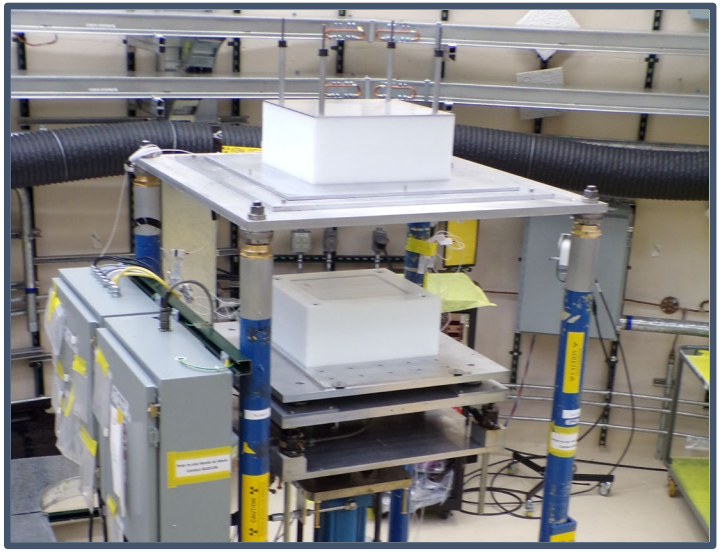
Meeting adjourned at 12:05pm ET.

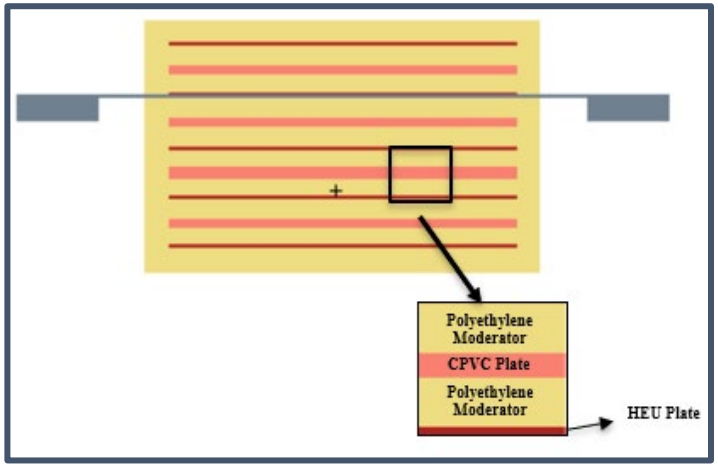
Los Alamos NATIONAL LABORATORY

Chlorine Critical Experiments, Solution Density Prediction, and Validation for NCS

K. Aldrich, J. Alwin, R. Bulso, N. Calhoun, T. Cutler, T. Robertson, R. Sartor

LA-UR-23-22946





Background

- NA-191 funded work on Integral Experiment, Density Law Evaluation & In-situ measurements (future work)
- Extensive collaboration across LANL
- Integral Experiment
  - Necessary for NCS validation
  - Design and execution of experiments – T. Cutler
  - Collaboration with Criticality Experiments Safety Committee – R. Sartor
- Density Law Evaluation
  - Required to be able to analyze plutonium solutions
  - UNM NCS Pipeline POC – N. Calhoun
  - Density Measurements – K. Aldrich
  - Density Law for plutonium nitrate solutions, UNM Research and NCSD Intern – T. Robertson
  - Density Law for plutonium chloride solutions, UNM Research and NCSD Staff Member – R. Bulso

Background

Solvent Extraction Contactors

Pure Pu Metal

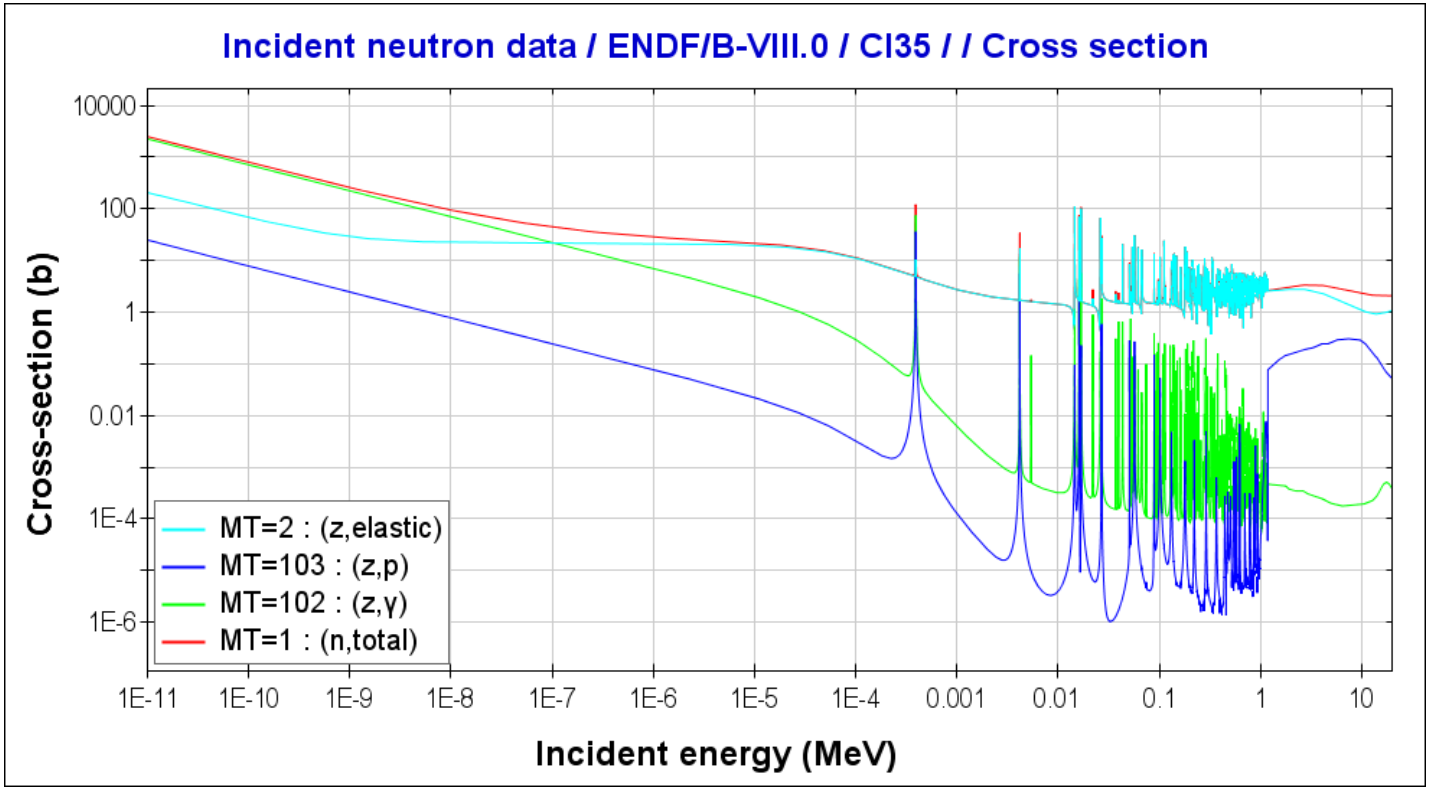
- Chlorine absorption important--
  - Pu Aqueous Chloride Processing at PF-4
  - Pu pyrochemical Pu processing at PF-4
  - Electrorefining of *uranium* using LiCl at Y-12
- Two proposals submitted to NCSP for FY20
  - NCSP opted to fund LLNL proposal with focus on HEU
  - Benefit in two complementary experiments with low correlations
    Different fuel, spectra, interstitial material strengthens validation

$PuCl_3$

- PF-4 interest in potential decreased conservatism in NCS limits
  - NA-191 funding and high priority: CWS, Density Law
  - Potential future work on In-situ experiments
- Very few benchmark experiments sensitive to Cl-35 (n,γ) exist that can be applied toward validation for NCS

Background: ^{35}Cl Cross-sections

- ^{35}Cl Main reactions, (n,γ) significant at thermal energy

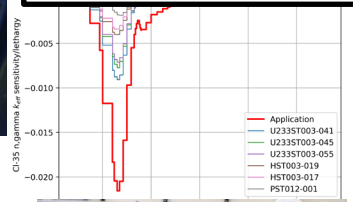


Integral Experiment Design & Execution
T. Cutler – NEN-2 LANL

Planet: Chlorine Worth Study in Support of PF-4 Operations

- Motivation
  - Aqueous Chloride Operations at PF-4 are important for Pu recovery from various salts and processes, but have conservative mass limits which don't account for absorption of neutrons in Cl
- Objective
  - Design and execute a critical experiment to validate Cl neutron absorption
  - Use ARCHIMEDES framework for experiment optimization with ML guided approach, which supports an accelerated timeline
- Execution
  - Use the ZPPR Pu plates with interleaved PVC/ CPVC and HDPE
  - Three configurations to match the full Pu-Cl concentration profile in Aq Cl Ops
  - Perform with sufficient detail to write ICSBEP benchmark with minimized experimental uncertainties
  - Major collaboration across many Divisions across LANL

Gap analysis between Aq Cl Ops and existing benchmarks

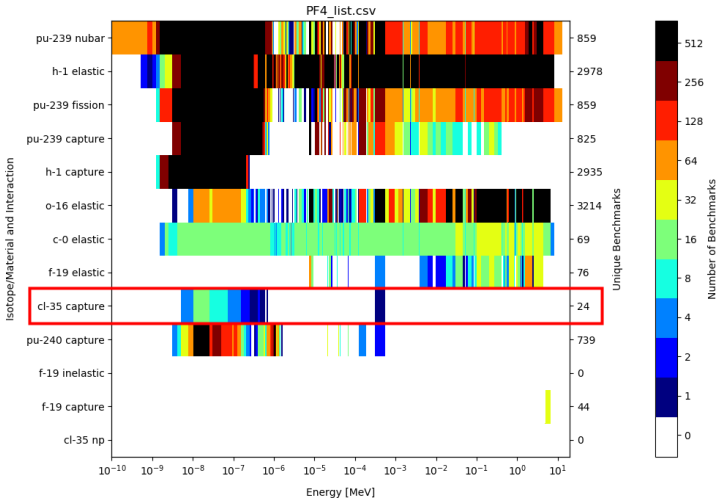


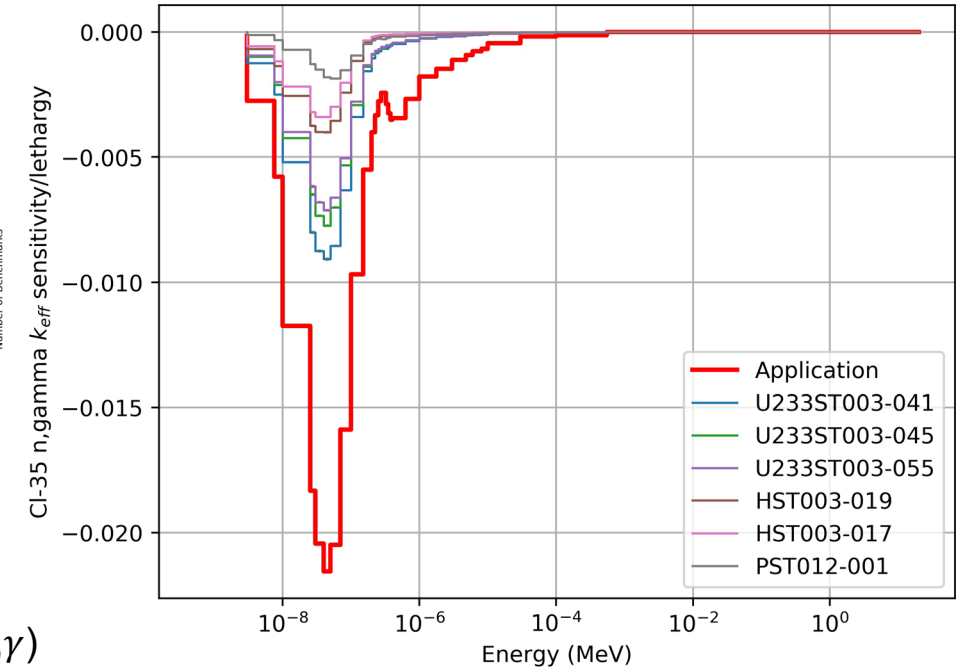
Single layer of CWS, showing PVC and HDPE

AMPP-4 personnel join NEN-2 in loading Pu plates for the experiment

CWS Config 1

Gap Analysis (Comparison to Existing Benchmarks)

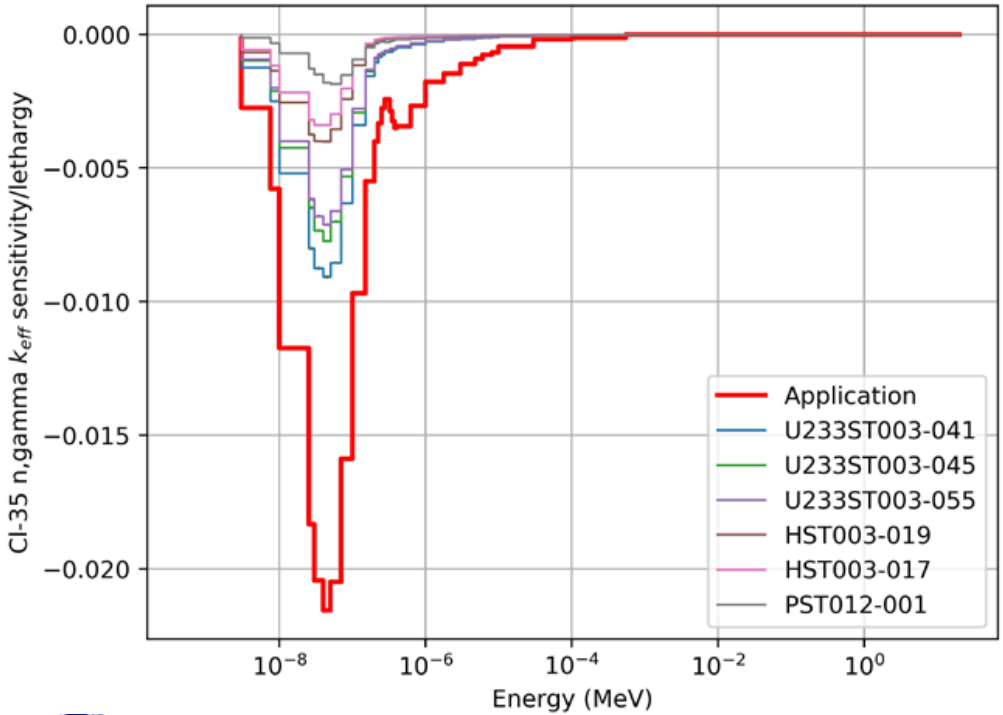


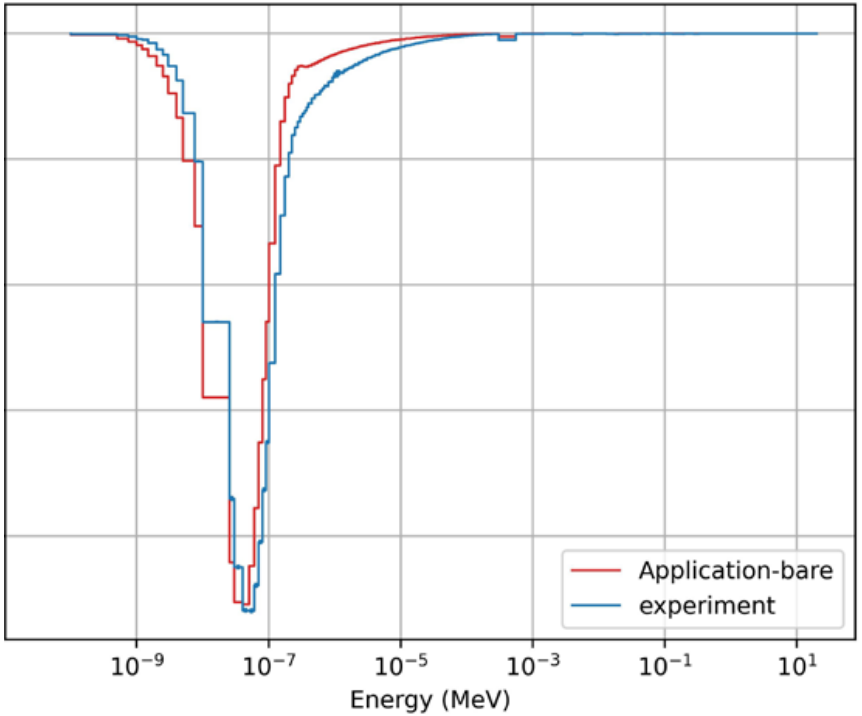


- Comparison to existing experiments
  - few benchmarks sensitive to Cl-35 (n,γ)
  - sensitivity of pre-existing benchmarks is much lower than the PF-4 Aqueous Chloride application
  - PST012 is most similar Pu experiment, has Lucoflex box for water reflection floating on plutonium nitrate solution

Designing optimized experiments

- Comparison of ^{35}Cl (n,γ) sensitivity for existing experiments (figure on left) versus optimally designed CWS experiment (figure on right)
  - CWS design same sensitivity as application



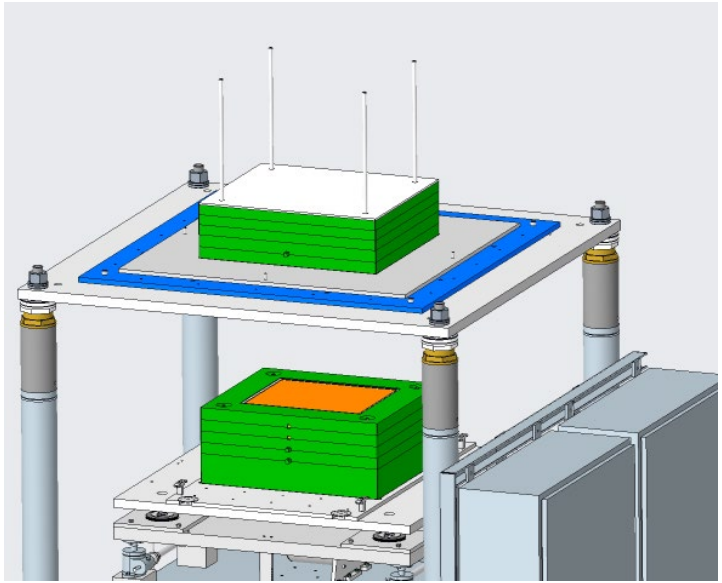


Designing optimized experiments

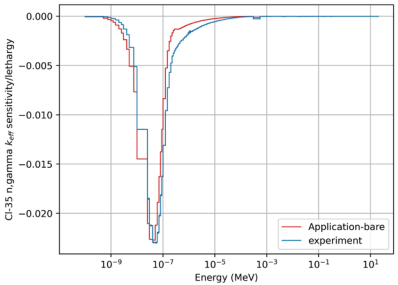
- Designed using EUCLID-predecessor framework (2019 ARCHIMEDES LDRD Reserve)
- Funded by NA-191
- Initial tasking June 2020; executed Dec 2021
- Near record timeline
- Benchmark planned for Spring 2023
- 3 configs covering full Pu concentration range
- Combinations of Pu, HDPE, PVC, and CPVC
- Specifically focused on maximizing partial c_k and minimizing overall experimental uncertainty
- Major collaboration between NEN, NCS, MRR, AMPP, XCP, CCS

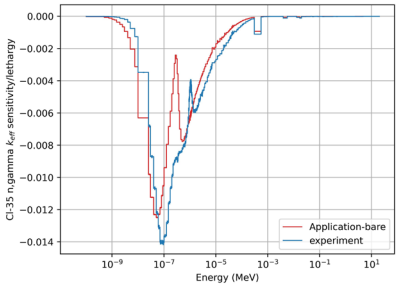
Final Designs

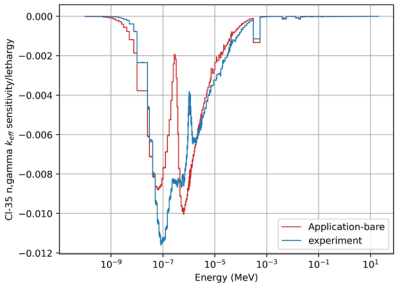
- Reflector: 3” HDPE (top, bottom, sides)
- Fuel: 5x4 (20 total per unit) ZPPR plates, ~105 g Pu per plate
- Moderator: HDPE (varying geometry)
- Cl Material: PVC or CPVC (varying geometry)
- Configurations:
  1. optimized for 30 g/L application (covers 20-100 g/L range)
     - Stack of HDPE-PVC-HDPE on ZPPR plates
  2. optimized for 300 g/L application (covers 300-400 g/L range)
     - ~7.9” diameter PVC cylinder inside HDPE on ZPPR plates
  3. optimized for 600 g/L application (covers 500-600 g/L range)
     - ~7.9” diameter CPVC cylinder inside HDPE on ZPPR plates



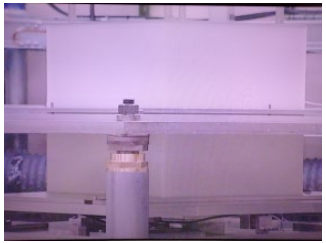
Optimized Experiment Configurations

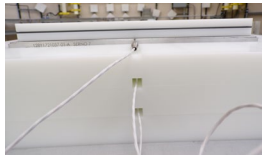




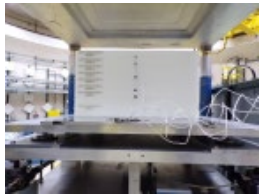


Configuration 1 20-100 g/L





Configuration 2 300-400 g/L



Configuration 3 500-600 g/L

Criticality Safety Experiments Committee (CESC) Collaboration
R. Sartor – NCS LANL and CESC Member

Collaboration on experiments with Criticality Experiments Safety Committee (CESC)

- CESC provides independent & objective safety review of criticality experiments performed at the National Criticality Experiments Research Center (NCERC)
- CESC met with NEN-2 staff to review CEF-EXP-019, *Planet Experiment Plan – Chlorine Worth Study*.
- Modest changes to the procedures suggested; CESC did not identify any safety concerns. Reflects NEN-2's attention and effort in developing the experiment plan.
- CESC observe NCERC activities annually, planned 2021 review with execution of CWS to observe assembly, remote operations, and disassembly of the experiment.

Loading Pu plates during the experiment

Plutonium Solution Density Measurements
K. Aldrich – CAAC LANL

Example k_{eff} Calculation for Aqueous Plutonium Solution – 600 g ^{239}Pu

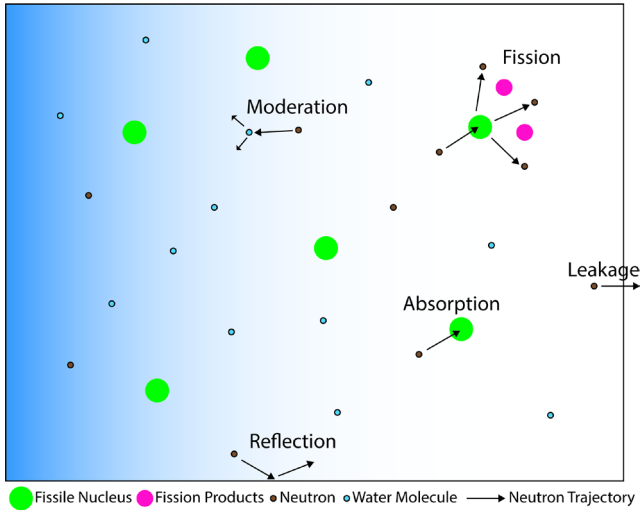
MCNP inputs: **material density**, **atomic percentages**, geometry, reflection, etc.

No chlorine is included in inputs

Pu – water mixture density is calculated from density of *α*-Pu (19.8 g/cm^3)

Repeat density calculation for desired concentration range

Output: k-eigenvalue (k_{eff})



Example Density Calculation 100 g/L:

$$0.100\ g\ Pu\ \div 19.8\ g/cm^3 = 0.005051\ cm^3$$

$$1.000\ cm^3 - 0.005051\ cm^3 = 0.99495\ cm^3$$

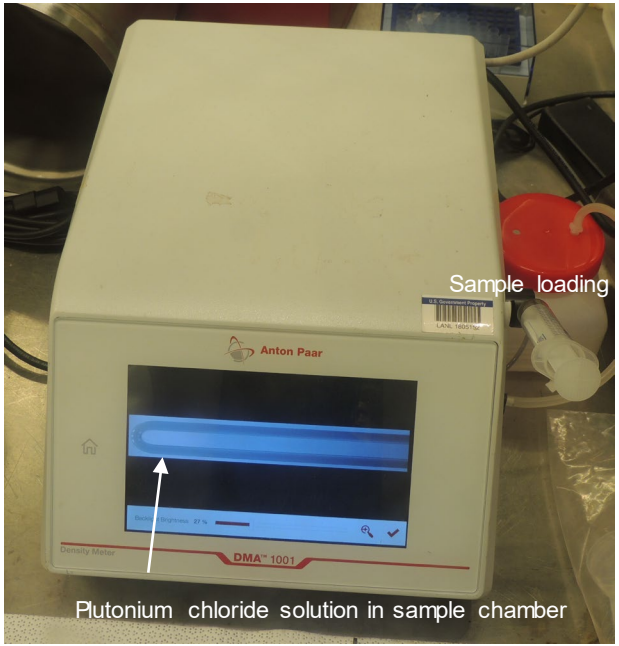
$$0.99495\ cm^3 \times 0.99187\ g/cm^3 = 0.99314\ g\ H_2O$$

$$0.99314\ g + 0.100\ g = 1.09319\ g/cm^3$$

Experimental Density Measurements

- Samples prepared from dissolution of high purity *α*-Pu metal in HCl
  - Well characterized for Pu/HCl concentrations
  - Used to prepare range of concentrations

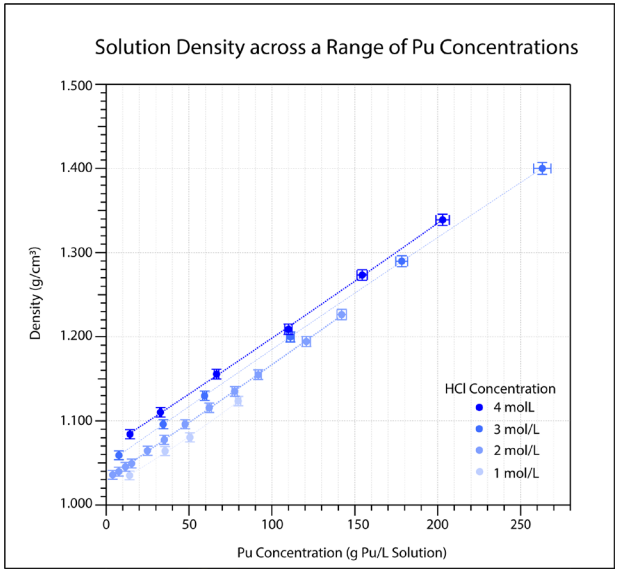
- Anton Parr 1001 Density Meter
  - Oscillating U-tube technique
  - Thermo-coupled measurements
  - Broad range of solutions can be measured (0 to 3 g/cm^3)

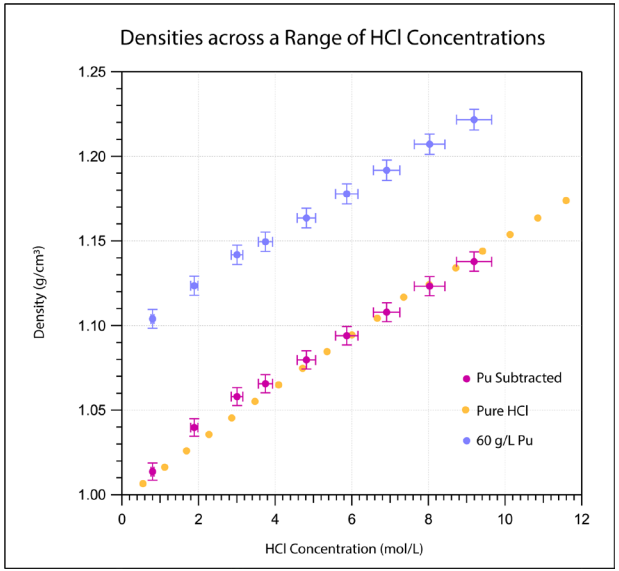


Commercial density meter utilized for solution measurements shown in a radiological glovebox. The U-shaped sample chamber is shown with plutonium chloride solution loaded via the syringe on the right.

Cross, J. N., et. al. *JRNC*, **2018**, 318, 1697.
Cross, J. N., Thompson, P., Kunsberg, D. J., *Plutonium Handbook, 2nd ed.*, **2019**, Ch. 46, 3343.

Experimental Density Data





Experimentally measured density values (average of triplicates) from the Anton Parr 1001 DMA solution density meter are plotted as a function of either [Pu] (left) or [HCl] (right), above. Error estimates combine statistical error and errors introduced via sample preparation. Measurements shown were taken at 25 °C.

Path Toward Pitzer Method Derived Density Law for $PuCl_3/HCl/H_2O$ Ternary Solutions

Empirical estimate of density law:

$$d = d_0 + A \cdot m_{Pu} + B \cdot m_H + C \cdot T + D \cdot m_{Pu} \cdot m_H + E \cdot m_{Pu} \cdot T + F \cdot (m_{Pu})^2 + G \cdot (m_H)^2$$

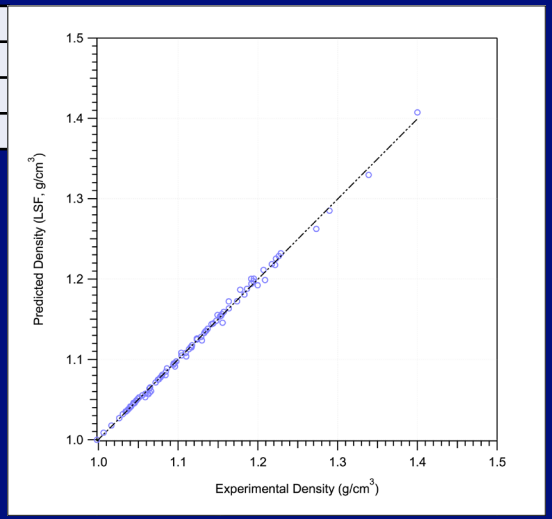
m_{Pu} = molality of Pu, m_H = molality of acid, T = temperature (°C)

Ordinary least squares fit applied to full set of data points (93 points) – results in a model with low residual errors:

Coefficients	
d_0	1.00739
A	0.35034
B	0.01598
C	-0.000303
D	-0.01614
E	-0.00063
F	0.04858
G	-0.00031

} Non-zero coefficients for multiplication terms

Residuals from LSF	
max	0.0108
min	-0.0089
avg	-0.001%



Weber, C. F., Hopper, C.M., *Nuclear Technology*, **2006**, 153, 1-8; Pitzer, K.S., *J. Phys. Chem.*, **1973**, 77, 268; Pitzer, K. S., Activity Coefficients in Electrolyte Solutions, 2nd ed., K. S. Pitzer (ed), *CRC Press*, **1991**.

UNM NCS Pipeline
N. Calhoun– NCS LANL

UNM Pipeline

- Bring awareness of the NCS career to our local communities
- Contract established 2021
- Establishes collaboration between faculty and staff at LANL and UNM
- Original scope: NCS undergrad/grad course
- Expanded scope: NCS undergrad/grad course and Graduate Student Project
- NCS to provide graduate students with project topic

UNM-Graduate Student Project

- NCS provides graduate students with project topic
- Mentor graduate students weekly
- Invite students to LANL meetings pertaining to project topic

UNM Graduate Student Project-Mentors

Dr. Christopher Perfetti

- UNM Assistant Professor 2018-Present
- Ph.D. Nuclear Engineering and Radiological Sciences **UM**
- NE410/NE510, NE499/NE515, NCS, Nuclear Reactor Theory, Nuclear Reactor Kinetics and Dynamics

Jennifer Alwin

- Senior Qualified NCS Analyst/NCS DL
- Educational background in ChE and NE
- 25 years at LANL
- MCNP Instructor
- Chair Criticality Experiments Safety Committee

Graduate Students

Tara Robertson

- B.S. Nuclear Engineering UNM (2021)
- Currently working on Masters in NE at UNM (exp. Grad 2023)
- SNL Intern & LANL Intern
- LANL NCSD Analyst – May 2023

Riley Bulso

- B.S. Nuclear Engineering RPI (2019)
- Currently working on Masters in NE at UNM (exp. Grad 2024)
- **4+** years NCS at LANL

Graduate Student Project

- For MCNP6 models
  - need to know geometry & materials in fissionable material processes
  - assumptions must be quantified for the impact to bias

- System with a significant amount of bias due to material modeling assumptions is in the area of aqueous plutonium processing
  - These are typically plutonium nitrate and plutonium chloride solutions
  - Currently modeled as fictitious plutonium metal-water mixtures

- Little is known about the actual density of the solution and/or no predictive capability approved for use at LANL for modeling them

```
c Water
m200 1001.80c 2.0
     8016.80c 1.0
mt200 lwtr.20t
c PU
m300 94239.80c 1.0
c
C -----------------------------------------
C Pu-239 Metal/Water Mechanical Mixture
C
C -----------------------------------------
C Pu Metal/Water Mechanical Mixture:  1.24 g/cc
m100  1001.80c   -0.0892702573697133
      1002.80c   -2.05190204144513e-05
      8016.80c   -0.708672563732072
      94239.80c  -0.2020366598778
mt100 lwtr.20t
      hwtr.20t
C 0
C Pu Metal/Water Mechanical Mixture: 18.09 g/cc
m400  1001.80c   -0.000573450074917905
      1002.80c   -1.3180911695121e-07
      8016.80c   -0.00455233743845233
      94239.80c  -0.994874080677513
mt400 lwtr.20t
      hwtr.20t
C 0
```

MCNP6 material cards with solution weight fractions H-1, H-2, O-16, Pu-239 for Pu metal-water mixture

Graduate Student Project Cont.

- 2 graduate students are working on the plutonium nitrate and plutonium chloride densities
- This research will fill the gap and develop an algorithm for use with MCNP6 to model the density of the solutions
- The method will be validated with experimental data for density and also validated with critical experiments modeled using MCNP6
- The broad objective of this research is aimed at implementing a plutonium nitrate and plutonium chloride density law, and to provide meaningful tools for which a working density law can be derived

Summary

- University pipeline benefits DOE Complex as a whole-students readily available to fill mission needs
- Internal to LANL- We have been able to see the benefits with retention rates and work output
- Impacts the local community in a positive manner
- Graduate Student Project- Will improve knowledge of solution densities and modeling conventions for all users of MCNP6

Plutonium Nitrate Solution Density Predictive Capability

T. Robertson – UNM Graduate Researcher/NCS LANL

Density Law Python Tool for MCNP- $Pu(NO_3)_4$ solution

- Used an empirical density equation using equation outlined in paper by Weber describing implementation in SCALE
  - Currently working on addition of Pitzer method.
- Created a python tool to predict the density of the solution using multiple inputs of plutonium and nitrate content (concentration, molarity, molality). The tool also includes abilities to calculate the material card atom densities and edit MCNP6.2 input files.
  - PuNSDensitySolver
  - PuNSDensityFunctions
- Validated and verified against benchmark data usi ICSBEP Handbook to find density fit to +/- 2.6%.

```
30  def Density1(mPu,mH,T):
31      """mPu and mH are in molality (mol solute/kg solvent) and T is in Celsius"""
32      if mPu>3.3 or mH<0 or mH>6.27 or T<0 or T>60:
33          print("ERROR: Data entered is out of bounds of equation range.")
34          return 0
35      else:
36          A=0.402234
37          B=0.029992
38          C=3.01282*(10**-5)
39          D=-0.017735
40          E=-4.7033*(10**-4)
41          F=-0.026282
42          G=-1.172*(10**-3)
43          do=0.997
44
45          return do+A*mPu+B*mH+C*T+D*mPu*mH+E*mPu*T+F*mPu*mPu+G*mH*mH
46
```

PuNSDensitySolver

```
7     import PuNSDensitySolver
8
```

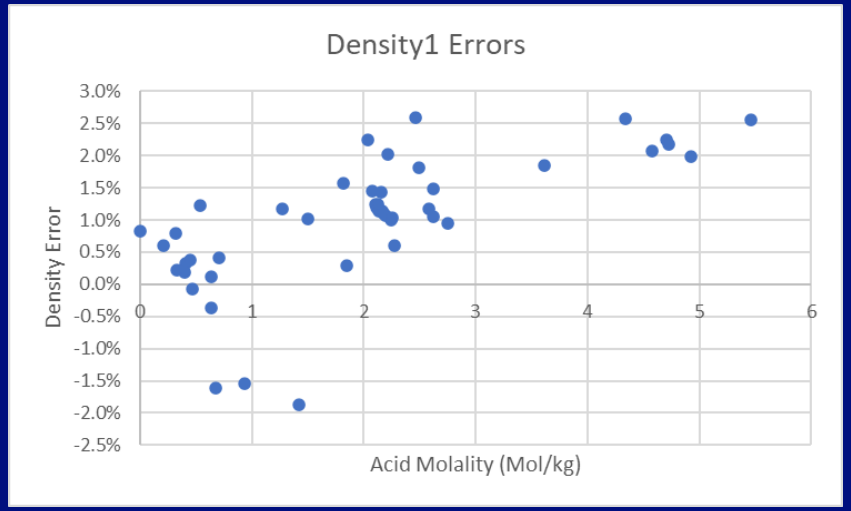
```
For Pu: Enter 1 to input molality (mol Pu/kg solvent), enter 2 to input Concentration (g Pu/L
solution), or enter 3 to input molarity (mol Pu/L Solution): 2

For H: Enter 1 to input molality (mol H/kg solvent), enter 2 to input Concentration (g H/L solution),
or enter 3 to input molarity (mol H/L Solution): 3

Enter Temperature of Solution in Celsius: 25

Enter Plutonium concentration (g Pu/L solution): 100

Enter HNO3 Molarity (mol HNO3/L solution): 2

Would you like to create a MCNP Material Card? (Y/N): n



Your solution density is:  1.2184983711302875  kg/L




Would you like to run another case? (Y/N):
```

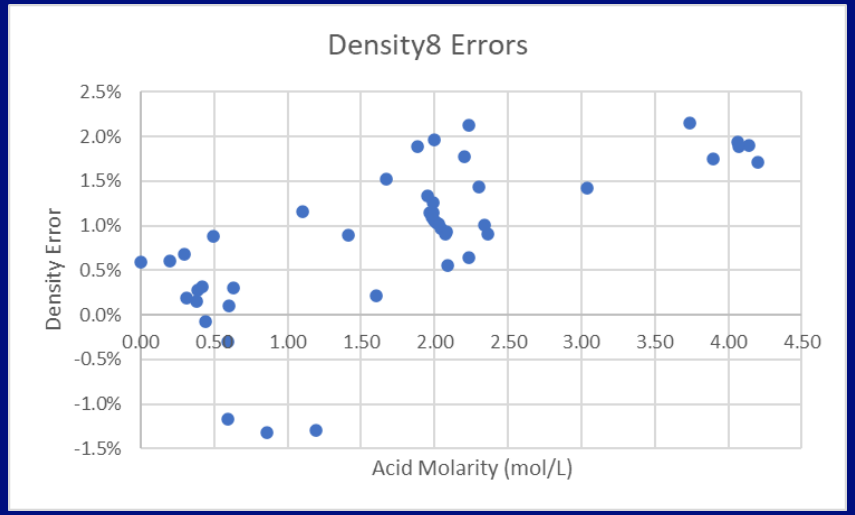
PuNSDensityFunctions

```
7   import PuNSDensityFunctions as PUNS
8
9   print(PUNS.Density8(100,2,25))
```

```
1.2184983711302875
```

Validation and Verification





Plutonium Chloride Solution Density Predictive Capability

R. Bulso – NCS LANL & UNM Graduate Researcher

Density Law Python Tool for MCNP-AQCL

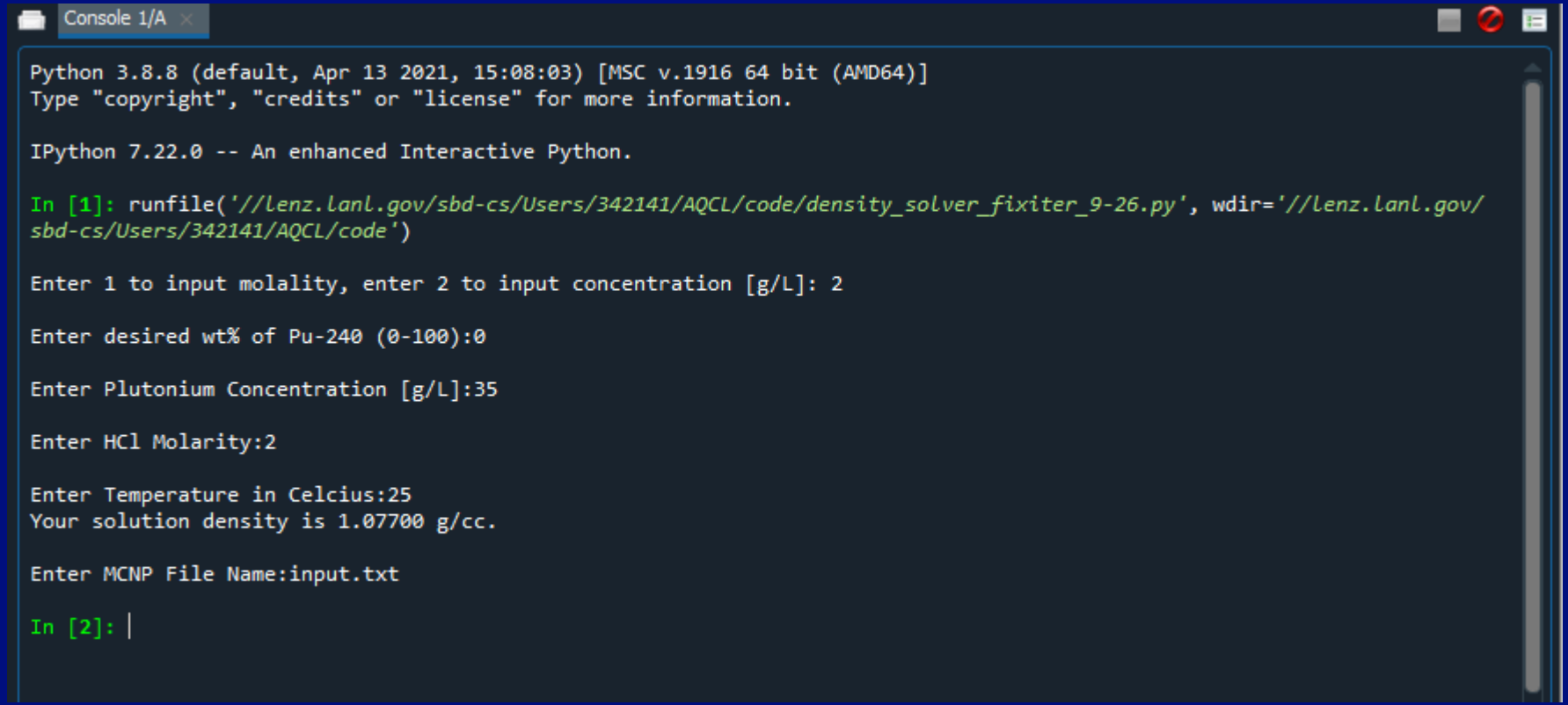
- Pitzer Method to determine solution density → material composition
  - Least square fit of density equation, populated with experimental data from C-AAC, used to determine the equations coefficients

- User inputs: amount of Pu, amount of HCl, solution temperature in Celsius, and name of MCNP file
  - Options to input molality or concentration [g/L] of Pu, and molality or molarity [moles/L] of HCl
  - Specify ^{240}Pu content as at% or wt%

- Outputs: Solution density, specified MCNP file with new material card

- Note: Pu is modeled in the Pu(III) valance state for conservatism. C-AAC data notes that the valance state of Pu (III or IV) has little to no effect on the bulk density of the solution.

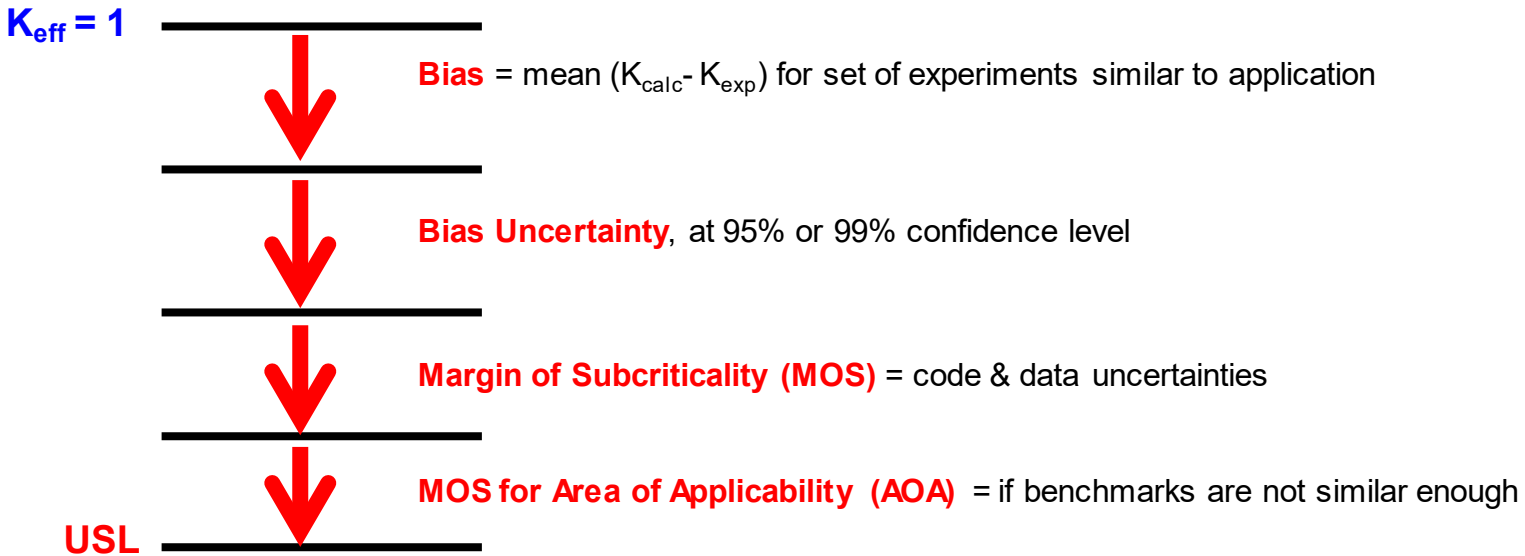
Density Law Python Tool for MCNP-AQCL



NCS Validation and Future Work
J. Alwin – XCP-7 LANL

Nuclear Criticality Safety (NCS) Validation

- Validation quantifies suitability of code system for use in NCS analyses by comparison with benchmark experiments → Upper Subcritical Limit
- Bias: difference between calculated and experimental k-effective
- Bias uncertainty: uncertainly to account for benchmarks, calculational models and methods,
- MOS: allowance beyond bias and bias uncertainty to ensure subcriticality



NCS Validation

- Bias & bias uncertainty: credible when the application (A) & chosen benchmarks (B) are neutronically similar
- Systems similarly sensitive to the same nuclear data → same bias
- The c_k correlation coefficient compares system, assessing potential for common bias for each nuclide, reaction, and energy group
- c_k = 1: two systems use same data in same way
- Sensitivities computed by MCNP6: Application, S_A, Benchmark, S_B
- Application variance due to nuclear data uncertainties: $Var_k(A) = \vec{S}_A \bar{C}_{xx} \vec{S}_A^T$
- Benchmark variance due to nuclear data uncertainties: $Var_k(B) = \vec{S}_B \bar{C}_{xx} \vec{S}_B^T$
- Covariance between A & B due to nuclear data uncertainties: $Cov_k(A,B) = \vec{S}_A \bar{C}_{xx} \vec{S}_B^T$
- Correlation between A & B due to nuclear data:

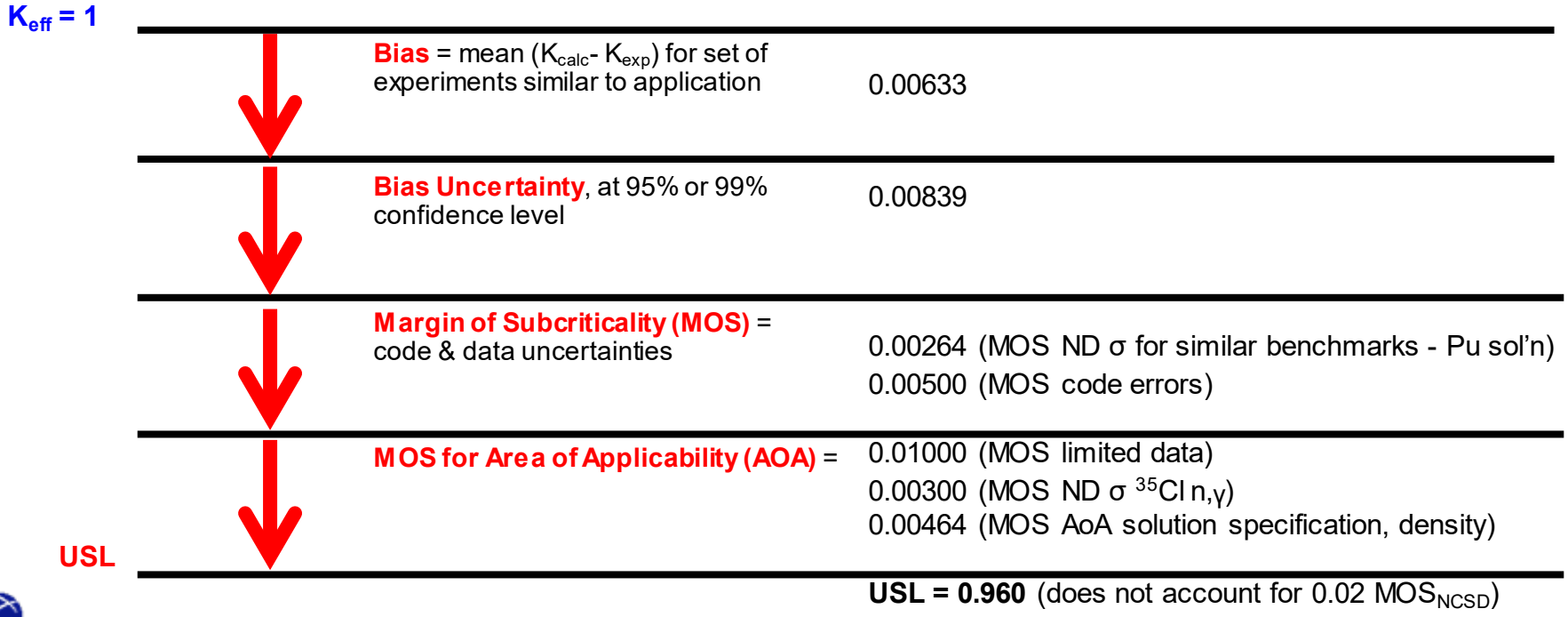
$$c_k(A,B) = \frac{Cov_k(A,B)}{\sqrt{Var_k(A)} \cdot \sqrt{Var_k(B)}} = \frac{\vec{S}_A \bar{C}_{xx} \vec{S}_B^T}{\sqrt{\vec{S}_A \bar{C}_{xx} \vec{S}_A^T} \cdot \sqrt{\vec{S}_B \bar{C}_{xx} \vec{S}_B^T}}$$

c_k and Partial c_k (17035 n,γ) Comparisons

Application/Model	CWS Configuration 1	CWS Configuration 2	CWS Configuration 3	TEX HEU Cl #1 8 layer
	Partial c_k Total c_k	Partial c_k Total c_k	Partial c_k Total c_k	Partial c_k Total c_k
Aqueous Chloride 30 g/L PF-4	0.9427 0.9436	0.9020 0.5578	0.8999 0.5178	0.9955 0.1435
Aqueous Chloride 300 g/L PF-4	0.8149 0.8701	0.9998 0.8327	0.9976 0.8212	0.6499 0.1791
Aqueous Chloride 600 g/L PF-4	0.7609 0.8526	0.9977 0.8225	0.9998 0.8097	0.5808 0.1798

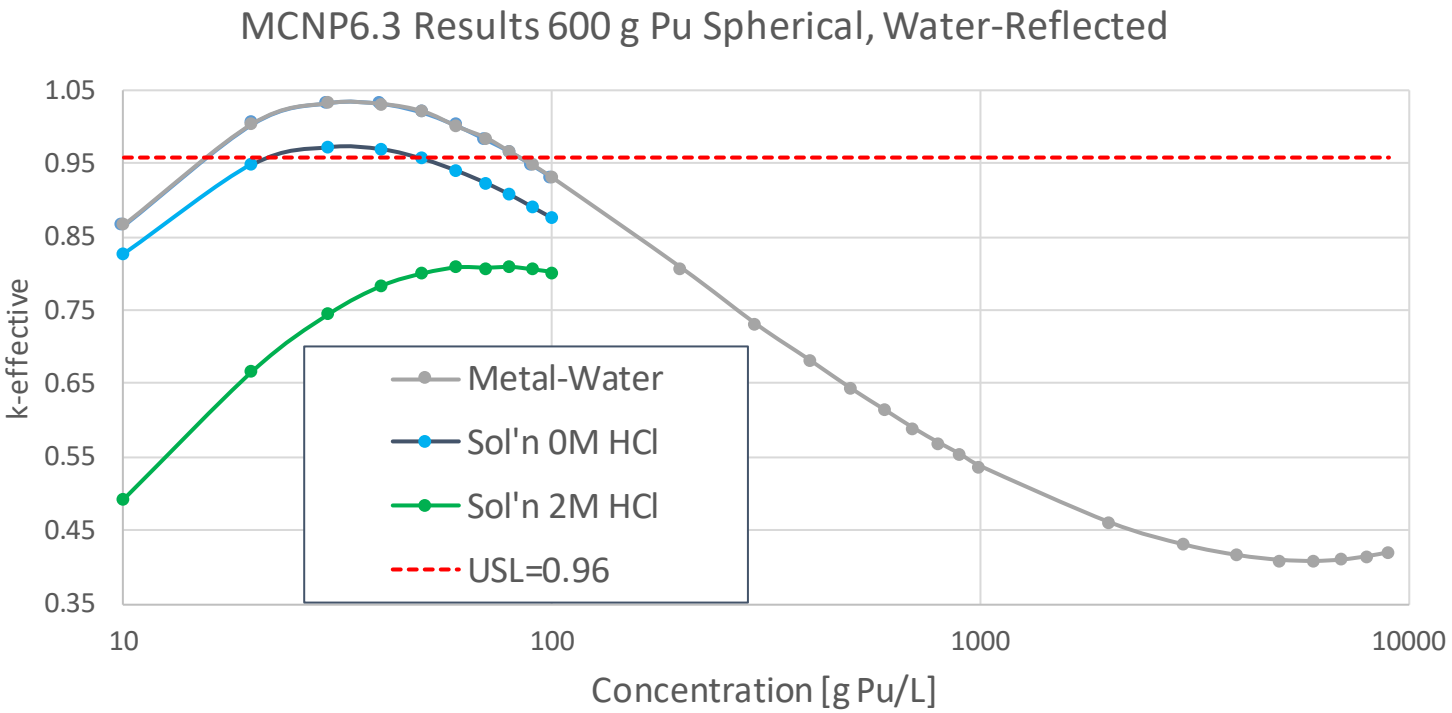
Nuclear Criticality Safety (NCS) Validation

- Whisper-1.1 **preliminary** results w/BLO covariances (low fidelity)
- MOS: allowance beyond bias and bias uncertainty to ensure subcriticality
- ANSI/ANS-8.1, DOE CSSG Response 14-02 *Validation with Limited Benchmark Data*



Potential Credit for Cl Absorption

- Potential mass limit differences Pu metal-water vs. $PuCl_3$ Solution, 600 g Pu
  - Non conservative case; spherical, reflected, Pu[0] →credit isotopic, limited reflection, geometry



Continuing/Future Work

- Integrate ENDF/B-VIII.0 covariance data
  - Important for accurate estimation of nuclear data uncertainty for $^{35}Cl(n,\gamma)$
- Integrate latest CWS benchmark input files into Whisper benchmark library
- Compare applications with CWS benchmark using Whisper
- Accept CWS experiments as benchmarks, ICSBEP approval
- Model application cases using density law
  - Understand k-effective differences
    - uncertainty in density law
    - credit for Cl in process steps
- Document validation strategy
  - Choosing similar benchmarks
  - For application cases in each process
  - ND uncertainty
- Understand standards requirements [ANSI/ANS-8.6] → in-situ poisons, etc.

Conclusions

- Collaboration across LANL on completing important work
  - Cl critical experiments
  - Pu solution density measurements
  - Establishing a predictive capability for density so that solutions can be modeled
- Multiple organizations
  - Strength of LANL
- Critical Experiment Successful
  - PF-4 operations involved in critical experiment
  - Impressive schedule
  - Near completion for acceptance as benchmark (ICSBEP)
- Work establishes capability to analyze Pu solutions more realistically
  - Solution vs. metal-water mixture
  - Contains neutrons absorbing materials as part of process
  - Acid necessary to create solution

Questions? …& Acknowledgements

- This work was supported by the U.S. Department of Energy through the Los Alamos National Laboratory. Los Alamos National Laboratory is operated by Triad National Security, LLC, for the National Nuclear Security Administration of U.S. Department of Energy (Contract No. 89233218CNA000001).

- CWS was funded under the Material Recycle and Recovery Program, NNSA Plutonium Program Office (NA-191), under Office of Production Modernization (NA-19), funded and managed by the National Nuclear Security Administration for the Department of Energy. Research on critical experiment design was supported by the U.S. Department of Energy LDRD program at Los Alamos National Laboratory.

- On behalf of LANL NCSD, we would like to thank the NCSP management for their continued support.

More Acknowledgements

Thank you:

Hutchinson	Jesson	NEN-2
Cutler	Theresa	NEN-2
Goda	Joetta	NEN-2
Grove	Travis	NEN-2
Walker	Jessie	NEN-2
Thompson	Nicholas	NEN-2
Wynne	Nicholas	NEN-2
Valdez	Kenneth	NEN-2
Martin	Justin	NEN-2
Amundson	Kelsey	NEN-2
Kleedtke	Noah	NEN-2
Smith	Travis	NEN-2
Michaud	Isaac	CCS-6
Alwin	Jennifer	XCP-7
Favorite	Jeffery	XCP-7
Salazar-Crockett	Alicia	NCS
Little	Robert	XCP-3
Romero	Christopher	E-1
Hayes	David	NEN-2
Bluhm	Brian	GS-NNS
Rench	Nicholas	NCERC-FO
Young	Suzzanne	NCERC-FO
Hoffman	Stanley	NCERC-FO
Harper	Arnold	RT-BSI
Perlstein	Daniel	NCERC-FO
Bunsen	James	AMPP-4
Aldrich	Kelly	C-AAC
Vu	Dung	C-AAC
Ambrosio	Gabrielle	AMPP-4
Kimball	David	AMPP-4
Berman	Leah	AMPP-4
Lopez	Christopher	AMPP-4
Worl	Laura	INP-MRR
Lynn	Alex	NCERC-FO
Blumberg	Paul	NCERC-FO
Bridgewater	Jon	AO
George	Jerry	RP-TA55
Jaegers	Peter	XTD-NTA
Mclaughlin	Tom	NEN-2
Sartor	Ray	NCS
Ziehm	Sue	JLON

↓Application	Benchmark →	CWS #1 30 g/l	CWS #2 300 g/l	CWS #3 600 g/l	TEX HEU Cl #1 6 layers	TEX HEU Cl #2 8 layers
Aqueous Chloride 30 g/L PF-4	$\sim C_{k\ 17035\ n,\gamma}$	0.942736	0.557797	0.517819	0.995484	0.855305
	$C_{k\ overall}$	0.943612	0.901996	0.899929	0.143512	0.133822
Aqueous Chloride 300 g/L PF-4	$\sim C_{k\ 17035\ n,\gamma}$	0.814859	0.999768	0.997648	0.649937	0.915636
	$C_{k\ overall}$	0.870086	0.832729	0.821191	0.179145	0.175662
Aqueous Chloride 600 g/L PF-4	$\sim C_{k\ 17035\ n,\gamma}$	0.760870	0.997733	0.999779	0.580765	0.876842
	$C_{k\ overall}$	0.852607	0.822491	0.809708	0.179837	0.179496
Y-12 case 7e	$\sim C_{k\ 17035\ n,\gamma}$	0.997269	0.844530	0.818185	0.949580	0.991472
	$C_{k\ overall}$	0.099850	0.103916	0.103432	0.776393	0.750561
Y-12 case 8a	$\sim C_{k\ 17035\ n,\gamma}$	0.953098	0.584529	0.545402	0.998047	0.871724
	$C_{k\ overall}$	0.154066	0.137912	0.133175	0.796197	0.742442
Y-12 case 8b	$\sim C_{k\ 17035\ n,\gamma}$	0.967873	0.626938	0.589294	0.999958	0.896599
	$C_{k\ overall}$	0.149072	0.134887	0.130556	0.807623	0.756429
Y-12 case 8c	$\sim C_{k\ 17035\ n,\gamma}$	0.978160	0.661189	0.624873	0.999366	0.915526
	$C_{k\ overall}$	0.140839	0.129349	0.125631	0.810930	0.763660
Y-12 case 8d	$\sim C_{k\ 17035\ n,\gamma}$	0.986490	0.694136	0.659223	0.996768	0.932629
	$C_{k\ overall}$	0.120857	0.114127	0.111594	0.795663	0.754602

What is adjustment?

Adjustment: mathematical process to update a nuclear data library with information from integral experiments. Usually, GLLS is used (e.g., Whisper at LANL).

$$\sigma^* = \sigma + (SC_{\sigma\sigma})^T \cdot (S^T C_{\sigma\sigma} S + C_{ee})^{-1} \cdot (y_e - y_c)$$

$$C^*_{\sigma\sigma} = C_{\sigma\sigma} - (SC_{\sigma\sigma})^T \cdot (S^T C_{\sigma\sigma} S + C_{ee})^{-1} \cdot (SC_{\sigma\sigma})$$

$\sigma \rightarrow$ ND mean
$C \rightarrow$ Covariance matrix
$y \rightarrow$ benchmark data
$S \rightarrow$ Sensitivity matrix

The resulting, adjusted libraries are application-specific libraries. The application space is represented by the integral experiments chosen for adjustment.

Users would gain with adjustment tool:

- Capability to produce their own application specific library,
- Fast inclusion of new integral exp. into nuclear-data libraries (days instead of year).