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Title:	MCNP Parametric Studies of Plutonium Metal and Various Interstitial Moderating Materials
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MCNP Parametric Studies of Plutonium Metal and Various Interstitial Moderating Materials

1. Summary

Nuclear Criticality Safety (NCS) has performed calculations evaluating the effect of different interstitial materials on 5.0-kg of plutonium metal. As with all non-fissionable interstitials, the results here illustrate that it requires significant quantities of oil to be intimately mixed with plutonium, reflected by a thick layer of full-density water, to achieve the same reactivity as that of solid plutonium metal.

2. Evaluation Method

2.1 Calculational Platform

The calculations were performed using MCNP6 Version 1.0 with ENDF/B-VII.1 nuclear data, including appropriate $S(\alpha, \beta)$, on the Moonlight High Performance Computing cluster. This is a verified and validated computational method as documented in Reference 1.

2.2 Computational Model

Table 1 lists the materials, properties, and cross sections that were used for the calculations in this document.

The model consisted of two concentric spheres. The inner sphere was a mixture of 5kg of ^{239}Pu in one of seven potential moderators. Total volume of the inner sphere was varied to allow for concentrations of Pu varying from pure metal to as close to pure moderator as MCNP6 could sustain a calculation for. The outer sphere comprised a 12-in thick tight-fitting water reflector.

The specifications for California (CA) oil, Texas (TX) oil and hydraulic oil are taken from a compendium provided by Pacific Northwest National Laboratory. [Ref. 2] Additionally, an idealized oil (based upon Spindura ® oil) is provided. Atom fractions and bulk densities for the oils are given in Table 1.

Table 1– Material Specifications

	CA oil	**TX oil**	**Hydraulic Oil**	**Idealized Oil**	**Beryllium**	**Carbon**
Density→ **ZAID ↓**	0.9550 g/cc	0.8750 g/cc	0.8710 g/cc	0.8576 g/cc	1.848 g/cc	2.25 g/cc
1001	.633782	.629388	.392857	.685714		
4009						
6000	.364349	.365220	.476190	.314286		
7014		.002578				
8016			.047619			
15031			.011905			
16032	.001776	.002449				
16033	.000014	.000019				
16034	.000079	.000120				
16036	.000001	.000002				
17035			.054115			
17037			.017314			

The idealized oil is based on Spindora ® oil; however, the material definition utilized in this study ignores the functional groups (the group of atoms, usually the non-hydro-carbon portion, which cause the characteristic chemical reactions), in favor of increasing the hydrogen density. The other significant point in this analysis is that the presence of non-NOCH functional groups or small quantities of additive or contaminants that would act as parasitic neutron absorbers, thus reducing the neutron multiplication of the mixture.

The hydraulic oil was calculated as an 84 atom chain, six atoms of which were Cl.

3. Calculational Results

Results of the parametric study are presented in Figure 1. By varying the plutonium concentration and holding the plutonium mass constant, the net affect is for the volume of the mixture to increase/decrease.

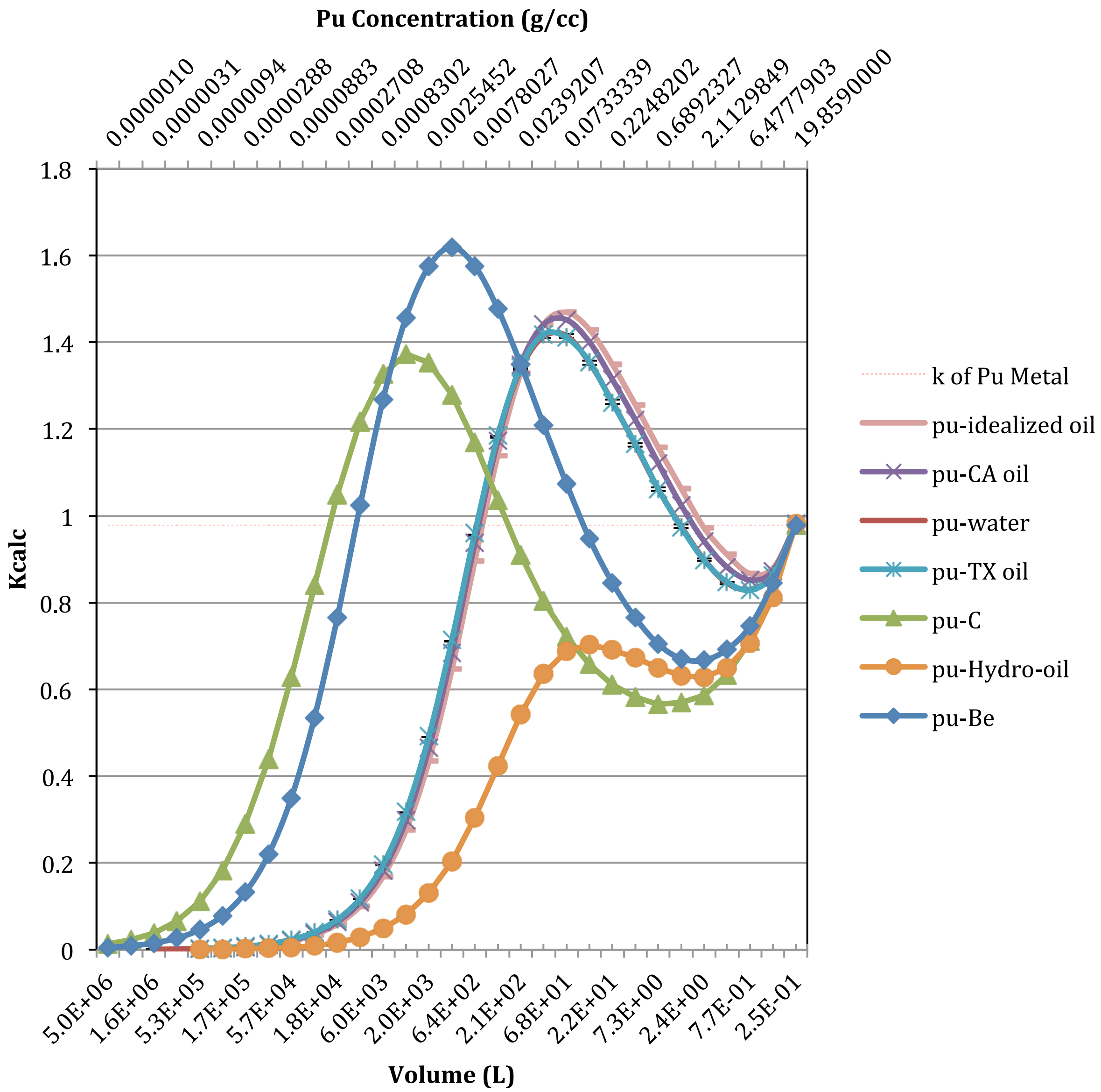

Figure 1. k_{calc} as a function of plutonium concentration in various moderators.

4. Observations

As can be seen in Figure 1, idealized oil, TX oil and CA oil had comparable effects to water with the idealized and CA oil being slightly more reactive than water for high plutonium concentrations. While the difference is not large, it is statistically significant in both cases. Of concern here is the hydrogen density of the oils. As can be seen in Table 1, the CA oil has a noticeably heavier bulk density than the other oils, leading to a higher hydrogen density. The other significant point in this analysis is that the presence of non-NOCH functional groups or small quantities of additive or contaminants can significantly reduce the reactivity of the system. The idealized oil has no such quantities and therefore has the highest k_{calc} of any system modeled.

5. Summary

This study examines multiple moderating materials, and their effect upon the neutron multiplication of 5,000-g ^{239}Pu.

The analytical results reported in this study represent valid bases for defining a variety of bounding cases for criticality safety limits.

6. References

1 **LA-UR-14-23352**, *Validation of MCNP6.1 for Criticality Safety of Pu-Metal, -Solution, and -Oxide Systems*, 2014-05-13.

2 **NCS-MEMO-14-039**, *Approval for Interim Use of MCNP6 Version 1.0,* 2014-10-06.

3 **PNNL-15870 Rev1,** *Compendium of Material Composition Data for Radiation Transport Modeling,* 2011-03-04

APPENDIX: Selected WORM Files

```
c  water reflected sphere of pu-239 metal mixed with water
c
c  constants:
c  atomic weight of water = <a_h2o=2*1.00794 + 15.9994>
c  atomic weight of pu-239 = <a_pu=239.052156>
c  water density = <h2o_den=0.9982> g/cm^3
c  plutonium metal density = <pu_den=19.86> g/cm^3
c
c  variables:
c  plutonium mass = <pu_mass=5000> g pu-239
c  plutonium concentration = <pu_conc=0.001:19859:log31> g pu-239/l
c  water mass = <h2o_mass=(pu_mass/pu_conc*1000-pu_mass/pu_den)*h2o_den|f> g
c
c  hydrogen to pu-239 ratio (h/x) = <h2o_mass/a_h2o/pu_mass*a_pu*2|f>
c
c  mixture volume = <mix_vol=pu_mass/pu_conc|f> l
c
c  mixture weight = <(pu_mass+h2o_mass)*0.002205|f> lbs
c
c  cell cards
1   1  -<(pu_mass+h2o_mass)/mix_vol/1000|f>    -1     imp:n=1
2   2  -0.9982   +1 -2  imp:n=1
3   0            +2     imp:n=0

c  surface cards
c  plutonium/water sphere
1  so  <((mix_vol*1000*3/4/pi)^(1/3))|f>
c  water reflector
2  so  <((mix_vol*1000*3/4/pi)^(1/3)+12*in)|f>

c  data cards
kcode 1000 1.0 25 275
ksrc  0.0 0.0 0.0
m1   94239.80c <pu_mass/mix_vol/1000/a_pu*an>
      8016.80c <h2o_mass/mix_vol/1000/a_h2o*an>
      1001.80c <h2o_mass/mix_vol/1000/a_h2o*an*2>
mt1   lwtr.20t
m2    8016.80c 1
      1001.80c 2
mt2   lwtr.20t
```

```
c  water reflected sphere of pu-239 metal mixed with hydraulic oil
c
c  constants:
c  atomic weight of oil = <a_oil=821.379381>
c  atomic weight of pu-239 = <a_pu=239.052156>
c  oil density = <oil_den=0.8710> g/cm^3
c  plutonium metal density = <pu_den=19.86> g/cm^3
c
c  variables:
c  plutonium mass = <pu_mass=5000> g pu-239
c  plutonium concentration = <pu_conc=0.001:19859:log31> g pu-239/l
c  oil mass = <oil_mass=(pu_mass/pu_conc*1000-pu_mass/pu_den)*oil_den|f> g
c
c  hydrogen to pu-239 ratio (h/x) = <oil_mass/a_oil/pu_mass*a_pu*33|f>
c
c  mixture volume = <mix_vol=pu_mass/pu_conc|f> l
c
c  mixture weight = <(pu_mass+oil_mass)*0.002205|f> lbs
c
c  cell cards
1   1  -<(pu_mass+oil_mass)/mix_vol/1000|f>    -1     imp:n=1
2   2  -0.9982   +1 -2  imp:n=1
3   0            +2     imp:n=0

c  surface cards
c  plutonium/oil sphere
1  so  <((mix_vol*1000*3/4/pi)^(1/3))|f>
c  water reflector
2  so  <((mix_vol*1000*3/4/pi)^(1/3)+12*in)|f>

c  data cards
kcode 1000 1.0 25 275
ksrc  0.0 0.0 0.0
m1   94239.80c <pu_mass/mix_vol/1000/a_pu*an>
      1001.80c <oil_mass/mix_vol/1000/a_oil*an*33>
      6000.80c <oil_mass/mix_vol/1000/a_oil*an*40>
      8016.80c <oil_mass/mix_vol/1000/a_oil*an*4>
      15031.80c <oil_mass/mix_vol/1000/a_oil*an>
      17035.80c <oil_mass/mix_vol/1000/a_oil*an*6*.7576>
      17037.80c <oil_mass/mix_vol/1000/a_oil*an*6*.2424>
mt1   poly.20t
m2    8016.80c 1
      1001.80c 2
mt2   lwtr.20t
```

```
c  water reflected sphere of pu-239 metal mixed with Theoretical oil
c
c  constants:
c  atomic weight of oil = <a_oil=156>
c  atomic weight of pu-239 = <a_pu=239.052156>
c  oil density = <oil_den=0.8576> g/cm^3
c  plutonium metal density = <pu_den=19.86> g/cm^3
c
c  variables:
c  plutonium mass = <pu_mass=5000> g pu-239
c  plutonium concentration = <pu_conc=0.001:19859:log31> g pu-239/l
c  oil mass = <oil_mass=(pu_mass/pu_conc*1000-pu_mass/pu_den)*oil_den|f> g
c
c  hydrogen to pu-239 ratio (h/x) = <oil_mass/a_oil/pu_mass*a_pu*.629388|f>
c
c  mixture volume = <mix_vol=pu_mass/pu_conc|f> l
c
c  mixture weight = <(pu_mass+oil_mass)*0.002205|f> lbs
c
c  cell cards
1   1  -<(pu_mass+oil_mass)/mix_vol/1000|f>    -1     imp:n=1
2   2  -0.9982   +1 -2  imp:n=1
3   0            +2     imp:n=0

c  surface cards
c  plutonium/oil sphere
1  so  <((mix_vol*1000*3/4/pi)^(1/3))|f>
c  water reflector
2  so  <((mix_vol*1000*3/4/pi)^(1/3)+12*in)|f>

c  data cards
kcode 1000 1.0 25 275
ksrc  0.0 0.0 0.0
m1   94239.80c <pu_mass/mix_vol/1000/a_pu*an>
      1001.80c <oil_mass/mix_vol/1000/a_oil*an*24>
      6000.80c <oil_mass/mix_vol/1000/a_oil*an*11>
mt1   poly.20t
m2    8016.80c 1
      1001.80c 2
mt2   lwtr.20t
```