

Cell: J4

Comment: STOCKMANH:
number of oxygens associated with each mole of element. NOTE that usually, O content of U,Pu,Np exceeds 2 per metal, as burnup proceeds.

Cell: K4

Comment: STOCKMANH:
We use the datao.ymp atomic weight, since we are only interested in the mols, and wan't eq6 to calculate moles from weight consistently

Cell: B5

Comment: Emma Parker:
Did not include due to limited thermodynamic data and in order to limit the number of elements in the simplified fuel composition, to enable EQ6 to run smoothly.

Cell: C5

Comment: Emma Parker:
This number designates the isotope. The first two digits are the element's atomic number, and the last three digits are the isotope number (atomic mass of isotope).

Cell: B6

Comment: Emma Parker:
Did not include due to an insignificant quantity. The cut off is E-05.

Cell: K18

Comment: STOCKMANH:
yes, should be 239, but eq6 uses 244 internally

Cell: B24

Comment: Emma Parker:
Did not include due to limited thermodynamic data and in order to limit the number of elements in the simplified fuel composition, to enable EQ6 to run smoothly.

Cell: B27

Comment: STOCKMANH:
No significant Cm in thermo database

Cell: B34

Comment: Emma Parker:
Did not include due to an insignificant quantity. The cut off is E-05.

Cell: B35

Comment: Emma Parker:
Did not include due to an insignificant quantity. The cut off is E-05.

Cell: B37

Comment: Emma Parker:
Did not include due to an insignificant quantity. The cut off is E-05.

Cell: B38

Comment: Emma Parker:
Did not include due to an insignificant quantity. The cut off is E-05.

Cell: B39

Comment: STOCKMANH:
assume escapes and is inert

Cell: B44

Comment: Emma Parker:
Included with REE below (modeled as Gd).

Cell: B46

Comment: Emma Parker:
Did not include due to limited thermodynamic data and in order to limit the number of elements in the simplified fuel composition, to enable EQ6 to run smoothly.

Cell: J47

Comment: STOCKMANH:
zerovalent in Pd-Rh-Ru-Mo-Tc nuggets

Cell: J48

Comment: STOCKMANH:
zerovalent in Pd-Rh-Ru-Mo-Tc nuggets

Cell: H50

Comment: STOCKMANH:
Include Ru, Rh, Pd, and Ag

Cell: B58

Comment: STOCKMANH:
Like Kr, assume lost or inert

Idealized summary to 4 decimal places, for fuel mwt defined as 100 g.

Elem.ideal	moles	moles, 4 place	eqpt wt. (data0.yml)	g. exact	g. from 4 place	basis species
U		3.6170E-01	0.3617	238.0289	8.6095E-01	UO ₂ **
Np		9.3516E-04	0.0009	237	2.2163E-01	Np****
Pu		2.6952E-03	0.0027	244	6.5769E-01	Pu****
Zr		5.3552E-04	0.0005	91.224	4.8852E-02	ZrO**
Mo		8.5711E-04	0.0009	95.94	8.2231E-02	MoO ₄ **
Tc		8.2715E-04	0.0008	98	8.1666E-02	TcO ₄ **
Ru		2.0113E-03	0.0020	101.07	2.0329E-01	RuO ₄ **
Cs		1.1804E-03	0.0012	132.90545	1.5402E-01	Cs*
Ba		1.0090E-03	0.0010	137.327	1.3857E-01	Ba**
Gd		3.4793E-03	0.0035	144.24	5.0198E-01	Gd****
O		7.3854E-01	0.7385	15.9904	1.1816E-01	H ₂ O or O ₂
			sum mwt=>		100	100.01

Equation to be in the form of



Charge balance

charge (right) 0.7460 = hh → 0.3617*(2) + 0.0009*(4) + 0.0027*(4) + 0.0005*(2) + 0.0009*(1) + 0.0020*(2) + 0.0013*(1) + 0.0010*(2) + 0.0035*(0)

water (right) 0.3720 = ww → hh * 0.5

oxygen gas 0.1866 = oo → ww * 0.5 + 0.5 * (O_R - O_L) → see below (O Balance)

*** Need "charge (right)" to be divisible by 4 without exceeding 4 decimal places (for eqpt to parse), adjusted moles of Cs

0.0001 = cs_inc

increasing the Cs by 0.0001 does the trick!

O Balance

O left side: 0.7385 = O_L

O right side

0.7387 = O_R

=> 0.3617*(2)+0.0009*(4)+0.0027*(4)+0.0005*(2)+0.0009*(1)+0.0020*(2)+0.0013*(1)+0.0010*(2)+0.0035*(0)

Eq6 Input Assumptions

10.02 Density fuel calculated in "CSNF WP.xls", tab "Volumes and Surface Areas"
9.981 Molar volume for eq6

Data0 input

```

-----below is section to add under solids in data0 file-----
CSNF_35at40_10K Complex
  sp_type = solid idealized
  ( )
  * mol.wt. = 100.010 g/mol
  VDP:Tr = 9.9810 cm**3/mol [source: 100.01/10.412]
  ****
  11 element(s):
    0.7385 O          0.0009 Zr          0.0013 Cs
    0.3617 U          0.0009 Mo          0.0010 Ba
    0.0009 Np         0.0008 Tc          0.0035 Gd
    0.0027 Pu         0.0020 Ru
  ****
  14 species in aqueous dissociation reaction:
  -1.0000 CSNF_35at40_10K          0.0020 RuO4--
  -0.3617 O2++                    0.0013 Cs+
  0.0009 Np++++                    0.0010 Ba++
  0.0027 Pu++++                    0.0035 Gd+++
  0.0005 ZrO++                     0.3730 H2O
  0.0009 MoO4--                    -0.1866 O2(g)
  0.0008 TcO4-                     -0.7460 H+
  *
  **** logK grid [0-25-60-100C 81.0132bar; 150-200-250-300C 8Paat-H2O]:
    500.0000 500.0000 500.0000 500.0000
    500.0000 500.0000 500.0000 500.0000
  ****
  * Note we use a large K of 50 to ensure solid is never stable
  
```

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Cell: C27
STOCKMANH
Comment: See 4 place Cs entry above

This sheet considers the elements that are considered Principal Isotopes in the Topical report, p. 3-30.
 The elements included on this page are the Principal isotopes that are not included in the fuel listed under tab "Simplified Fuel Composition"

Values come from CAL-UDC-NU-000006 REV00, Case 10 from Table III-1, LPM1, 3.5% enrichment 40 GWd/mtU

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			gram-atoms	mols idealized	O factor	at. wt. Data0.ymp	mass	mols. 100g	
Th	90232		1.87E-04						
Pa	91233		9.27E-09						
U	92233	233.039522	8.12E-04						
U	92234	234.040904	4.33E-02						
U	92235	235.043915	1.15E+00						
U	92236	236.045637	7.14E-01						
U	92237		7.06E-15						
U	92238	238.05077	1.02E+02						
Np	93235		0.00E+00						
Np	93236		0.00E+00						
Np	93236		1.22E-07						
Np	93237	237.048056	2.68E-01						
Np	93238		7.17E-33						
Pu	94237		0.00E+00						
Pu	94238	238.049511	5.30E-26						
Pu	94239	239.052146	5.93E-01						
Pu	94240	240.053882	1.07E-01						
Pu	94241	241.056737	2.29E-07						
Pu	94242	242.058725	7.39E-02						
Am	95241	241.056714	6.94E-06						
Am	95242	242.059502	3.88E-26						
Am	95243	243.061367	7.62E-03						
Cm	96242		1.01E-28						
Cm	96243		0.00E+00						
Cm	96244		0.00E+00						
Cm	96245		1.36E-04						
Cm	96246		9.64E-06						
Cm	96247		8.95E-07						
Cm	96248		1.00E-07						
H	1003		0.00E+00						
Li	3006	6.0151247	9.82E-07						
Li	3007	7.0160039	4.55E-08						
Be	4009	9.0121855	6.80E-08						
As	33075	74.9215964	4.66E-05						
Kr	36080		2.36E-08						
Kr	36082		2.91E-04						
Kr	36083		1.49E-02						
Kr	36084		4.16E-02						
Kr	36086		6.46E-02						
Y	39089		1.55E-01						
Zr	40093	91.22	1.54E-01						
Nb	41093	92.906382	6.98E-04						
Mo	42095	94.905839	2.46E-01						
Tc	43099	98.90627501	2.37E-01						
Ru	44101	100.905576	2.37E-01						
Am				7.62E-03	2		243	1.85E+00	0.0065

Cell: J6

Comment: STOCKMANH:

number of oxygens associated with each mole of element. NOTE that usually, O content of U,Pu,Np exceeds 2 per metal, as burnup proceeds.

Cell: K6

Comment: STOCKMANH:

We use the datao.ymp atomic weight, since we are only interested in the mols, and wan't eq6 to calculate moles from weight consistently

Cell: B7

Comment: Emma Parker:

Did not include due to limited thermodynamic data and in order to limit the number of elements in the simplified fuel composition, to enable EQ6 to run smoothly.

Cell: C7

Comment: Emma Parker:

This number designates the isotope. The first two digits are the element's atomic number, and the last three digits are the isotope number (atomic mass of isotope).

Cell: B8

Comment: Emma Parker:

Did not include due to an insignificant quantity. The cut off is E-05.

Cell: H52

Comment: STOCKMANH:

Include Ru,Rh,Pd, and Ag

Cell: B60

Comment: STOCKMANH:

Like Kr, assume lost or inert

idealized summary to 4 decimal places, for fuel mwt defined as 100 g.

Elem_ideal	mols	mols, 4 place	eq0 at wt. (data0 yme)	g, exact	g, from 4 place	basis species
Am		6.5133E-03	0.0065	243	1.5827E+00	Am ⁺⁺⁺
Rh		1.2736E-01	0.1274	102.9005	1.3108E+01	Rh ⁺⁺⁺
Ag		2.3388E-02	0.0234	107.9682	2.5241E+00	Ag ⁺
Nd		3.3827E-01	0.3383	144.24	4.8792E+01	Nd ⁺⁺⁺
Sm		1.2204E-01	0.1220	150.36	1.8350E+01	Sm ⁺⁺⁺
Eu		2.4863E-02	0.0250	151.964	3.7991E+00	Eu ⁺⁺⁺
O		7.4094E-01	0.7409	15.9994	1.1854E+01	H ₂ O or O ₂
			sum mwt=>		100	100.01

Equation to be in the form of:

Fuel + hh * H⁺ + oo * O₂(g)

→

0.0065 * Am⁺⁺⁺ + 0.1274 * Rh⁺⁺⁺ + 0.0234 * Ag⁺ + 0.3383 * Nd⁺⁺⁺
 + 0.1220 * Sm⁺⁺⁺ + 0.0250 * Eu⁺⁺⁺
 + ww * H₂O

Charge Balance

charge (right)

water (right)

oxygen gas

1.8810 = hh = 0.0065*(3) + 0.1274*(3) + 0.0234*(1) + 0.3383*(3) + 0.1220*(3) + 0.0250*(3)
 0.9405 = ww = hh * 0.5
 0.0998 = oo = ww * 0.5 + 0.5 * (O_R - O_L) --- see below (O Balance)

O Balance

O left side

0.7409 = O_L

O right side

0 = O_R

EQ6 Input Assumptions

10.02 Density fuel calculated in "CSNF WP.xls"; tab "Volumes and Surface Areas"
 9.981 Molar volume for eq6

Data0 Input

====Below is section to add under solids in data0 file=====

Principal_Isotopes Complex

sp.type = solid idealized

[]

* mol.wt. = 100.010 g/mol

V0PrTr = 9.9810 cm³/mol [source: 100.01/10.412]

7 element(s):

0.0065 Am 0.1274 Rh 0.0234 Ag

0.3383 Nd 0.1220 Sm 0.0250 Eu

10 species in aqueous dissociation reaction:

-1.0000 Principal_Isotopes 0.0065 Am⁺⁺⁺

0.1274 Rh⁺⁺⁺ 0.0234 Ag⁺

0.3383 Nd⁺⁺⁺ 0.1220 Sm⁺⁺⁺

0.0250 Eu⁺⁺⁺ 0.9405 H2O

-0.0998 O2(g) -1.8810 H⁺

*

**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:

500.0000 50.0000 500.0000 500.0000

500.0000 500.0000 500.0000 500.0000

* Note we use a large K of 50 to ensure solid is never stable

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Calculate Fraction of CSNF containing principal isotopes not covered in CSNF fuel composition

0.3617 =moles U per mole of CSNF_35640_10K
 3.81E-03 =ratio of moles of Nd in starting fuel to moles of U in starting fuel
 0.3383 =moles Nd per mole of Principal_Isotopes
 4.08E-03 = Moles of Principal_Isotopes per mole of CSNF_35640_10K =
 (moles U per mole CSNF) x (moles Nd per mole U in starting fuel) / (moles Nd per mole Principal_Isotopes)
 This is the value to multiply by the moles and surface area of CSNF_35640_10K to determine
 the number of moles and surface area of Principal_Isotopes for input into EQ6 file for sensitivity run

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