

# Calculation of the radiological term for a PWR Severe Accident using ASTEC

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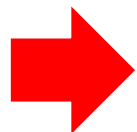
## Motivation

- Determine decay heat from realistic initial FP files
- Compare the capability of FP retention for different release paths
- Deliver realistic source terms for RODOS calculations  
(RODOS calculates the FP distribution outside the containment)

# Prediction of nuclide inventories

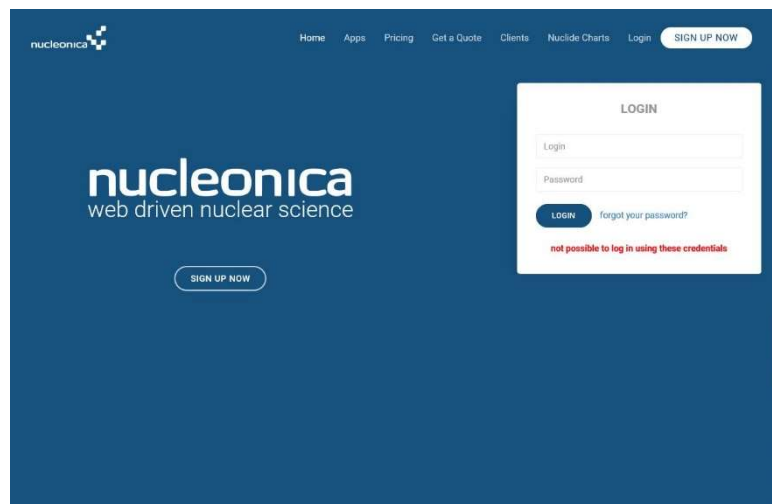
## ASTEC has the capabilities:

- to determine the residual power after the SCRAM from a given initial nuclide file
- to determine the decay chains of the isotopes in the initial nuclide file
- To calculate the transport of the FP in nuclide file through the primary/secondary circuits and the containment after a failure of the fuel rod cladding



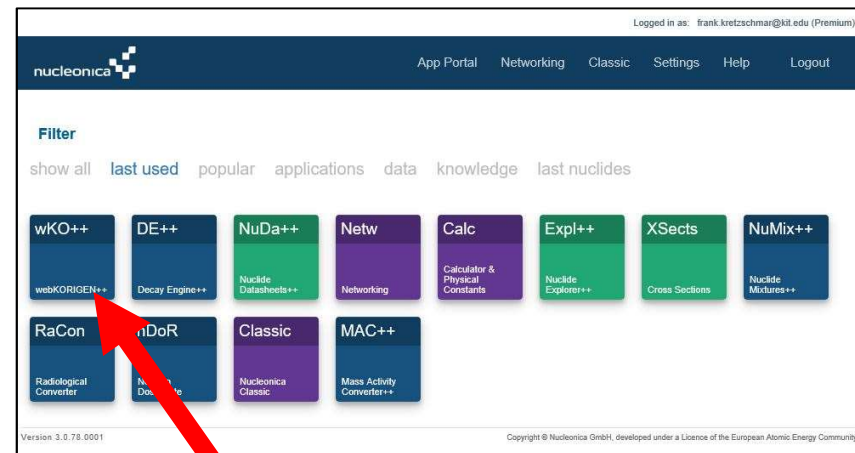
There is a need, to generate a **realistic** initial FP file for ASTEC calculations

# Prediction of nuclide inventories



<https://www.nucleonica.com/>

1 year license costs  $\approx$  600 Euro



webKORIGEN

# Prediction of nuclide inventories

Step 1: Calculation Mode   Step 2: Reactor / Operation   Step 3: Input Summary and Run   Step 4: Display Results   Step 5: Log files

**Reactor type**

PWR  
 BWR  
 EFR

**Reactor Parameters**

Burnup ( $MW_{th} \cdot d / kg_{HM}$ ):

Total initial heavy metal mass ( $t_{HM}$ ):

Electrical efficiency (%):

Derived Power values  
Specific Power: 30.49 MW /  $t_{HM}$   
Thermal Power: 0.13 GW  
Electrical Power: 0.04 GW

**Initial Fuel and Neutron Spectrum**

UOX

MOX

Nuclide	Weight (%)
Pu238/Pu (w/o)	<input type="text" value="2.6"/>
Pu239/Pu (w/o)	<input type="text" value="50.5"/>
Pu240/Pu (w/o)	<input type="text" value="27.8"/>
Pu241/Pu (w/o)	<input type="text" value="11.5"/>
Pu242/Pu (w/o)	<input type="text" value="7.6"/>
Am241/Pu (w/o)	<input type="text" value="1.0"/>

Uranium matrix  
 Natural  
 Depleted

**Irradiation and decay parameters**

No. of cycles:

Length of cycle:  d

Load factor (%):

Cooling time before reprocessing:  y

Decay time after reprocessing:  y

**Reprocessing ratio (%)**

Uranium:

Plutonium:

Neptunium:

Americium:

Curium:

webKORIGEN - input mask



# Prediction of nuclide inventories

## Result of webKORIGEN calculation

webKorigen++: Nuclides during 328 d irradi. of 4.305 tHM PWR UOX

Material quantity over time

	Time(d)	0.00E+00	1.20E+01	7.52E+01	1.38E+02	2.02E+02	2.65E+02	3.28E+02	3.28E+02
Nuclide	MatIndex	Mass (g)							
U238	922380	4.11E+06	4.10E+06	4.10E+06	4.10E+06	4.09E+06	4.09E+06	4.08E+06	4.08E+06
U235	922350	1.98E+05	1.96E+05	1.86E+05	1.77E+05	1.68E+05	1.60E+05	1.52E+05	1.52E+05
Pu239	942390	0.00E+00	5.06E+02	3.90E+03	6.86E+03	9.43E+03	1.17E+04	1.36E+04	1.36E+04
U236	922360	0.00E+00	3.54E+02	2.17E+03	3.89E+03	5.53E+03	7.08E+03	8.57E+03	8.57E+03
Xe136	541360	0.00E+00	9.44E+01	6.06E+02	1.12E+03	1.64E+03	2.16E+03	2.68E+03	2.68E+03
Xe134	541340	0.00E+00	7.14E+01	4.51E+02	8.30E+02	1.21E+03	1.59E+03	1.96E+03	1.96E+03
Ba138	561380	0.00E+00	6.42E+01	4.03E+02	7.40E+02	1.08E+03	1.41E+03	1.74E+03	1.74E+03
Pu240	942400	0.00E+00	2.82E+00	1.41E+02	4.23E+02	7.95E+02	1.23E+03	1.70E+03	1.70E+03
La139	571390	0.00E+00	6.16E+01	3.88E+02	7.12E+02	1.03E+03	1.35E+03	1.67E+03	1.67E+03
Cs137	551370	0.00E+00	5.94E+01	3.73E+02	6.84E+02	9.95E+02	1.30E+03	1.61E+03	1.61E+03
Ce140	581400	0.00E+00	1.12E+01	2.87E+02	6.13E+02	9.39E+02	1.26E+03	1.59E+03	1.59E+03
Cs133	551330	0.00E+00	2.69E+01	3.36E+02	6.53E+02	9.67E+02	1.28E+03	1.58E+03	1.58E+03
Ce142	581420	0.00E+00	5.62E+01	3.54E+02	6.51E+02	9.45E+02	1.24E+03	1.53E+03	1.53E+03
Nd143	601430	0.00E+00	1.09E+01	2.63E+02	5.55E+02	8.38E+02	1.11E+03	1.38E+03	1.38E+03
U234	922340	1.51E+03	1.50E+03	1.47E+03	1.44E+03	1.41E+03	1.38E+03	1.35E+03	1.35E+03
Pr141	591410	0.00E+00	6.59E+00	1.79E+02	4.45E+02	7.34E+02	1.03E+03	1.32E+03	1.32E+03
Mo100	421000	0.00E+00	4.08E+01	2.57E+02	4.74E+02	6.91E+02	9.09E+02	1.13E+03	1.13E+03
Tc99	430990	0.00E+00	2.90E+01	2.51E+02	4.73E+02	6.91E+02	9.08E+02	1.12E+03	1.12E+03
Xe132	541320	0.00E+00	2.53E+01	2.35E+02	4.50E+02	6.68E+02	8.91E+02	1.12E+03	1.12E+03
Zr96	400960	0.00E+00	4.18E+01	2.61E+02	4.77E+02	6.92E+02	9.05E+02	1.12E+03	1.12E+03
Zr94	400940	0.00E+00	4.18E+01	2.61E+02	4.76E+02	6.89E+02	9.00E+02	1.11E+03	1.11E+03
Mo98	420980	0.00E+00	3.97E+01	2.49E+02	4.59E+02	6.70E+02	8.80E+02	1.09E+03	1.09E+03
Zr93	400930	0.00E+00	3.82E+01	2.49E+02	4.55E+02	6.58E+02	8.57E+02	1.05E+03	1.05E+03
Nd145	601450	0.00E+00	3.83E+01	2.44E+02	4.47E+02	6.45E+02	8.41E+02	1.03E+03	1.03E+03
Mo97	420970	0.00E+00	3.44E+01	2.33E+02	4.31E+02	6.27E+02	8.22E+02	1.02E+03	1.02E+03
Ru101	441010	0.00E+00	3.64E+01	2.30E+02	4.24E+02	6.19E+02	8.14E+02	1.01E+03	1.01E+03
Ce144	581440	0.00E+00	5.32E+01	3.07E+02	5.21E+02	7.01E+02	8.52E+02	9.79E+02	9.79E+02
Zr92	400920	0.00E+00	3.65E+01	2.32E+02	4.24E+02	6.12E+02	7.96E+02	9.76E+02	9.76E+02
Sr90	380900	0.00E+00	3.57E+01	2.20E+02	3.97E+02	5.70E+02	7.36E+02	8.99E+02	8.99E+02
Zr91	400910	0.00E+00	2.64E+00	7.75E+01	2.11E+02	3.70E+02	5.39E+02	7.10E+02	7.10E+02
Ru102	441020	0.00E+00	2.40E+01	1.52E+02	2.83E+02	4.15E+02	5.50E+02	6.86E+02	6.86E+02
Mo95	420950	0.00E+00	2.00E-01	3.15E+01	1.31E+02	2.83E+02	4.65E+02	6.61E+02	6.61E+02
Cs135	551350	0.00E+00	2.35E+01	1.52E+02	2.79E+02	4.04E+02	5.27E+02	6.50E+02	6.50E+02
Pu241	942410	0.00E+00	2.83E+01	1.75E+02	3.45E+02	5.09E+02	6.84E+02	8.56E+02	8.56E+02

not in list for decay heat

webKorigen++: Nuclides during 328 d irradi. of 4.305 tHM PWR UOX

Material quantity over time

	Time(d)	0.00E+00	1.20E+01	7.52E+01	1.38E+02	2.02E+02	2.65E+02	3.28E+02	3.28E+02
Nuclide	MatIndex	Decay heat (W)							
U238	922380	1.05E-01	1.05E-01	1.05E-01	1.05E-01	1.04E-01	1.04E-01	1.04E-01	1.04E-01
U235	922350	3.46E-02	3.43E-02	3.26E-02	3.10E-02	2.94E-02	2.79E-02	2.65E-02	2.65E-02
Pu239	942390	0.00E+00	2.93E+00	2.25E+01	3.96E+01	5.45E+01	6.74E+01	7.87E+01	7.87E+01
U236	922360	0.00E+00	1.84E-03	1.13E-02	2.02E-02	2.87E-02	3.68E-02	4.45E-02	4.45E-02
Xe136	541360	0.00E+00	3.46E-17	2.22E-16	4.10E-16	6.00E-16	7.90E-16	9.82E-16	9.82E-16
Xe134	541340	0.00E+00	1.70E-13	1.08E-12	1.98E-12	2.88E-12	3.78E-12	4.68E-12	4.68E-12
Pu240	942400	0.00E+00	5.97E-02	2.98E+00	8.95E+00	1.68E+01	2.60E+01	3.59E+01	3.59E+01
Cs137	551370	0.00E+00	1.15E+01	7.20E+01	1.32E+02	1.92E+02	2.52E+02	3.12E+02	3.12E+02
Ce142	581420	0.00E+00	4.75E-14	3.00E-13	5.50E-13	7.99E-13	1.05E-12	1.29E-12	1.29E-12
U234	922340	8.07E-01	8.04E-01	7.88E-01	7.72E-01	7.56E-01	7.40E-01	7.24E-01	7.24E-01
Mo100	421000	0.00E+00	5.29E-16	3.33E-15	6.15E-15	8.97E-15	1.18E-14	1.46E-14	1.46E-14
Tc99	430990	0.00E+00	4.95E-04	4.29E-03	8.07E-03	1.18E-02	1.55E-02	1.92E-02	1.92E-02
Zr96	400960	0.00E+00	1.58E-16	9.89E-16	1.81E-15	2.62E-15	3.43E-15	4.23E-15	4.23E-15
Zr94	400940	0.00E+00	3.59E-13	2.24E-12	4.09E-12	5.92E-12	7.73E-12	9.52E-12	9.52E-12
Mo98	420980	0.00E+00	1.92E-12	1.21E-11	2.22E-11	3.24E-11	4.26E-11	5.28E-11	5.28E-11
Zr93	400930	0.00E+00	2.19E-05	1.42E-04	2.60E-04	3.76E-04	4.91E-04	6.03E-04	6.03E-04
Ce144	581440	0.00E+00	2.02E+02	1.17E+03	1.98E+03	2.66E+03	3.24E+03	3.72E+03	3.72E+03
Sr90	380900	0.00E+00	1.01E+01	6.25E+01	1.13E+02	1.62E+02	2.10E+02	2.56E+02	2.56E+02
Cs135	551350	0.00E+00	2.87E-05	1.86E-04	3.40E-04	4.92E-04	6.43E-04	7.92E-04	7.92E-04
Pu241	942410	0.00E+00	2.54E-04	9.00E-02	4.95E-01	1.32E+00	2.55E+00	4.16E+00	4.16E+00
Nd144	601440	0.00E+00	3.04E-14	1.20E-12	3.95E-12	8.05E-12	1.33E-11	1.97E-11	1.97E-11
Pm147	611470	0.00E+00	4.70E+00	7.46E+01	1.46E+02	2.10E+02	2.67E+02	3.18E+02	3.18E+02
Nd148	601480	0.00E+00	3.44E-16	2.17E-15	3.98E-15	5.78E-15	7.58E-15	9.38E-15	9.38E-15
Rb87	370870	0.00E+00	1.25E-09	7.78E-09	1.41E-08	2.03E-08	2.63E-08	3.22E-08	3.22E-08
Np237	932370	0.00E+00	1.37E-04	2.24E-03	5.35E-03	9.28E-03	1.40E-02	1.93E-02	1.93E-02
Zr95	400950	0.00E+00	4.96E+03	2.25E+04	3.12E+04	3.53E+04	3.72E+04	3.79E+04	3.79E+04
Te130	521300	0.00E+00	8.97E-22	5.73E-21	1.07E-20	1.57E-20	2.09E-20	2.61E-20	2.61E-20
Y91	390910	0.00E+00	5.66E+03	2.59E+04	3.49E+04	3.86E+04	3.98E+04	4.00E+04	4.00E+04
Np239	932390	0.00E+00	1.89E+05	1.99E+05	2.04E+05	2.08E+05	2.12E+05	2.16E+05	2.16E+05
Ce141	581410	0.00E+00	3.45E+03	1.24E+04	1.46E+04	1.51E+04	1.52E+04	1.52E+04	1.52E+04
Nd150	601500	0.00E+00	3.22E-17	2.04E-16	3.80E-16	5.58E-16	7.39E-16	9.22E-16	9.22E-16
I129	531290	0.00E+00	6.22E-07	4.92E-06	9.92E-06	1.52E-05	2.06E-05	2.61E-05	2.61E-05
Nb95	410950	0.00E+00	4.85E+02	1.05E+04	2.07E+04	2.71E+04	3.06E+04	3.24E+04	3.24E+04
Ce90	380900	0.00E+00	5.23E-03	2.22E-02	3.87E-02	5.20E-02	6.45E-02	7.45E-02	7.45E-02

Nuclide masses

Nuclide decay heats

# Prediction of nuclide inventories

Keminventar											
Brennelement-Typ		Anzahl	Masse (kg) pro frischem Brennelement								
			Uran 234	Uran 235	Uran 238	Pu 238	Pu 239	Pu 240	Pu 241	Pu 242	Am 241
U-BE		48	0.2266	24.7572	513.2162	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
U-Gd-BE		81	0.218	23.8012	507.8808	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MOX		64	0	1.1490	498.4145	0.5418	21.5302	9.0878	2.8487	1.8692	0.3588
ursprünglich frische Masse, die schon eine gewisse Anzahl an Zyklen durchlaufen haben											
Anzahl Zyklen	Brennelement-Typ	Anzahl	Masse (kg) pro frischem Brennelement								
			Uran 234	Uran 235	Uran 238	Pu 238	Pu 239	Pu 240	Pu 241	Pu 242	Am 241
1	U-BE	8	1.8128	198.0576	4105.7296	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	U-Gd-BE	16	3.4880	380.8192	8126.0928	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	MOX	16	0.0000	18.3840	7974.6320	8.6688	344.4832	145.4048	45.5792	29.9072	5.7408
2	U-BE	8	1.8128	198.0576	4105.7296	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	U-Gd-BE	16	3.4880	380.8192	8126.0928	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	MOX	16	0.0000	18.3840	7974.6320	8.6688	344.4832	145.4048	45.5792	29.9072	5.7408
3	U-BE	8	1.8128	198.0576	4105.7296	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	U-Gd-BE	16	3.4880	380.8192	8126.0928	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	MOX	16	0.0000	18.3840	7974.6320	8.6688	344.4832	145.4048	45.5792	29.9072	5.7408
4	U-BE	8	1.8128	198.0576	4105.7296	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	U-Gd-BE	16	3.4880	380.8192	8126.0928	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	MOX	16	0.0000	18.3840	7974.6320	8.6688	344.4832	145.4048	45.5792	29.9072	5.7408
5	U-BE	8	1.8128	198.0576	4105.7296	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	U-Gd-BE	16	3.4880	380.8192	8126.0928	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	MOX	0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6	U-BE	8	1.8128	198.0576	4105.7296	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	U-Gd-BE	1	0.2180	23.8012	507.8808	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	MOX	0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

## Example Core inventory of a generic German PWR

# Prediction of nuclide inventories

							1. cycle					
U-BE							U-Gd-BE					
Name	Value Mass	Sum Mass	Part Mass	Decay value	Sum Decay	Part Decay	Name	Value Mass	Sum Mass	Part Mass	Dec	
4	U238	4,082293E+03	4,082293E+03	9,478301E-01	1,041790E-01	1,041790E-01	8,464427E-09	U238	8,079726E+03	8,079726E+03	9,496645E-01	2,04
5	U235	1,517502E+02	4,234043E+03	9,830636E-01	2,651765E-02	1,306967E-01	1,061896E-08	U235	2,899798E+02	8,369706E+03	9,837478E-01	5,06
6	Pu239	1,362027E+01	4,247663E+03	9,862260E-01	7,866387E+01	7,879457E+01	6,401970E-06	Pu239	2,735722E+01	8,397063E+03	9,869633E-01	1,58
7	U236	8,567809E+00	4,256231E+03	9,882152E-01	4,452970E-02	7,883910E+01	6,405588E-06	U236	1,680773E+01	8,413871E+03	9,889388E-01	8,73
8	Xe136	2,682749E+00	4,258914E+03	9,888381E-01	9,815427E-10	7,883910E+01	6,405588E-06	Xe136	5,323584E+00	8,419194E+03	9,895645E-01	1,94
9	Xe134	1,961616E+00	4,260876E+03	9,892936E-01	4,678675E-06	7,883910E+01	6,405589E-06	Xe134	3,876591E+00	8,423071E+03	9,900202E-01	9,24
10	Ba138	1,742369E+00	4,262618E+03	9,896981E-01	0,000000E+00	7,883910E+01	6,405589E-06	Pu240	3,467758E+00	8,426539E+03	9,904277E-01	7,33
11	Pu240	1,695948E+00	4,264314E+03	9,900919E-01	3,588870E+01	1,147278E+02	9,321505E-06	Ba138	3,441744E+00	8,429980E+03	9,908323E-01	0,00
12	La139	1,669579E+00	4,265984E+03	9,904795E-01	0,000000E+00	1,147278E+02	9,321505E-06	La139	3,297214E+00	8,433278E+03	9,912198E-01	0,00
13	Cs137	1,612618E+00	4,267596E+03	9,908540E-01	3,118097E+02	4,265375E+02	3,465569E-05	Cs137	3,187598E+00	8,436465E+03	9,915945E-01	6,16
14	Ce140	1,585246E+00	4,269181E+03	9,912220E-01	0,000000E+00	4,265375E+02	3,465569E-05	Ce140	3,130822E+00	8,439596E+03	9,919625E-01	0,00
15	Cs133	1,582724E+00	4,270764E+03	9,915895E-01	0,000000E+00	4,265375E+02	3,465569E-05	Cs133	3,126891E+00	8,442723E+03	9,923300E-01	0,00
16	Ce142	1,528391E+00	4,272293E+03	9,919444E-01	1,292041E-06	4,265375E+02	3,465569E-05	Ce142	3,018330E+00	8,445741E+03	9,926848E-01	2,55
17	Nd143	1,376237E+00	4,273669E+03	9,922639E-01	0,000000E+00	4,265375E+02	3,465569E-05	Nd143	2,712552E+00	8,448454E+03	9,930036E-01	0,00
18	U234	1,351458E+00	4,275020E+03	9,925777E-01	7,239860E-01	4,272615E+02	3,471452E-05	Pr141	2,607971E+00	8,451062E+03	9,933101E-01	0,00
19	Pr141	1,320298E+00	4,276341E+03	9,928842E-01	0,000000E+00	4,272615E+02	3,471452E-05	U234	2,592224E+00	8,453654E+03	9,936148E-01	1,38
20	Mo100	1,128088E+00	4,277469E+03	9,931461E-01	1,464697E-08	4,272615E+02	3,471452E-05	Mo100	2,230618E+00	8,455885E+03	9,938770E-01	2,89
21	Tc99	1,122151E+00	4,278591E+03	9,934067E-01	1,916519E-02	4,272807E+02	3,471607E-05	Tc99	2,216858E+00	8,458102E+03	9,941375E-01	3,78
22	Xe132	1,117774E+00	4,279709E+03	9,936662E-01	0,000000E+00	4,272807E+02	3,471607E-05	Xe132	2,213340E+00	8,460315E+03	9,943977E-01	0,00
23	Zr96	1,115963E+00	4,280824E+03	9,939253E-01	4,230908E-09	4,272807E+02	3,471607E-05	Zr96	2,203259E+00	8,462518E+03	9,946566E-01	8,35
24	Zr94	1,107640E+00	4,281932E+03	9,941825E-01	9,515857E-06	4,272807E+02	3,471608E-05	Zr94	2,185186E+00	8,464703E+03	9,949135E-01	1,87
25	Mo98	1,089951E+00	4,283022E+03	9,944356E-01	5,277648E-05	4,272807E+02	3,471608E-05	Mo98	2,154659E+00	8,466858E+03	9,951667E-01	1,04
26	Zr93	1,053678E+00	4,284076E+03	9,946802E-01	6,030526E-04	4,272813E+02	3,471613E-05	Zr93	2,078055E+00	8,468936E+03	9,954110E-01	1,18
27	Nd145	1,032408E+00	4,285108E+03	9,949199E-01	0,000000E+00	4,272813E+02	3,471613E-05	Nd145	2,037397E+00	8,470973E+03	9,956505E-01	0,00
28	Mo97	1,016073E+00	4,286124E+03	9,951558E-01	0,000000E+00	4,272813E+02	3,471613E-05	Mo97	2,006821E+00	8,472980E+03	9,958863E-01	0,00
29	Ru101	1,009300E+00	4,287134E+03	9,953902E-01	0,000000E+00	4,272813E+02	3,471613E-05	Ru101	1,996874E+00	8,474977E+03	9,961210E-01	0,00
30	Ce144	9,794143E-01	4,288113E+03	9,956176E-01	3,719745E+03	4,147026E+03	3,369412E-04	Ce144	1,932099E+00	8,476909E+03	9,963481E-01	7,33
31	Zr92	9,763533E-01	4,289089E+03	9,958442E-01	0,000000E+00	4,147026E+03	3,369412E-04	Zr92	1,924309E+00	8,478834E+03	9,965743E-01	0,00
32	Sr90	8,985841E-01	4,289988E+03	9,960529E-01	2,556823E+02	4,402709E+03	3,577151E-04	Sr90	1,769090E+00	8,480603E+03	9,967822E-01	5,03
33	Zr91	7,104881E-01	4,290698E+03	9,962178E-01	0,000000E+00	4,402709E+03	3,577151E-04	Zr91	1,400241E+00	8,482003E+03	9,969468E-01	0,00
34	Ru102	6,864954E-01	4,291385E+03	9,963772E-01	0,000000E+00	4,402709E+03	3,577151E-04	Ru102	1,360104E+00	8,483363E+03	9,971067E-01	0,00
35	Mo95	6,613657E-01	4,292046E+03	9,965308E-01	0,000000E+00	4,402709E+03	3,577151E-04	Pu241	1,308260E+00	8,484671E+03	9,972604E-01	8,68
36	Cs135	6,495483E-01	4,292696E+03	9,966816E-01	7,921756E-04	4,402709E+03	3,577152E-04	Mo95	1,305303E+00	8,485977E+03	9,974139E-01	0,00
37	Pu241	6,257883E-01	4,293322E+03	9,968269E-01	4,156209E+00	4,406866E+03	3,580529E-04	Cs135	1,265787E+00	8,487242E+03	9,975626E-01	1,54
38	Nd146	5,955485E-01	4,293917E+03	9,969652E-01	0,000000E+00	4,406866E+03	3,580529E-04	Nd146	1,177755E+00	8,488420E+03	9,977011E-01	0,00
39	Y89	5,780540E-01	4,294495E+03	9,970994E-01	0,000000E+00	4,406866E+03	3,580529E-04	Y89	1,138634E+00	8,489559E+03	9,978349E-01	0,00
40	Nd144	5,361983E-01	4,295031E+03	9,972239E-01	1,968146E-05	4,406866E+03	3,580529E-04	Nd144	1,062214E+00	8,490621E+03	9,979598E-01	3,89
41	Sr88	5,357080E-01	4,295567E+03	9,973483E-01	0,000000E+00	4,406866E+03	3,580529E-04	Sr88	1,054927E+00	8,491676E+03	9,980837E-01	0,00
42	Rh103	5,189093E-01	4,296086E+03	9,974687E-01	0,000000E+00	4,406866E+03	3,580529E-04	Rh103	1,029167E+00	8,492705E+03	9,982047E-01	0,00
43	Xe131	4,846971E-01	4,296571E+03	9,975813E-01	0,000000E+00	4,406866E+03	3,580529E-04	Xe131	9,587256E-01	8,493664E+03	9,983174E-01	0,00



# Prediction of nuclide inventories

1. cycle											
U-BE							U-Gd-BE				
	Name	Value Mass	Sum Mass	Part Mass	Decay value	Sum Decay	Part Decay	Name	Value Mass	Sum Mass	Part Mass
46	Nd148	4,586229E-01	4,297962E+03	9,979044E-01	9,375266E-09	4,725043E+03	3,839044E-04	Nd148	9,067412E-01	8,496421E+03	9,986414E-01
47	Rb87	3,846243E-01	4,298347E+03	9,979937E-01	3,221962E-02	4,725075E+03	3,839071E-04	Rb87	7,574330E-01	8,497178E+03	9,987305E-01
48	Np237	3,152382E-01	4,298662E+03	9,980669E-01	1,931970E-02	4,725094E+03	3,839086E-04	Np237	6,347665E-01	8,497813E+03	9,988051E-01
49	Zr95	3,064944E-01	4,298969E+03	9,981381E-01	3,793030E+04	4,265539E+04	3,465703E-03	Zr95	6,045485E-01	8,498417E+03	9,988761E-01
50	Sm150	<del>3,022871E-01</del>	<del>4,299271E+03</del>	<del>9,982083E-01</del>	<del>0,000000E+00</del>	<del>4,265539E+04</del>	<del>3,465703E-03</del>	Pd105	6,028763E-01	8,499020E+03	9,989470E-01
51	Pd105	<del>3,005399E-01</del>	<del>4,299572E+03</del>	<del>9,982781E-01</del>	<del>0,000000E+00</del>	<del>4,265539E+04</del>	<del>3,465703E-03</del>	Sm150	5,993716E-01	8,499620E+03	9,990174E-01
52	Kr86	2,947507E-01	4,299866E+03	9,983465E-01	0,000000E+00	4,265539E+04	3,465703E-03	U239	3,116572E-03	8,499623E+03	9,990178E-01
53	Te130	2,505613E-01	4,300117E+03	9,984047E-01	2,612602E-14	4,265539E+04	3,465703E-03	Y96	5,521231E-07	8,499623E+03	9,990178E-01
54	Y91	2,262699E-01	4,300343E+03	9,984572E-01	3,995438E+04	8,260977E+04	6,711952E-03	Np239	4,499133E-01	8,500073E+03	9,990707E-01
55	Np239	2,223358E-01	4,300566E+03	9,985088E-01	2,161024E+05	2,987122E+05	2,427003E-02	Rb92	3,301515E-07	8,500073E+03	9,990707E-01
56	Ce141	2,174200E-01	4,300783E+03	9,985593E-01	1,516874E+04	3,138809E+05	2,550247E-02	Cs140	9,533895E-06	8,500073E+03	9,990707E-01
57	Nd150	2,037530E-01	4,300987E+03	9,986066E-01	9,224695E-10	3,138809E+05	2,550247E-02	Cs138	3,415858E-04	8,500073E+03	9,990707E-01

not in U-Gd-BE

In line 748 of U-Gd-BE

Process of ordering, summarizing masses and decay heats and referring masses to decay heats must be automatized!

# Prediction of nuclide inventories



EXCEL procedure written  
to bring the information from  
webKORIGEN calculations in  
a usable form

# Prediction of nuclide inventories

BQ842

Name:		1 cycl U-BE				1 cycl U-Gd-BE				1 cycl MOX-BE				2 cycl U-BE			
therm. Power (W):		1.30E+08				2.60E+08				2.60E+08				1.30E+08			
		Mass		Decay Heat		Mass		Decay Heat		Mass		Decay Heat		Mass		Decay Heat	
		Name	Value (kg)	Name	Value (W)	Name	Value (kg)	Name	Value (W)	Name	Value (kg)	Name	Value (W)	Name	Value (kg)	Name	Value (W)
Sum of Column:		4303.77		1.230734E+07		8507.98		2.432929E+07		8569.84		2.169317E+07		4303.09		1.208562E+07	
Total Mass (kg):		103110.89															
Total thermal Power (W):		3.140E+09															
Total Decay Heat (W):		2.822E+08															

Inventory Output

Name:		1 cycl U-BE				1 cycl U-Gd-BE				1 cycl MOX-BE				2 cycl U-BE			
therm. Power (W):		1.30E+08				2.60E+08				2.60E+08				1.30E+08			
		Mass		Decay Heat		Mass		Decay Heat		Mass		Decay Heat		Mass		Decay Heat	
		Name	Value (kg)	Name	Value (W)	Name	Value (kg)	Name	Value (W)	Name	Value (kg)	Name	Value (W)	Name	Value (kg)	Name	Value (W)
Sum of Column:		4303.77		1.230734E+07		8507.98		2.432929E+07		8569.84		2.169317E+07		4303.09		1.208562E+07	
Sn113		3.437281E-25				Sn113		8.184294E-25		Po212		6.047705E-24		Tc95m		5.419691E-24	
Tc95		8.665400E-26				Tc95		1.884546E-25		Sn113m		2.227619E-24		Tc95		8.404183E-25	
Po214		4.264708E-26				Po214		8.183508E-26						Po214		1.732853E-25	
						Po213		3.385954E-26						Po213		8.558814E-26	
														In113m		4.914998E-26	



# Prediction of nuclide inventories

F20									
1.06289785E-12									
	A	B	C	D	E	F	G	H	I
	Name	Mass (kg)	Mass/Total Mass	Sum Mass (kg)	Sum Mass/Total Mass	Decay (W)	Sum Decay (W)	Sum Decay/Total Decay	
2	U238	9.608549E+04	8.213267E-01	96085.49	8.213267E-01	2.451196E+00	2.451196E+00	8.685876E-09	
3	O16	1.387726E+04	1.186211E-01	109962.75	9.399478E-01	0.000000E+00	2.451196E+00	8.685876E-09	
4	U235	1.321980E+03	1.130012E-02	111284.73	9.512479E-01	2.310798E-01	2.682276E+00	9.504713E-09	
5	Pu239	1.096675E+03	9.374242E-03	112381.41	9.606221E-01	6.336212E+03	6.338895E+03	2.246203E-05	
6	Pu240	6.103860E+02	5.217503E-03	112991.79	9.658396E-01	1.291344E+04	1.925233E+04	6.822113E-05	
7	Pu241	3.154883E+02	2.696754E-03	113307.28	9.685364E-01	2.096483E+03	2.134881E+04	7.565007E-05	
8	U236	3.072914E+02	2.626688E-03	113614.57	9.711631E-01	1.597834E+00	2.135041E+04	7.565573E-05	
9	Xe136	1.928484E+02	1.648444E-03	113807.42	9.728115E-01	7.051535E-14	2.135041E+04	7.565573E-05	
10	Pu242	1.531935E+02	1.309479E-03	113960.62	9.741210E-01	5.366846E+01	2.140408E+04	7.584591E-05	
11	Xe134	1.362575E+02	1.164712E-03	114096.87	9.752857E-01	3.250856E-10	2.140408E+04	7.584591E-05	
12	Ba138	1.181051E+02	1.009548E-03	114214.98	9.762953E-01	0.000000E+00	2.140408E+04	7.584591E-05	
13	Cs137	1.108835E+02	9.478178E-04	114325.86	9.772431E-01	2.141810E+04	4.282218E+04	1.517415E-04	
14	Ce140	1.105628E+02	9.450773E-04	114436.42	9.781882E-01	0.000000E+00	4.282218E+04	1.517415E-04	
15	La139	1.090943E+02	9.325241E-04	114545.52	9.791207E-01	0.000000E+00	4.282218E+04	1.517415E-04	
16	Cs133	1.034018E+02	8.838660E-04	114648.92	9.800046E-01	0.000000E+00	4.282218E+04	1.517415E-04	
17	Ce142	1.017803E+02	8.700048E-04	114750.70	9.808746E-01	8.613589E-11	4.282218E+04	1.517415E-04	
18	Pr141	9.696459E+01	8.288411E-04	114847.67	9.817034E-01	0.000000E+00	4.282218E+04	1.517415E-04	
19	Xe132	9.210600E+01	7.873105E-04	114939.77	9.824907E-01	0.000000E+00	4.282218E+04	1.517415E-04	
20	Mo100	8.187488E+01	6.998561E-04	115021.65	9.831906E-01	1.062898E-12	4.282218E+04	1.517415E-04	
21	Nd144	8.055633E+01	6.885854E-04	115102.20	9.838791E-01	2.959421E-09	4.282218E+04	1.517415E-04	
22	Mo98	7.729260E+01	6.606874E-04	115179.50	9.845398E-01	3.740706E-09	4.282218E+04	1.517415E-04	
23	Nd143	7.554826E+01	6.457770E-04	115255.04	9.851856E-01	0.000000E+00	4.282218E+04	1.517415E-04	
24	Ru101	7.391029E+01	6.317758E-04	115328.95	9.858174E-01	0.000000E+00	4.282218E+04	1.517415E-04	
25	Tc99	7.294023E+01	6.234839E-04	115401.89	9.864409E-01	1.245566E+00	4.282342E+04	1.517459E-04	
26	Zr96	7.129463E+01	6.094175E-04	115473.19	9.870503E-01	2.703352E-13	4.282342E+04	1.517459E-04	
27	Mo97	6.758589E+01	5.777157E-04	115540.77	9.876280E-01	0.000000E+00	4.282342E+04	1.517459E-04	
28	Zr94	6.724979E+01	5.748427E-04	115608.02	9.882028E-01	5.775316E-10	4.282342E+04	1.517459E-04	
29	Nd145	6.193298E+01	5.293953E-04	115669.96	9.887322E-01	0.000000E+00	4.282342E+04	1.517459E-04	
30	Zr93	6.116716E+01	5.228492E-04	115731.12	9.892551E-01	3.499654E-02	4.282346E+04	1.517460E-04	
31	Mo95	5.794662E+01	4.953204E-04	115789.07	9.897504E-01	0.000000E+00	4.282346E+04	1.517460E-04	
32	Ru102	5.697641E+01	4.870272E-04	115846.05	9.902374E-01	0.000000E+00	4.282346E+04	1.517460E-04	
33	Ru104	5.476351E+01	4.681116E-04	115900.81	9.907056E-01	0.000000E+00	4.282346E+04	1.517460E-04	
34	Zr92	5.421153E+01	4.633934E-04	115955.02	9.911689E-01	0.000000E+00	4.282346E+04	1.517460E-04	

Result of ordering

# Prediction of nuclide inventories

Out\_ISOTOP - Editor

Datei Bearbeiten Format Ansicht ?

SRG ISOTOP									
'U238'	8.21326708E-01	'O16'	1.18621073E-01	'U235'	1.13001164E-02	'Pu239'	9.37424227E-03	'Pu240'	5.21750252E-03
'Pu241'	2.69675427E-03	'U236'	2.62668794E-03	'Xe136'	1.64844374E-03	'Pu242'	1.30947899E-03	'Xe134'	1.16471231E-03
'Ba138'	1.00954750E-03	'Cs137'	9.47817842E-04	'Ce140'	9.45077273E-04	'La139'	9.32524088E-04	'Cs133'	8.83865962E-04
'Ce142'	8.70004808E-04	'Pr141'	8.28841109E-04	'Xe132'	7.87310518E-04	'Mo100'	6.99856137E-04	'Nd144'	6.88585390E-04
'Mo98'	6.60687409E-04	'Nd143'	6.45777037E-04	'Ru101'	6.31775842E-04	'Tc99'	6.23483934E-04	'Zr96'	6.09417506E-04
'Mo97'	5.77715686E-04	'Zr94'	5.74842731E-04	'Nd145'	5.29395326E-04	'Zr93'	5.22849152E-04	'Mo95'	4.95320442E-04
'Ru102'	4.87027183E-04	'Ru104'	4.68111588E-04	'Zr92'	4.63393364E-04	'Cs135'	4.24013823E-04	'Rh103'	3.92042845E-04
'Zr91'	3.90757481E-04	'Pu238'	3.82165594E-04	'Pd105'	3.78210886E-04	'Nd146'	3.76509372E-04	'Sr90'	3.74152055E-04
'Y89'	2.97416988E-04	'Xe131'	2.81872589E-04	'Am243'	2.80054477E-04	'Np237'	2.79048943E-04	'Nd148'	2.70775929E-04
'Ce144'	2.47465464E-04	'Sr88'	2.36162668E-04	'Am241'	2.23179016E-04	'Pd107'	2.13735454E-04	'Pd106'	1.92195228E-04
'Sm150'	1.87854949E-04	'Te130'	1.78582007E-04	'Rb87'	1.70019688E-04	'Pd104'	1.54593897E-04	'Pm147'	1.51710270E-04
'Nd150'	1.45890565E-04	'Pd108'	1.44933739E-04	'U234'	1.43032566E-04	'Ru106'	1.34535418E-04	'Kr86'	1.31858489E-04
'I129'	1.29745887E-04	'Cm244'	1.11491340E-04	'Sm148'	9.65444813E-05	'Sm152'	9.57127082E-05	'Eu153'	9.43757336E-05
'Cs134'	7.74734550E-05	'Rb85'	7.53585140E-05	'Kr84'	7.16317053E-05	'Ru100'	6.84952823E-05	'Sm147'	6.47538057E-05
'Np239'	5.51619245E-05	'Zr95'	5.39376334E-05	'Gd156'	5.38102044E-05	'U239'	3.82045155E-07	'Y96'	4.93186391E-11
'Nb100'	1.58111082E-11	'Cs138'	3.31631028E-08	'Cs140'	8.85518632E-10	'I134'	6.01816760E-08	'Y98'	3.48743219E-12
'Y97'	2.86619516E-11	'Nb98'	3.10831061E-11	'Rb92'	2.43234533E-11	'Nb102'	7.93006191E-12	'Tc104'	9.63890989E-09
'Sr95'	1.75682468E-10	'La144'	4.85854286E-10	'Nb101'	7.59590871E-11	'Xe137'	3.67014035E-09	'Zr99'	2.32351125E-11
'Y94'	9.99401395E-09	'La142'	7.83643733E-08	'Xe139'	4.37805128E-10	'Y95'	5.91805349E-09	'Cs139'	8.40675160E-09
'La140'	2.28016352E-06	'Cs141'	2.80504109E-10	'Ba143'	1.75990648E-10	'Rb91'	3.46454054E-10	'Nb103'	9.89309337E-12
'Mo103'	7.32380096E-10	'Tc106'	2.11598712E-10	'Sr93'	3.59279674E-09	'Rb93'	2.56791611E-11	'Tc102'	4.28361177E-11
'Te135'	1.53707715E-10	'I136'	5.60399146E-10	'Cs142'	1.16324861E-11	'I137'	2.04048960E-10	'Zr101'	1.41810406E-11
'I132'	9.79741528E-08	'I136m'	2.44092029E-10	'Rb90'	6.67805464E-10	'Ba141'	1.58740294E-08	'I135'	3.89309547E-07
'Sr96'	5.88083868E-12	'Mo101'	9.89732184E-09	'Sr94'	6.17452115E-10	'Zr100'	6.63752111E-11	'Mo105'	2.25145021E-10
'Xe138'	1.27277794E-08	'La143'	1.14740096E-08	'Y99'	5.49857481E-12	'Tc105'	3.64917563E-09	'Nb99'	1.14264041E-10
'Cm242'	4.48858411E-05	'Y92'	8.94629030E-08	'Tc103'	5.94982473E-10	'Xe140'	1.07662655E-10	'Kr90'	1.48454155E-10
'Kr89'	8.01108815E-10	'La145'	2.16515303E-10	'Kr91'	2.85742597E-11	'Y93'	3.03025723E-07	'Rb89'	4.27110807E-09
'Rb94'	5.97132807E-12	'Ba139'	7.69562482E-08	'Ba144'	1.07863426E-10	'La141'	2.05711354E-07	'Zr98'	3.31928220E-10
'Sr97'	1.06330792E-12	'Rb88'	3.69115664E-09	'I138'	2.43866569E-11	'I133'	1.27804523E-06	'Ba142'	8.85045862E-09
'Nb104'	1.12862156E-11	'Ba145'	1.96614029E-11	'Pr144'	1.04715785E-08	'Mo104'	4.92119821E-10	'Te133'	6.61329052E-09
'Tc107'	8.22547507E-11	'Cs143'	6.58706294E-12	'Nb97'	4.15963457E-08	'Te133m'	2.69411544E-08	'Br88'	2.86676047E-11
'Zr97'	5.77254451E-07	'Br86'	9.80496591E-11	'Xe141'	5.87569049E-12	'Te134'	3.71571277E-08	'Tc101'	9.62202356E-09
'Zr102'	1.00272055E-11	'Nb99m'	6.34800045E-10	'Sb133'	8.12300820E-10	'Br87'	1.09559495E-10	'Sb132'	6.14133668E-10
'Ce145'	1.67541786E-09	'Sr91'	2.18242106E-07	'La146'	2.13525368E-11	'Sr92'	6.82445352E-08	'Pr148'	6.25822418E-10
'Te136'	6.80985462E-11	'Pr146'	7.68349691E-09	'Rh106'	1.30567733E-10	'Ru105'	1.29733422E-07	'Mo106'	3.14128204E-11
'Pr145'	2.04003559E-07	'Tc108'	8.49023027E-12	'Rh108'	5.28046927E-11	'Kr92'	3.58764898E-12	'Sb131'	7.09991620E-09
'Pr147'	4.96258117E-09	'Ce147'	3.40121812E-10	'Ru107'	1.05849274E-09	'Mo99'	2.75873904E-06	'Ce143'	1.62085787E-06
'Sb132m'	7.04587154E-10	'Br89'	5.91075006E-12	'Kr88'	3.46391795E-08	'Kr87'	1.13953261E-08	'Rb90m'	3.70005969E-10
'La147'	1.29585966E-11	'Ba140'	1.69292494E-05	'Rb95'	3.78914058E-13	'Nb95'	2.91455862E-05	'Rh104'	1.88936875E-10
'Sb134m'	1.35289553E-11	'Y91'	3.20624836E-05	'Te131'	8.57201341E-09	'Pr150'	1.44345174E-11	'Se85'	3.39056818E-11
'Mo107'	4.54914655E-12	'Zr103'	1.44057254E-12	'Ce149'	1.33606609E-11	'Nb100m'	3.45422240E-12	'Nb97m'	4.80084354E-10
'Cs144'	1.18127404E-12	'Nb105'	3.28101153E-12	'Y100'	5.30281667E-13	'Pr149'	4.69187039E-10	'Ru103'	3.65213852E-05
'Ce148'	2.49872996E-10	'I139'	3.56594864E-12	'Se86'	1.65698138E-11	'Sr89'	2.07141451E-05	'Sb130'	4.15342513E-09
'Te137'	3.03978018E-12	'Ba146'	4.64528632E-12	'Pr143'	1.55827165E-05	'Mo102'	5.49693144E-09	'Sr98'	6.65269346E-13
'Tc100'	3.09255375E-11	'Kr93'	7.92337987E-13	'Rh107'	6.14210990E-09	'Br90'	1.08321539E-12	'Se87'	3.32631871E-12

Generation of STRU ISOTOP by the EXCEL procedure



# Extension of Input (VESSEL+Primary)

Additional moduls to be activated

STRU CALC\_OPT

SC1 MODULIST

'CESAR'

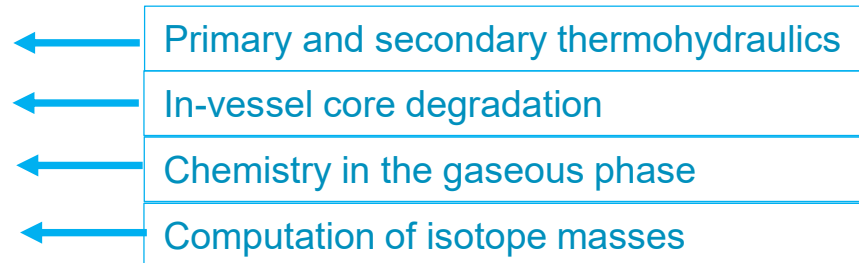
'ICARE'

'SOPHAERO'

'ISODOP'

TERM

END



# Extension of Input (VESSEL+Primary)

Additional moduls to be activated

STRU FP\_HEAT

SRG ISOTOP

TERM

END

Other Fields, like  
FP, FRAQ, TIME, POWE  
are not needed anymore

## Extension of Input (Containment)

STRU CONTAINM

STRU ZONE

STRU GEOM

CDRY

concrete dry area

CWET

concrete wet area

PDRY

painted dry area

PWET

painted wet area

SDRY

steel dry area

SWET

steel wet area

END

END

END

# Extension of Input (Containment)

```
STRU WALL
  NAME 'WA_SEP'
  MATE 'SSTEEL'
  MODEL 0
  TYPE 'OTHER'
  THIC 0.13m
  V 5.28
  VOLUME 'SEP'
  STRU GEOM
    S_exch 39.70
    L 5.8
    D_h 4.8
    surf_lat 39.70
    surf_set 0.0
  END
  STRU GEOM
    S_exch 41.55
  END
  STRU THER
    T_wall 286.0C
  END
END
```

Mandatory, if TYPE 'OTHER'

# Determination of isotopes released from the containment

Problem:

Masses of isotops flowing through CONNs are not available for the user

But following pieces of information are available:

List of isotope names:

BASE : PHYSICAL : BANK : INAME

List of isotope masses in the containment:

BASE : FP\_HEAT : CONTAINMENT : MI

Cumulative mass of elements through CONN:

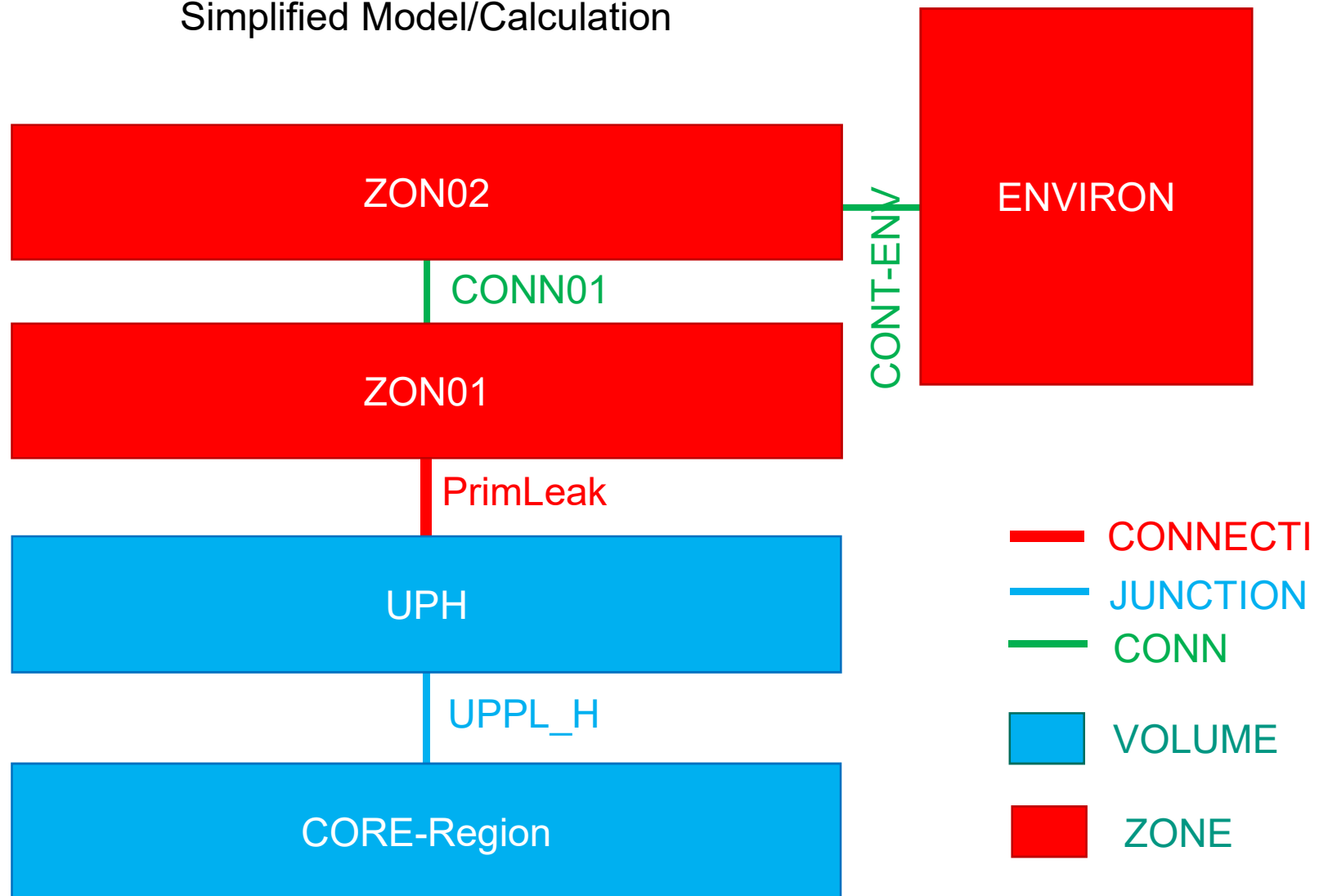
BASE : CONTAINM : CONN 'name' : FPDI : 'name of element'

These pieces of information make it possible to determine the mass of an isotope which has left the containment



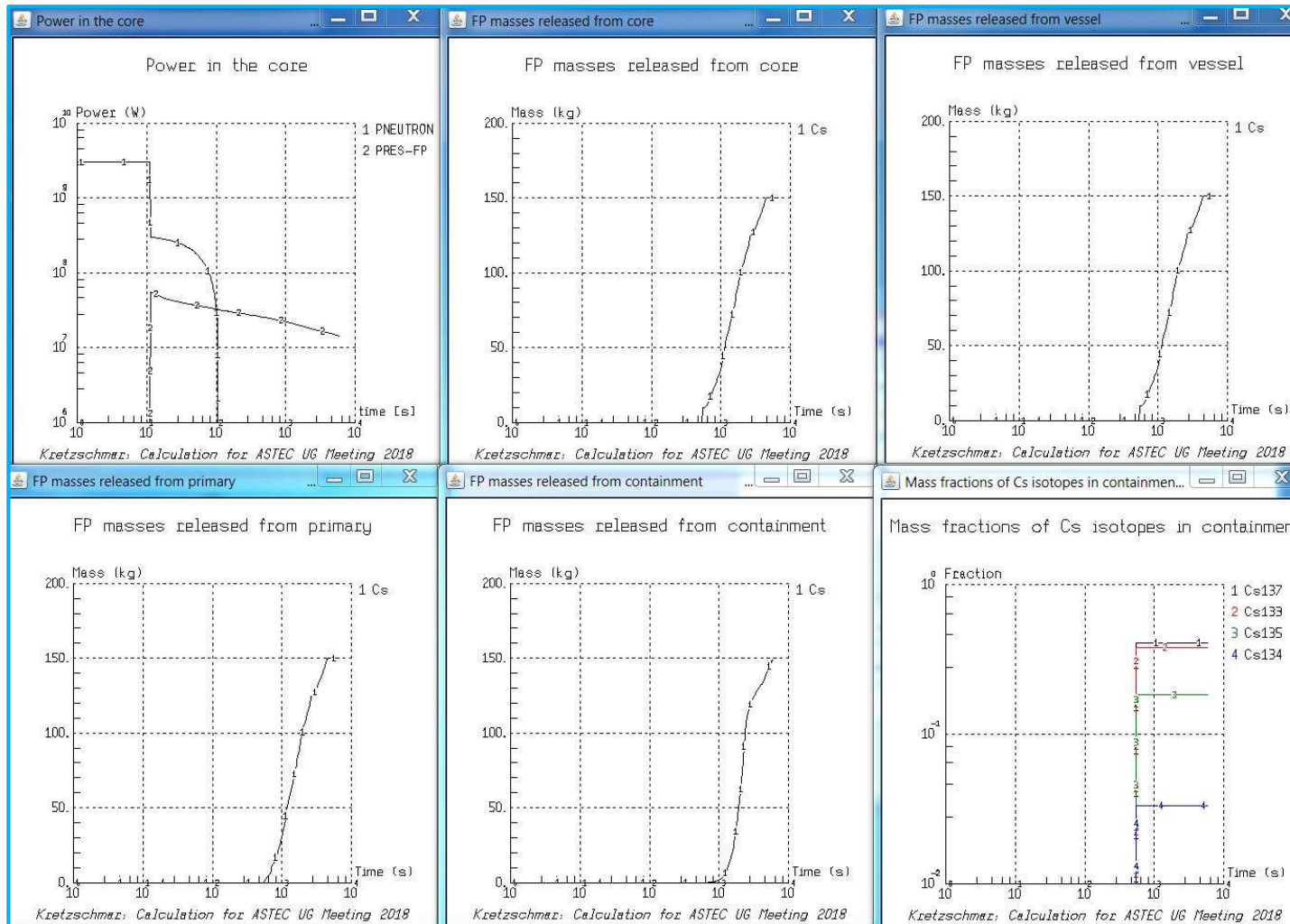
# Extension of Input (V+P+Containment)

Simplified Model/Calculation



# Extension of Input (V+P+Containment)

## Simplified Model/Calculation



## Outlook

- Include models for FPs in inputs for other reactor types
- Include models for the core melt in the reactor pit
- Include models for the chemistry in the containment
- Calculation of more complex scenarios