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)

04/10/18   Frank Kretzschmar

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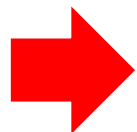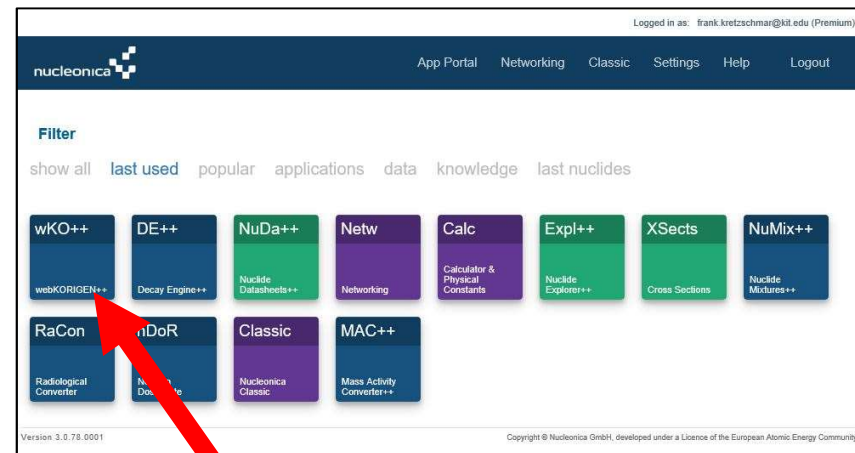
There is a need, to generate a **realistic** initial FP file for ASTEC calculations

Prediction of nuclide inventories

https://www.nucleonica.com/
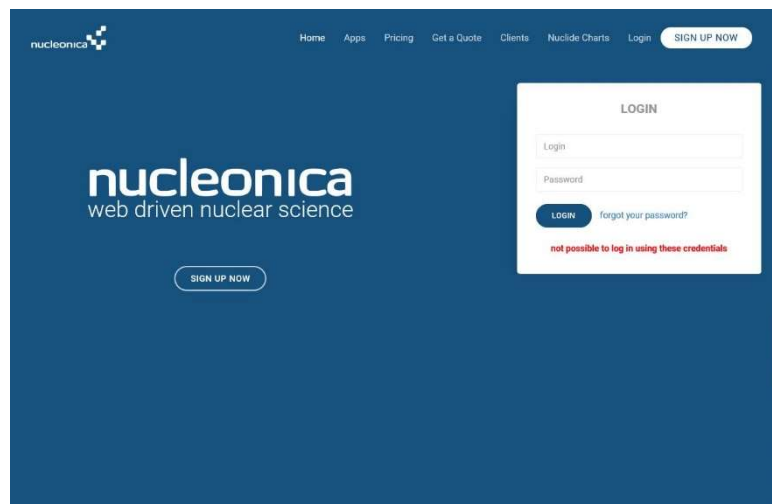
1 year license costs ≈ 600 Euro

webKORIGEN

Prediction of nuclide inventories

webKORIGEN - input mask

Prediction of nuclide inventories

Result of webKORIGEN calculation

Nuclide masses

Nuclide decay heats

Prediction of nuclide inventories

			Kerninventar								
	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

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Prediction of nuclide inventories

	Name	Value Mass	Sum Mass	Part Mass	Decay value	Sum Decay	Part Decay	Name	Value Mass	Sum Mass	Part Mass	Dec
1											1. cycle	
2				U-BE							U-Gd-BE	
3	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	2,00
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	5,00
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+04	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

Tabelle1 | Tabelle2 | Tabelle3 | ⊕

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
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
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
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
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
Sm150	3,022871E-01	4,299271E+03	9,982083E-01	0,000000E+00	4,265539E+04	3,465703E-03	Pd105	6,028763E-01	8,499020E+03	9,989470E-01
Pd105	3,005399E-01	4,299572E+03	9,982781E-01	0,000000E+00	4,265539E+04	3,465703E-03	Sm150	5,993716E-01	8,499620E+03	9,990174E-01
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
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
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
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
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
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 refering masses to decay heats must be automatized!

Frank Kretzschmar

Prediction of nuclide inventories

171201_SRG_ISOTO...

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

Prediction of nuclide inventories

Prediction of nuclide inventories

	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	

Cell reference: F20 — 1.06289785E-12

Result of ordering

Prediction of nuclide inventories

Generation of STRU ISOTOP by the EXCEL procedure

Extension of Input (VESSEL+Primary)

Additional moduls to be activated

```
STRU CALC_OPT

    SC1 MODULIST
       'CESAR'          ←   Primary and secondary thermohydraulics
       'ICARE'          ←   In-vessel core degradation
       'SOPHAERO'       ←   Chemistry in the gaseous phase
       'ISODOP'         ←   Computation of isotope masses
    TERM


END
```
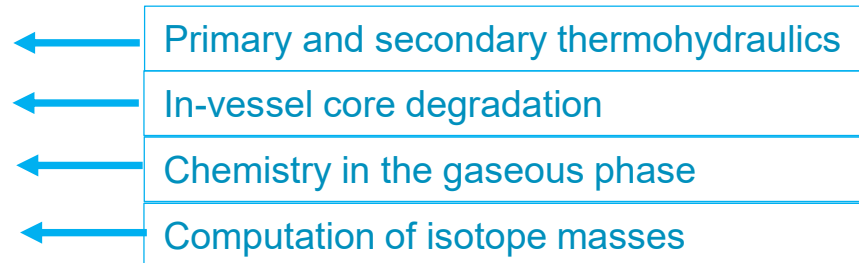
Extension of Input (VESSEL+Primary)

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

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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 isotop names:
BASE : PHYSICAL : BANK : INAME

List of isotop masses in the containment:
BASE : FP_HEAT : CONTAINMENT : MI
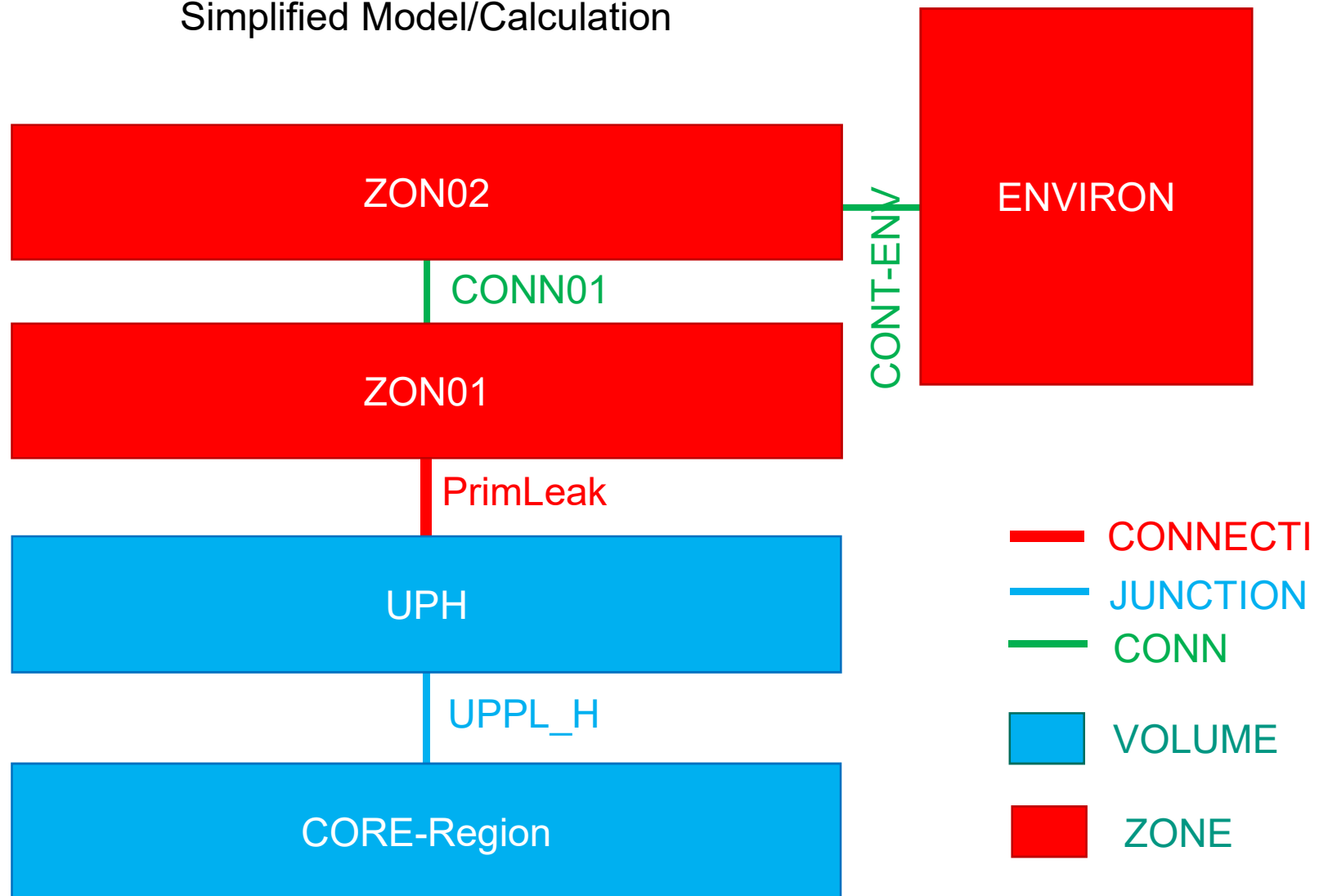
Cumulative mass of elements through CONN:
BASE : CONTAINM : CONN ´name´ : FPDI : ´name of element´

These pieces of information make it possible to determine the mass of an isotop which has left the containment
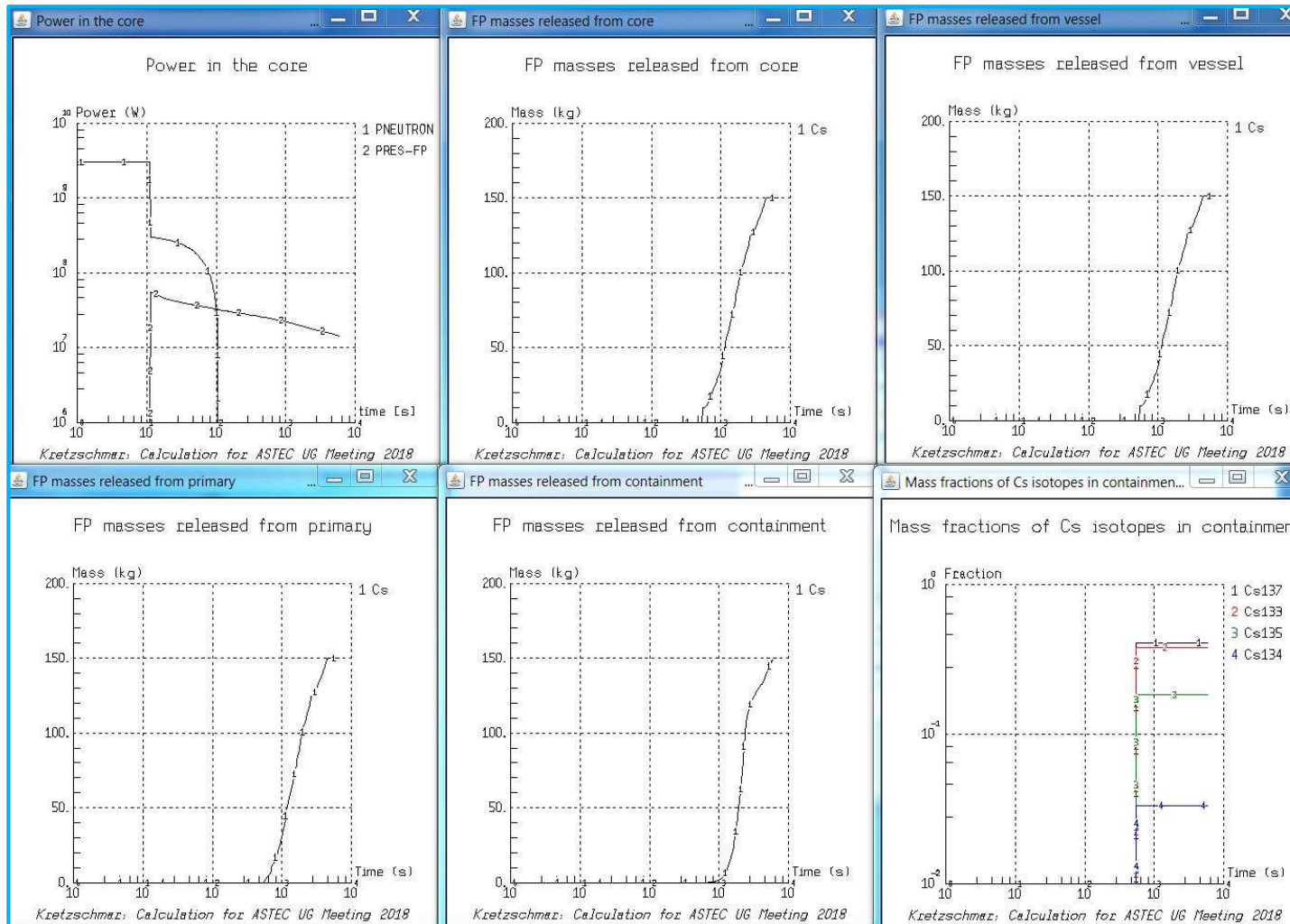
Extension of Input (V+P+Containment)

Simplified Model/Calculation

Extension of Input (V+P+Containment)

Simplified Model/Calculation

Outlook

- Include models for FPs in inputs for other rector types

- Include models for the core melt in the reactor pit

- Include models for the chemistry in the containment

- Calculation of more complex scenarios

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