

Nuclear Data Libraries and Mixture Definitions

SCALE 6.3.3

ORNL is managed by UT-Battelle, LLC for the US Department of Energy



U.S. DEPARTMENT OF
ENERGY

Learning goals

- Obtain overview of available nuclear data libraries in SCALE
- Understand the different options on how to define a material:
 - Basic standard composition
 - Compounds
 - Weight percent mixture
 - Fissile solutions
- Learn how SCALE considers Thermal Scattering Law (TSL) data

Nuclear data libraries



SCALE's nuclear data libraries

- The AMPX code system is used to prepare (almost*) all of SCALE's nuclear data libraries
- The key nuclear data libraries are as follows:
 - Continuous-energy (CE) cross section libraries
 - Multi-group (MG) cross section libraries
 - Multi-group covariance libraries (uncertainty and correlation data)
 - Other important libraries: fission yields, decay data, activation, etc.
- SCALE 6.3 libraries were prepared based on evaluated nuclear data libraries: ENDF/B-VII.1 and ENDF/B-VIII.0
- All nuclear data libraries are stored in one directory: “data” within the SCALE installation folder
- SCALE searches for libraries via the `DATA` environmental variable

Relevant cross section libraries for this learning module

- “v7.1” indicates ENDF/B-VII.1; “v8.0” ENDF/B-VIII.0
- CE cross section libraries:
 - `ce_v7.1_endf.xml` (old-style xml file)
 - `ce_v8.0_endf.h5` (new HDF5 format)
- MG cross section libraries:
 - *Fine-group thermal*: `scale.rev05.xn252v7.1`
`scale.rev01.xn252v8.0`
 - *Broad-group LWR*: `scale.rev04.xn56v7.1`
 - *Fine-group SFR*: `scale.rev00.xn302v7.1`, `v8.0-302`
 - *Very fine-group*: `v7.1-1597`, `v8.0-1597`
 - *And many more coupled neutron–gamma libraries*
- The CE and MG libraries can be called via their explicit file name or via their alias (see later when we talk about input file development)

Typical SCALE inputs reference a library "alias" like **v7.1-252** or **ce_v7.1**.

All library aliases are defined in the file **FileNameAliases.txt** in the SCALE installation directory.

Cross section libraries and their use

- CE cross section libraries:
 - Point-wise tabulated values of cross sections on a fine energy mesh
 - Used by CENTRM for self-shielding and by KENO/Shift for neutron transport in CE mode
- MG cross section libraries:
 - Libraries contain flux-weighted averages of point-wise data over energy groups
 - **Problem-independent** MG libraries are distributed with SCALE
 - **Self-shielding calculation is required** to convert a problem-independent into a **problem-dependent** MG library for neutron transport calculations

Self-shielding must be requested through the “celldata” block, which enables XSPROC calculation

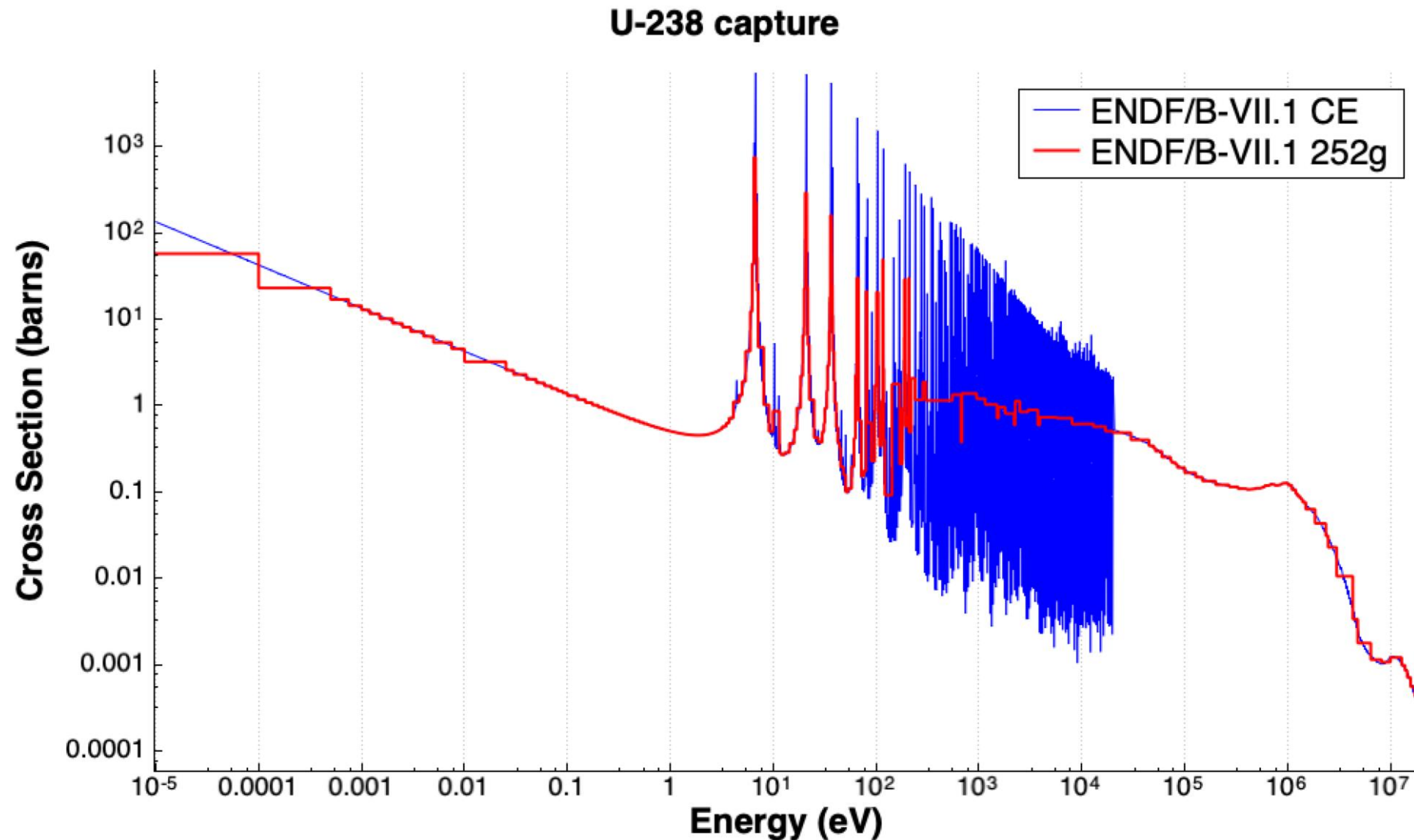
Comments on CE vs. MG

- CE
 - No need for “celldata” input block
 - Accurate representation of cross sections
 - Accurate calculation of energy distribution of integral quantities such as flux and reaction rates
 - CE Monte Carlo calculations require longer execution times to reach the same uncertainty as the corresponding MG Monte Carlo calculation
- MG
 - Generally shorter overall execution times (problem dependent)
 - Always shorter times in Monte Carlo modules for equivalent uncertainty
 - Accurate resonance self-shielding is not always possible

Hands-on: Cross section visualization

1. Open CE library *ce_v7.1_endf.xml*
2. Open MG library *scale.rev05.xn252v7.1*
3. Plot CE data of U-238 capture
4. Add plot of MG U-238 capture data into the same plot as the CE data

Hands-on: Cross section visualization



Composition definition



Mixtures in the COMPOSITION block

- Mixtures for many of SCALE's sequences (CSAS, TRITON, MAVRIC, XSPROC, etc.) are defined in the COMPOSITION block
- There is a range of ways to define a mixture
- These different types to define a mixture were developed to allow simple user inputs for a range of typical material descriptions
- Selecting the "right" input type can dramatically simplify user effort and the input—and it can enable easier error detection
- A mixing table listing the densities of individual nuclides in atoms/barn-cm for each mixture can be generated directly in Fulcrum to double-check mixture definitions
 - Click drop-down next to “Run”, then “Mixing Table”

Standard composition types

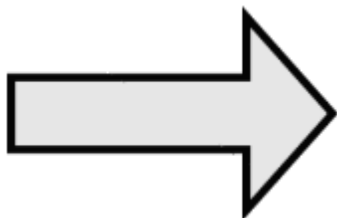
- Basic standard compositions
 - Individual nuclides
 - Elements with user-defined isotopic distribution
 - Some frequently used compounds/alloys (UO_2 , SS304, others)
- Compounds
 - User-specified compounds (atoms per molecule/compound)
- Weight percent mixtures
 - User-specified weight percent mixtures
- Fissile solutions
 - Nitrate and fluoride solutions of U, Pu, and Th as well as associated excess acid

Basic standard compositions



The standard composition library

- Contained in the data directory: `scale.rev40.sclib`
- This library contains information on isotopes, elements, compounds, alloys and mixtures:
 - SCALE IDs
 - Natural abundances of elements
 - Composition of alloys and mixtures (e.g., UO_2 or SS304)
 - Theoretical densities
 - Masses (in amu)
- SCALE module **compoz** can be used to convert the library to a regular text file and to create a new standard composition library
- The content is also displayed in the SCALE manual in section 7.2 “Standard composition library”



Besides Fulcrum's autocomplete windows, this is where you can find out which assumptions SCALE makes for the different compounds, alloys, and mixtures.

Basic standard composition input data

- Standard composition name
- Mixture number
- Theoretical density (optional)
 - Keyworded: DEN=
- Density multiplier (optional)
- Temperature (K) (optional)
- Isotopic distribution (optional)
- end

You can stop once you've supplied everything you need, but you must provide the END!

```
uranium 1 1.0 293 92235 96.0 92238 4 end
dry-air 2 end
h2o 3 den=1.0 1.0 597 end
```

Basic standard composition – autocomplete via Fulcrum

- Fulcrum provides autocomplete capability
 - **Ctrl-Space** opens drop down menu
- Select “stdcomp” option with data you want to provide
 - Replace example data with appropriate data
 - OR choose “configurable” and fill in fields

Autocomplete choices

The screenshot shows the SCALE 6.3.2 software interface. The main window displays a script file named 'new.inp' with the following content:

```
1 =csas5 parm=( )
2 title-goes-here
3 v7.1-252
4
5 read comp
6
7 ' TODO: define comp
8 uranium 1 1.0 293 92235 96.0 92238 4 end
9 dry-air 2 1.0 end
10
11 stdcomp - basic (configurable)
12 stdcomp - basic
13 stdcomp - basic + volume fraction
14 stdcomp - basic + volume fraction + temperature
15 stdcomp - basic + volume fraction + temperature + isotopics
16 stdcomp - basic + atomic density (configurable)
17 stdcomp - basic + atomic density
18 stdcomp - basic + atomic density + temperature
19 wtptcomp - basic (configurable)
20 wtptcomp - basic
21 wtptcomp - basic + volume fraction
22 wtptcomp - basic + volume fraction + temperature
23 wtptcomp - basic + volume fraction + temperature + isotopics
24 atomcomp - basic (configurable)
25 atomcomp - basic
26 atomcomp - basic + volume fraction
27 atomcomp - basic + volume fraction + temperature
28 atomcomp - basic + volume fraction + temperature + isotopics
29 solution - rho + density + temperature + volume fraction
30 solution - molar + density + temperature + volume fraction
31 solution - massfrac + density + temperature + volume fraction
32 solution - molefrac + density + temperature + volume fraction
33 solution - molality + density + temperature + volume fraction
```

An autocomplete dropdown menu is open at line 10, showing a list of available commands and their options. The list includes 'stdcomp' with various configuration options, 'wtptcomp', and 'atomcomp'. The status bar at the bottom indicates 'Line: 10, Col: 1' and the file path '/csas5/comps'. The bottom right corner shows 'Validation' and 'Messages' buttons.

Autocomplete example

- Need to specify: B₄C as mixture 3: $\rho=2.46$ g/cm³, 30 wt% ¹⁰B
- Autocomplete provides:
 - `uo2 1 1.0 293 92234 0.5 92235 5.0 92238 94.5 end`
- Change to:
 - `b4c 3 DEN=2.46 1.0 293 5010 30 5011 70 end`

Configurable example

- Same mixture 3, B₄C: $\rho=2.46 \text{ g/cm}^3$, 30 wt% ¹⁰B

stdcomp - basic (configurable)

Composition: b4c

Mixture: 3

☒ Theoretical Density: 2.460000

☒ Volume Fraction: 1.000000

☒ Temperature: 293.000000

☒ Isotopic Weight Percents

	+/-	Isotope	Weight Percent
1	+ -	5010	30.000000
2	+ -	5011	70.000000

Add row

b4c 3 den=2.460000 1.0 293.0
5010 30.0
5011 70.0 end

Results Log Template

OK Cancel

Simple use of density multiplier

- UO_2 pellets pressed to 96% of theoretical density (TD)
 - Two equivalent definitions:
 - `UO2 1 den=10.5216 1 293 end`
 - `UO2 1 0.96 293 end`
 - **den=** is keyword construct
 - 0.96 is multiplied by the default theoretical density (TD) (or supplied density) to determine density in mixture

Density and density multiplier

- Theoretical density for each material has a default value that can be changed with DEN=
- Variable name for density multiplier is VF (volume fraction), though it isn't always a volume fraction
- Density for each component is determined as TD times density multiplier
- Examples:

```
h2o 1 0.7 293 end [default  $\rho=0.9982$ ]
```

```
h2o 2 den=0.69874 1 293 end
```

Mixing basic compositions with density multipliers

- Multiple basic compositions can be used in the same mixture by providing the same mixture number
- The amount of each basic composition in the overall mixture can be controlled with the density multiplier for each component
- Must be done correctly – be careful

Example for mixing basic compositions

- Consider a mixture of 80 vol% water and 20 vol% UO_2
- Input would look like:

h2o	2	0.8	300	end
uo2	2	0.2	300	end
- Mixture 2 total mass density is calculated as:

$$\rho_{\text{H}_2\text{O}} = 0.9982 \times 0.8 = 0.79856$$

$$\rho_{\text{UO}_2} = 10.96 \times 0.2 = 2.192$$

$$\rho_{\text{MIX}=2} = 0.79856 + 2.192 = 2.99056$$

- The total mass density for each mixture is provided in the mixing table

Alternative approach

- Assume we know the mass density and the mass fractions
 - $\rho = 2.99056 \text{ g/cm}^3$
 - $\text{H}_2\text{O wt\%} = 26.703$
 - $\text{UO}_2 \text{ wt\%} = 73.297$
- Then the input looks like:

```
h2o          1 den=2.99056 0.26703 300 end
uo2          1 den=2.99056 0.73297 300 end
```

- Now the density multiplier is a mass fraction!

Nuclide density comparison between the two approaches

```
h2o          1 den=2.99056 0.26703 300    end
uo2          1 den=2.99056 0.73297 300    end

h2o          2 0.8 300    end
uo2          2 0.2 300    end
```

	Mixture 1	Mixture 2
Mass density (g/cm ³)	2.9906	2.9906
H-1 (a/b-cm)	5.338292e-002	5.338230e-002
O-16 (a/b-cm)	3.638303e-002	3.638276e-002
U-234 (a/b-cm)	2.640060e-007	2.640071e-007
U-235 (a/b-cm)	3.521722e-005	3.521737e-005
U-238 (a/b-cm)	4.853083e-003	4.853104e-003

²H, ¹⁷O and ¹⁸O are also reported—more on that later!

Entering number densities

- Density multiplier of 0 is a flag for SCALE that the next input is a number density in atoms/barn-cm

```
h          1  0  0.0667531  300  end

pu-238     1001  0  4.747e-07  293.000  end
pu-239     1001  0  1.068e-04  293.000  end
pu-240     1001  0  1.577e-05  293.000  end
pu-241     1001  0  5.626e-06  293.000  end
pu-242     1001  0  6.187e-07  293.000  end
rh-103     1001  0  1.104e-05  293.000  end
```

Caution on default densities

- The default density for all isotopes is 1.0 g/cm³ and, thus, likely not helpful
- The default density for all elements that are gases at room temperature is also 1.0 g/cm³, which is also unlikely to be helpful

Example elemental data

ID	Symbol	Name	Mass (amu)	Density	Isotopic Distribution	Atom %
6000	c	CARBON	12.0107	2.1	6012	98.93
					6013	1.07
24000	cr	CHROMIUM	51.9961	7.2	24050	4.345
					24052	83.789
					24053	9.501
					24054	2.365
1000	h	HYDROGEN	1.0079	1.0	1001	99.9885
					1002	0.0115
26000	fe	IRON	55.845	7.86	26054	5.845
					26056	91.745
					26057	2.119
					26058	0.282
92000	u	URANIUM	238.0289	19.05	92234	0.0054
					92235	0.7204
					92238	99.2742

From Table 7.2.2 Isotopes and their natural abundances

Comments on isotope treatment in previous SCALE versions

- SCALE 6.3 expands all elements to isotopes according to their natural abundance
 - If a nuclear data library does not have a cross section for a specific nuclide, then it is removed from the composition definition
 - O-18 is an exception, where the ENDF/B-VII.1 cross section is treated as zero
- Certain SCALE versions prior to SCALE 6.2/6.3 expanded H and O to H-1 and O-16, respectively
- Certain SCALE versions prior to SCALE 6.2/6.3 expanded Pu differently:
 - In earlier versions, SCALE has allowed Pu to be specified without an isotopic description, and it was assumed 100% Pu-239
 - This is no longer allowed; any material in the standard comp library including Pu (PuO_2 , PuC, $\text{Pu}(\text{NO}_3)_4$, PuF_4 , PuN) needs a user-specified isotopic distribution
 - Pu is not recognized (it has no natural abundance)
 - Plutoniumalp/plutoniumdlt or isotopes can be used
 - Configurable window in Fulcrum does not provide 94AAA options for isotopic composition
 - Type nuclide IDs (e.g., 94239) into fields directly

Examples of compound data

Name	Description	Density	ID	Atoms Per Molecule
al2o3	Aluminum oxide	3.97	13000	2
			8000	3
b4c	Boron carbide: B4C; natural Isotopic distribution obtained by default	2.52	5000	4
			6000	1
balsa	Balsa wood: C ₆ H ₁₀ O ₅	0.125	6000	6
			1000	10
			8000	5
benzene	Benzene with a S(α,β) thermal kernel	0.8765	5006000	6
			6001001	6

From Table 7.2.4 Compounds

Examples of alloy/mixture data

Name	Description	Density	Nuclide	Weight %
CARBONSTEEL	Carbon steel	7.8212	26000 6000	99.0 1.0
REG-CONCRETE	Regulatory concrete (developed for U.S. NRC)	2.3	26000 1000 13000 20000 8000 14000 11000	1.4 1.0 3.4 4.4 53.2 33.7 2.9
SS304S	Stainless steel-304 (using standard nuclides instead of special weighted nuclides)	7.94	6000 14000 15000 24000 25000 26000 28000	0.08 1.0 0.045 19.0 2.0 68.375 9.5

From Table 7.2.5 Alloys/mixtures

Void specification

- Mixture 0 is always void
 - Does not need to be specified in the composition block
- Void has no cross section – it is simply empty space
- Void can be specified in geometry data as necessary
- Volumes within the model that are void must be specified as such – void is NOT assumed in space with undefined material
- It can be used as many times as necessary in unit cell data specifications

Thermal scattering kernels



Thermal scattering kernels

- Cross sections of several nuclides are generated with thermal scattering kernels (TSL data)
- These can have a significant impact on calculated results
- **The selection of TSL data is done in SCALE by choosing the correct, corresponding nuclide identifier**
- Some examples:
 - H, Be, D, Fe, O, C cross sections are available with various TSLs
 - Carbon:
 - Free-gas, i.e. carbon cross section data: *c*
 - Carbon cross section data + graphite TSL data: *c-graphite*
 - Hydrogen:
 - Free-gas, i.e. hydrogen cross section data: *hfreegas*
 - Hydrogen cross section data + TSL data is available for various options: *h* (*h* in *h2o*), *h-benzene*, *h-cryo_ortho*, *h-cryo_para*, *h-liquid_ch4*, *h-poly*, *h-solid_ch4*, *h-zrh2*
- See STDCMP section of the manual for available cross sections

H-poly data thermal scattering

- SCALE 6.2 and earlier has incorrect **h-poly** due to an error in ENDF
 - Note that the default *h-1* is tied to thermal scattering for H₂O and was processed correctly
- Error in scattering can cause k_{eff} mispredictions of 1% or more
 - Patch available for SCALE 6.2 CE data from <https://code.ornl.gov/scale/sse/sdl-2021-024/-/releases>
- With new ENDF/B-VIII.0 TSLs, this error also applies to **h-lucite** and **si-***
- Assessment has shown that as long as CENTRM is used in XSPROC (instead of BONAMI), the error is significantly reduced compared to 6.2
- CE **h-poly**, **h-lucite**, and **si-*** data are fixed in SCALE 6.3.1 data patch
- MG **h-poly** and **h-lucite** data are fixed in SCALE 6.3.2 data patch

New data relevant for advanced reactors



Graphite

- Graphite = carbon cross section data + graphite TSL data
- ENDF/B-VII.1:
 - Carbon available only as element (*last element for which this was the case!*): **c**
 - Graphite TSL data only available for graphite as perfect crystal, i.e., 0% porosity: **c-graphite** or **graphite**
- ENDF/B-VIII.0:
 - Carbon isotopic data: **c-12**, **c-13**, **c***
 - Graphite TSL data available for graphite at different porosities:
 - 0%: **c12-graphite**, **c13-graphite**, **c-graphite***
 - 10%: **c12-10_graph**, **c13-10_graph**, **c-10_graph***
 - 30%: **c12-30_graph**, **c13-30_graph**, **c-30_graph***
- Note: Graphite data with 20% porosity planned to be included in future ENDF/B releases

We recommend the use of 0% porosity data.
See K. Ramic, et al. (2025), Carbon, 244,
120619, [10.1016/j.carbon.2025.120619](https://doi.org/10.1016/j.carbon.2025.120619)

New TSL data in ENDF/B-VIII.0

- ENDF/B-VII.1: SiO_2 , ZrH_2
- ENDF/B-VIII.0: SiO_2 , **SiC** , ZrH_2 , **YH_2**

Exercise: Basic standard composition



Exercises

- We will do one example together for each group of exercises
- Keep your inputs in a specific location, as many of the example specifications are drawn from the exercises you will be working on later
- We will create models using the T-XSEC sequence with the "v7-56" library

Criticality safety – Problem 1 – together

- Uranium metal
 - Density = 18.74 g/cm^3
 - Mixture temperature: 293 K
 - Enrichment:
 - 1.0202 w/o ^{234}U
 - 93.7112 w/o ^{235}U
 - 5.2686 w/o ^{238}U

Criticality safety – Problem 2

- Aluminum metal
 - Density = 2.702 g/cm^3
- Uranium oxide
 - 95% theoretical density
 - Mixture temperature: 293 K
 - Enrichment:
 - 4.95 w/o ^{235}U
 - 95.05 w/o ^{238}U

Criticality safety – Problem 3

- Homogeneous mixture of UF_4 and paraffin
 - Mixture density 3.8655 g/cm^3
 - UF_4 – 88.62 wt%
 - Enrichment:
 - 2.0 w/o ^{235}U
 - 98.0 w/o ^{238}U
 - Paraffin – 11.38 wt%
 - Mixture temperature 27°C

Remember, the density multiplier functions as a *mass fraction* if the overall mixture density is specified.

Criticality safety – Problem 3a

- Homogeneous mixture of UF_4 and paraffin
 - UF_4 – 51.13 vol%
 - Enrichment:
 - 2.0 w/o ^{235}U
 - 98.0 w/o ^{238}U
 - Paraffin – 48.87 vol%
 - Mixture temperature 27 °C

Remember, the density multiplier can function as a volume fraction.

Reactor physics – Problem 4

- Uranium dioxide (UO_2)
 - 95% theoretical density (TD)
 - Enrichment:
 - 4.95 wt% ^{235}U
 - 95.05 wt% ^{238}U
 - 900 K

Reactor physics – Problem 5

- UO_2 + gadolinium oxide
 - 4 wt% enriched in ^{235}U
 - 6 wt% Gd_2O_3
 - 10.50 g/cm^3
 - 900 K

Reactor physics – Problem 6

- Dry-air
 - SCALE default density
 - 850 K

Reactor physics – Problem 7

- Zirc-2
 - SCALE standard density (6.56 g/cm³)
 - 600 K

Reactor physics – Problem 8

- Water + soluble boron
 - 0.75 g/cm³
 - 900 ppm natural boron
 - 540 K

Exercise solutions: Basic standard compositions



Criticality Safety

Problem 1

```
u          1 den=18.74 1 293
          92235 93.7112
          92238 5.2686
          92234 1.0202   end
```

Problem 2

```
a1          2 end
uo2         3 0.95 293
          92235 4.95
          92238 95.05   end
```

Problem 3

```
uf4         4 den=3.8655 0.8862 300.15
          92235 2
          92238 98   end
paraffin    4 den=3.8655 0.1138 300.15   end
```

Problem 3a

```
uf4         4 0.5113 300.15
          92235 2
          92238 98   end
paraffin    4 0.4887 300.15   end
```

Reactor physics

Problem 4

```
uo2          1  0.95  900
                                     92235  4.95
                                     92238  95.05      end
```

Problem 5

```
uo2          2  den=10.5  0.94  900
                                     92235  4
                                     92238  96      end
```

Problem 6

```
gd2o3        2  den=10.5  0.06  900      end
```

```
dry-air       10  1  850      end
```

Problem 7

```
zirc2         20  1  600      end
```

Problem 8

```
h2o           30  den=0.75  1.0000  540      end
boron          30  den=0.75  0.0009  540      end
```

Note that the addition of boron as mass fraction to the water without adjusting the H₂O mass fraction causes a slight increase in the total mixture density (here: 0.7507 g/cm³). This is standard practice for lattice physics problems in which few-group cross sections are generated for core simulators. However, the accurate way would be to adjust the mass fraction for H₂O to 0.9991 to achieve a mixture mass density of the target 0.75 g/cm³.

Compounds



Atom compounds

- *atomname* – “atom” prefix is required as a flag to SCALE
- Mixture number
- Theoretical density
- Number of elements
- Nuclide ID and number of atoms
- Density multiplier
- Temperature (K) (optional)
- Isotopic distribution (optional)
- end

IFBA – ZrB₂ at 6.1 g/cm³ (45 wt% ¹⁰B)

```
atomIFBA 7 6.1 2
40000 1
5000 2
1.0 293
5010 45 5011 55
end
```

Integers required

Atom compounds

- Autocomplete and configurable also work for atom compounds (atomcomp)
- Default atomcomp is “atomuo2”

The screenshot shows the 'atomcomp - basic (configurable)' window. The 'Properties' section on the left has 'Atom Count Composition' expanded, showing 'Element Atom Counts' with an 'Add' button and two 'Remove' buttons. The main area contains fields for Name (IFBA), Mixture (7), Theoretical Density (6.100000), Density Multiplier (1.000000), and Temperature (293.000000). The bottom text area displays the configuration: atomIFBA 7 6.1 2, 40000 1, 5000 2, 1.0 293.0, 5011 55.0 5010 45.0 end. Buttons for Results, Log, Template, OK, and Cancel are at the bottom.

The screenshot shows the 'atomcomp - basic (configurable)' window with the 'Element' dropdown set to '5000' and 'Atom Count' set to '2'. The 'Isotopics' checkbox is checked. The 'Element Atom Counts' section shows two entries: 5011 with a weight percent of 55.000000 and 5010 with a weight percent of 45.000000. The bottom text area displays the configuration: atomIFBA 7 6.1 2, 40000 1, 5000 2, 1.0 293.0, 5011 55.0 5010 45.0 end. Buttons for Results, Log, Template, OK, and Cancel are at the bottom.

Exercise: Compounds



Problem 1 – together!

- Sodium bicarbonate (NaHCO_3)
 - Temperature 22 °C
 - Density = 2.1 g/cm³

Problem 2

- Calcium fluoride (CaF_2)
 - Temperature 610 °F (approximately 594 K)
 - Density = 3.18 g/cm³
 - Enrichment:
 - 96 w/o ⁴⁰Ca
 - 4 w/o ⁴⁸Ca

Exercise solutions: Compounds



Problem 1

```
atomnahco3 1 2.1 4
      11000 1
      1000 1
      6000 1
      8000 3
              1.0 295.15
end
```

Problem 2

```
atomcaf2          7  3.18  2
                                20000 1
                                9000  2
                                1.0 594.26
                                20040 96
                                20048  4  end
```

Weight percent mixture



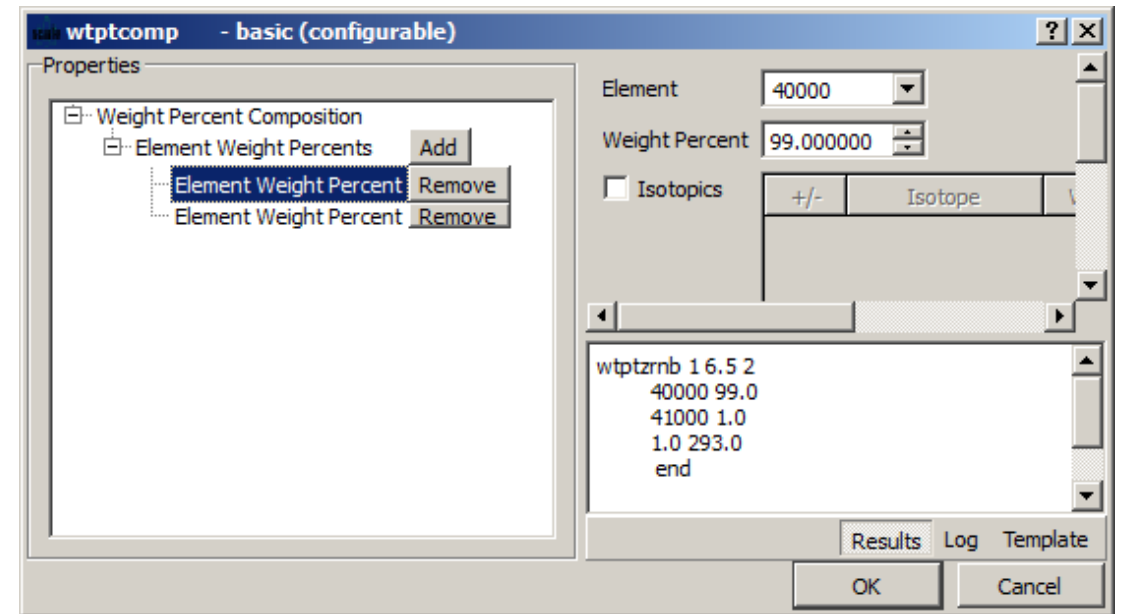
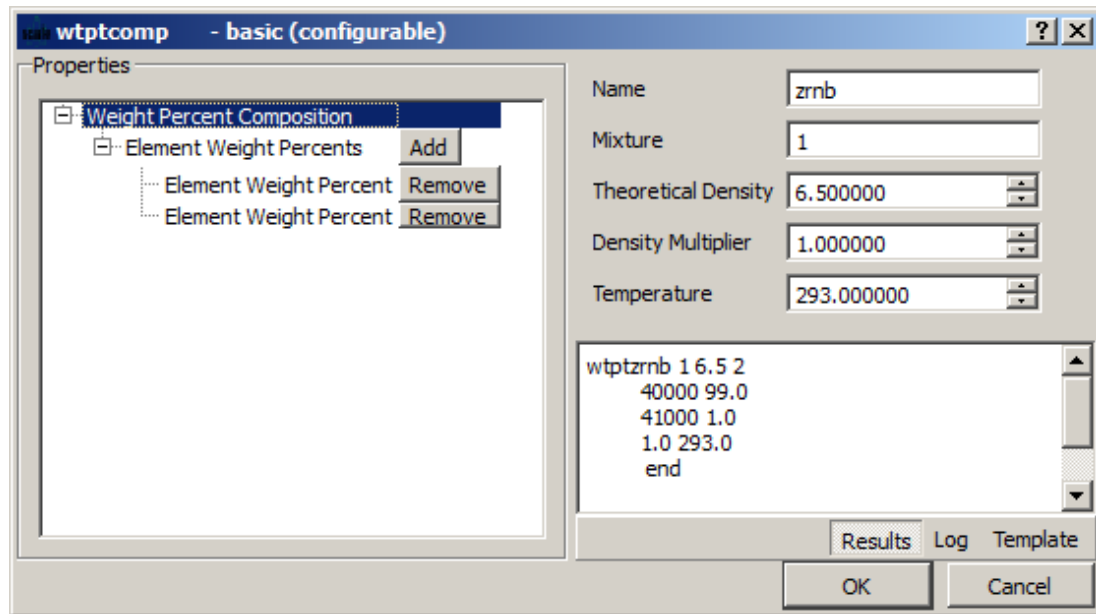
Weight percent mixture

- *wtptname* – “wtpt” prefix is required as a flag to SCALE
- Mixture number
- Theoretical density
- Number of elements
- Nuclide ID and weight percent
- Density multiplier
- Temperature (K) (optional)
- Isotopic distribution (optional)
- end

```
wtptzrn 1 6.5 2  
40000 99.0  
41000 1.0  
1.0 293  
end
```

Weight percent mixture

- Autocomplete and configurable also work for weight percent mixtures (wtptcomp)
- Default wtptcomp is “wtptuo2”



Exercise: Weight percent mixture



Problem 3

- Concrete
 - Overall density 2.32 g/cm^3
 - Constituent elements (w/o)
 - 48.49 w/o O (8000)
 - 23.31 w/o Ca (20000)
 - 15.5 w/o Si (14000)
 - 5.52 w/o C (6000)
 - 2.17 w/o Al (13000)
 - 1.37 w/o K (19000)
 - 1.25 w/o Mg (12000)
 - 1.01 w/o Fe (26000)
 - 0.75 w/o H (1000)
 - 0.63 w/o Na (11000)
 - Material temperature 293 K

Exercise solutions: Weight percent mixture



Problem 3

```
wtptconc      6  2.32  10
                26000 1.01
                1000 0.75
                6000 5.52
                8000 48.49
                12000 1.25
                13000 2.17
                14000 15.5
                19000 1.37
                11000 0.63
                20000 23.31
                1.0 293  end
```

Concrete is a common material, but no two concretes are the same. Without an assay of the particular concrete relevant to your safety case, studies should be performed to identify a conservative composition for your application. Magnason's concrete is a fictitious composite intended to bound all real concretes for criticality safety applications. See also recent work by Richard Taylor [1] and EPRI [2] on generic concrete compositions.

- [1] R. G. Taylor (2016), "Characteristics of Thick Concrete Neutron Reflection," Doctoral Dissertation, University of Tennessee, Knoxville. https://trace.tennessee.edu/utk_graddiss/4173/
[2] EPRI reference

Fissile solutions



Fissile solution components

Component Name	Nuclides in component		
UO ₂ (NO ₃) ₂	Nitrate solutions	92000	8000 7000
Th(NO ₃) ₄		90000	8000 7000
Pu(NO ₃) ₄		94000	8000 7000
HNO ₃		1001	7000 8000
UO ₂ F ₂	Fluoride solutions	92000	9019 8000
ThF ₄		90000	9019 8000
PuF ₄		94000	9019 8000
HF			1001 9019

From Table 7.2.6. Table of available solution components

Fissile solution input example

- More complex composition definition compared to all other discussed options
- Multiple components are allowed/used in each solution
 - One or two salts and potentially excess acid
 - HNO_3 for nitrate solutions and HF for fluoride solutions
- *solution ... end solution* construct within composition block
- Many inputs keyworded within solution block

Fissile solution input

```
SOLUTION MIX=5 RHO[UO2(NO3)2]=225 92235 91 92238 8 92234 0.8 92236 0.2  
MOLAR[HNO3]=0.6 TEMPERATURE=293 END SOLUTION
```

- **MIX**=mixture number – only mixture type with keyword
- **RHO**[]=mass of fissile component per liter of solution, in this case gU/L, gPu/L, or gTh/L
 - Followed by enrichment of fissile component
- **MOLAR**[]=excess acid molarity
- **TEMPERATURE**=temperature (K)
 - Temperature must be > 273.15 K → Don't freeze the solution!

Fissile solution input (cont.)

- Overall solution density can also be input
- SCALE can also solve for the density if “?” is entered: `density=?`
- Isotopic distributions can follow any other specification
 - For example, uranium enrichment on previous slide
- One or two fuel salts are allowed
 - Excess acid can be input as third component if needed

Exercise: Fissile solutions



Problem 1 – together!

- **UO₂F₂ solution**

- Specific gravity 2.0289
 - Assume water density at lab conditions is exactly 1 g/cm³
- 907.01 gm U/l
- Enrichment:
 - U-235 5.0 %
 - U-238 95.0 %

Problem 2

- Uranyl nitrate solution
 - Unknown density – let SCALE calculate it
 - 334.77 gU/l
 - Excess nitric acid 0.521 M
 - Enrichment:
 - 1.022 w/o ^{234}U
 - 93.172 w/o ^{235}U
 - 0.434 w/o ^{236}U
 - 5.372 w/o ^{238}U

Exercise solutions: Fissile solutions



Problem 1

```
solution mix=1 rho[uo2f2]=907.01 92235 5.0 92238 95  
          density=2.0289 temp=293 volfrac=1.0  
end solution
```

Problem 2

```
solution      mix=5  rho[uo2(no3)2]=334.77  92234  1.022
                                           92235  93.172
                                           92236  0.434
                                           92238  5.372

              molar[hno3]=0.521
              density=?  temperature=293  vol_frac=1

end solution
```

Composition specification summary



SUMMARY

- SCALE includes several options for defining mixtures in the composition block for use in neutron transport models
- The options to define a mixture were developed to simplify definitions for typical materials
- SCALE automatically calculates nuclide densities for all mixtures definitions
- The mixing table should be used to double-check the input

```
read comp
h2o 1 den=2.99056 0.26703 300 end
uo2 1 den=2.99056 0.73297 300 end
'
h2o 2 0.8 300 end
uo2 2 0.2 300 end
'
b4c 3 den=2.460000 1.0 293.0
      5010 30.0
      5011 70.0 end
'
atomIFBA 4 6.1 2
      40000 1
      5000 2
      1.0 293.0
      5010 45.0 5011 55.0 end
'
wtptzrnb 5 6.5 2
      40000 99.0
      41000 1.0
      1.0 293.0 end
'
solution mix=6 rho[uo2f2]=1.0 92235 4.5
92238 95.5
      density=1.0 temp=300 volfrac=1.0
end solution
end comp
```