Statement of Problem

Expressions have been formulated to calculate atom number densities starting from basic reactor geometrical data. These expressions will be programmed by the Math Department. The resulting code, called INPUT, will prepare the calculated number densities on input cards for MUFT and TNS.

Results and Conclusions

The INPUT code will prepare and output number densities in several different ways depending upon the data which the user has at his disposal to input to the code, and whether the output is needed for MUFT or TNS input.

If number density cards are desired for regions of cores for which the number densities have previously been calculated, the user can simply input* information specifying core, and core region desired and what type of output cards are to be prepared (MUFT and TNS at present). Provision will be made to

* See appendix for input and output details.
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add new sets of number densities to the program library as they are obtained. It will also be possible to incorporate new output formats into the code, if in the future extensive use is made of programs other than MUFT and TNS for cross section preparation. If the user wishes to modify one or more of the stored number densities (e.g. reduced fuel loading, etc.) this modifying factor will, of course, have to be input to the code.

In order to handle cases in which number densities are desired for cores in which the number densities have not already been calculated; a library of elements will be included. This will be composed of the MUFT and TNS libraries plus HfC, TiC, NbC, and B4C. This library will contain the density ($\rho$) and atomic mass (Matm) of each of these elements. Avogadro's number (No) will also have to be stored. Provision will be made for adding new elements to this library as they are needed.

The library of elements will be used in several different ways to calculate number densities depending on the information the user has available for input. However, in each case, the user must have at least one of the following sets of data available for the region or regions in which number densities are desired.

1. The volume fractions of the elements in the region
2. The geometry of the region and the total masses of the elements present
3. The weight per cents of the elements present.

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Method of Analysis

For the case in which the volume fractions for a given region are known and number densities for that region are desired the user simply inputs the volume fractions of the various elements present along with the element identification numbers*. Number densities for this region can then be calculated from:

\[
\text{Number Density} = \frac{\rho N_a}{M_{\text{atm}}} = \text{N. D. for each element}
\]

These will be called "macroscopic" number densities.

However, the user may have at his disposal volume fractions for two or more reactor components or regions and may want these regions or components to be "smeared out" into a single region or cell. For example, suppose the user wishes to consider a cell composed of one unfueled element surrounded by six fueled elements as below:

* See Appendix
In this case it is known that from the point of view of a cell composed of these seven components the volume fraction of fueled elements = 6/7 = $\mathcal{V}_F$, and the volume fraction of unfueled elements = 1/7 = $\mathcal{V}_U$.

Suppose further that the user knows that for an unfueled element the volume fraction of carbon = 3/4 = $\mathcal{V}_{UC}$, and the volume fraction of niobium = 1/4 = $\mathcal{V}_{UNb}$; and that for a fueled element the volume fraction for carbon = 5/8 = $\mathcal{V}_{FC}$, the volume fraction for niobium = 1/8 = $\mathcal{V}_{FNb}$, and the volume fraction of U235 = 1/4 = $\mathcal{V}_F U_{235}$. Then the "smeared out" volume fraction for carbon will be:

$$\mathcal{V}_C = \mathcal{V}_{UC} \mathcal{V}_{UF} + \mathcal{V}_F \mathcal{V}_{FC} = \frac{1}{7} \cdot \frac{3}{4} + \frac{6}{7} \cdot \frac{5}{8} = \frac{9}{14}$$

The number density of carbon in this cell would then be calculated from:

$$N_{DC} = (\rho C Na/ Matm)\mathcal{V}_C$$

The number densities of U235 and Nb would be calculated in a completely similar fashion. These will be known as "microscopic" number densities.

As was stated above, the user may also input the geometry of the region or regions along with the masses of the various elements in each region. In this case he will first specify the geometry desired (hex, slab, cylinder, sphere, cylindrical, shell, spherical shell); the dimensions and the weights of the elements in question. The code will then calculate the volume of the region from the type of geometry and dimensions:

<table>
<thead>
<tr>
<th>Geometry</th>
<th>Volume</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hex</td>
<td>$3 s^2 L$</td>
</tr>
<tr>
<td>Slab</td>
<td>LTH</td>
</tr>
<tr>
<td>Cylinder</td>
<td>$\pi r^2 L$</td>
</tr>
</tbody>
</table>
Sphere \[ \frac{4}{3} \pi r^3 \]
Cylindrical Shell \[ \pi L (r_2^2 - r_1^2) \]
Spherical Shell \[ \frac{4}{3} (r_o^3 - r_i^3) \]

The code will then use this calculated volume \( = V_{\text{reg}} \) to obtain a density over the region for each element \( \rho_{\text{el}} \)

\[
\rho_{\text{el}} = \frac{\text{Mass of Element}}{V_{\text{reg}}} \]

The number densities for each element are then calculated from:

\[
N. D. \text{ el} = \rho_{\text{el}} \frac{\text{Na}}{\text{Matm}}
\]

These calculations may also be performed either "microscopically" or "macroscopically".

Finally the user may input up to four different elements in a given region along with the weight fractions of these elements in that region, and obtain number densities for that region. For example, suppose the user has elements A and B with weight fractions \( w/o A \), \( w/o B \). The code, then, first calculates volume fractions for A and B as follows:

\[
\text{VF}_A \frac{\rho_A}{w/o A} = \text{VF}_B \frac{\rho_B}{w/o B} \tag{1}
\]

and

\[
\text{VF}_A + \text{VF}_B = 1 \tag{2}
\]

so

\[
\text{VF}_A = \frac{\text{w/o A}}{\text{w/o B}} \frac{\rho_B}{\text{VF}_B} \tag{A}
\]

from (2)

\[
\text{VF}_B = \frac{1}{\text{w/o A}} \frac{\rho_B + 1}{\text{w/o B}} \tag{B}
\]

\[
\text{VF}_A = 1 - \text{VF}_B
\]
These volume fractions are then used to calculate the corresponding number densities.

\[
\text{N.D.}_A = \frac{\rho_A N_A}{\text{Matm}} \cdot VF_A \\
\text{N.D.}_B = \frac{\rho_B N_A}{\text{Matm}} \cdot VF_B
\]

If the maximum of four elements are included equations (1) and (2) become for elements A, B, C, D;

\[
\frac{VF_A \rho_A}{\text{w/o A}} = \frac{VF_B \rho_B}{\text{w/o B}} = \frac{VF_C \rho_C}{\text{w/o C}} = \frac{VF_D \rho_D}{\text{w/o D}}
\]

(3)

\[
VF_A + VF_B + VF_C + VF_D = 1
\]

(4)

These equations are then solved for the volume fractions and the corresponding number densities are calculated. This calculation also can be performed either "microscopically" or "macroscopically".

It should be mentioned that in case one of the "elements" included in a region is really a compound (e.g. HfC, TiC, etc.) the calculated number density of the compound is added to any elements already present which appear in the compound. For example, if a region contains Nb, C, Hf, and HfC and the calculated number densities are:

\[
\begin{align*}
\text{NDNb} &= .003 \\
\text{NDc} &= .02 \\
\text{NDHf} &= .01 \\
\text{NDHfC} &= .001
\end{align*}
\]

Then the output will give .021 as the total number density of carbon in the region and .011 as the total number density of hafnium.

SIGNED  
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Appendix

Since the input code has not been programmed yet, the information
given below is a tentative plan for putting data into the code.

Card I:  
L1  
1 denotes library search  
2 denotes calculation  
L2  
1 denotes calculation, given volume fraction  
2 denotes calculation, given geom & weights  
3 denotes calculation, given weight per cents  
L3  
1 denotes microscopic calculation  
2 denotes macroscopic calculation

Card II:  
Reactor type (IRX)  
Region (IRG)  
Case (ICS)  
1 denotes NRX-A-1  
2 denotes KIWI B-1  
3 denotes KIWI B-2  
4 denotes KIWI B-4  
10 denotes radial region 10  
11 denotes axial region 1  
12 denotes axial region 2  
30 denotes axial region 20  
N\text{CH} denotes No. of densities to be Changed (1-12 at present)  
\text{ITP}\text{NPR}\text{OB}\text{V}\text{OLFR}\text{MACROSCOPIC CALCULATION, GIVEN VOLUME FRACTION}}
MICROSCOPIC CALCULATION, GIVEN VOLUME FRACTION

Card II: \( \text{ITP} \) \( \text{NPRB} \) denotes problem No.
1 denotes TNS
2 denotes MUFT

Card III: \( \text{NVF} \) denotes No. of volume fractions being input/region.
\( \text{NTPS} \) denotes No. of regions that are similar.

Card IV: \( (\text{NVF} + 3) \) \( \text{NELM} \) denotes the signal no. of the element no. density being calculated.
\( \text{VOLFR} \) denotes the volume fraction density being calculated.

MACROSCOPIC CALCULATION, GIVEN GEOMETRIES AND WEIGHTS

Card II: \( \text{NWT} \) denotes no. of weights being input.
\( \text{ITP} \) \( \text{NPRB} \) denotes problem no.
1 denotes TNS
2 denotes MUFT

\( \text{DIM1, DIM2, DIM3} \) denote
1 denotes slab dimensions of particular geometry.
2 denotes sphere geometry.
3 denotes cylinder
4 denotes hex
5 denotes cylindrical shell

Card III: \( (\text{NGW} + 2) \) \( \text{NELM} \) denotes signal no. of element no. density to be calculated.
\( \text{WT} \) denotes weight of element present.

MICROSCOPIC CALCULATION, GIVEN GEOMETRIES AND WEIGHTS

Card II: \( \text{ITP} \) \( \text{NPRB} \) denotes problem no.
1 denotes TNS
2 denotes MUFT

Card III: \( \text{NWT} \) denotes no. of weights input/volume
\( \text{IGEM} \) denotes type of geom. (see macro. case)
\( \text{DIM1, DIM2, DIM3} \) denote dimensions of geometry.

Card IV: \( (\text{NWT} + 3) \) \( \text{NELM} \) denotes signal no. of element no. densities to be calculated.
\( \text{WT} \) denotes weight of element present.