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INNOVATIVE METHOD TO CALCULATE THE ATOMIC DENSITIES OF ANY COMPOUND MIXED WITH A MODERATOR

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INTRODUCTION

Atomic densities – what for ?

- Are basic input data of any criticality calculation code
- For homogeneous fissile material, they are varying with the amount of moderator present inside the material

How to obtain them ?

- Experimental density laws, isopiestic laws, chemical analysis …
- If the total volume and the total mass of the mixture are respectively the sum of the volume and the sum of the mass, of each of its components, analytical expression can be determined. We will call it “Volume addition law”

“Volume addition law”

- Applicable for metals, oxides, carbides, nitrides and alloy mixtures
- Limitation: must be determined case by case (and is specific to a moderator).
- Sample for mixed oxide : $C(UPuO_2) = \dfrac{1}{\dfrac{1}{d_{UPuO_2}} + \dfrac{1}{2}\dfrac{M_{H_2O}}{M_{UPuO_2}}\dfrac{1}{d_{H_2O}}\dfrac{H}{UPu}}$
- And for $C(^{235}U + Pu)$? $C(^{235}U + Pu) = \dfrac{1-(1-E)(1-t)}{\dfrac{M_{UPuO_2}}{M_{UPu}}\dfrac{1}{d_{UPuO_2}} + \dfrac{1}{2}\dfrac{M_{H_2O}}{M_{UPu}}\dfrac{1}{d_{H_2O}}\dfrac{H}{U+Pu}}$
- And expressed as $\dfrac{H}{^{235}U + Pu}$ ratio ?

$$C(^{235}U + Pu) = \frac{1-(1-E)(1-t)}{\dfrac{M_{UPuO_2}}{M_{UPu}}\dfrac{1}{d_{UPuO_2}} + \dfrac{1}{2}\dfrac{M_{H_2O}}{M_{UPu}}\dfrac{1}{d_{H_2O}}\dfrac{H}{^{235}U + Pu}(1-\%at_{^{235}U,U}\,\%at_{U,U+Pu})}$$

- As user imagination is limitless, how can we give freedom to user so that any relation between concentration and moderator to fuel ratio can be used ?

Is it possible to determinate a generalized analytical relation ?

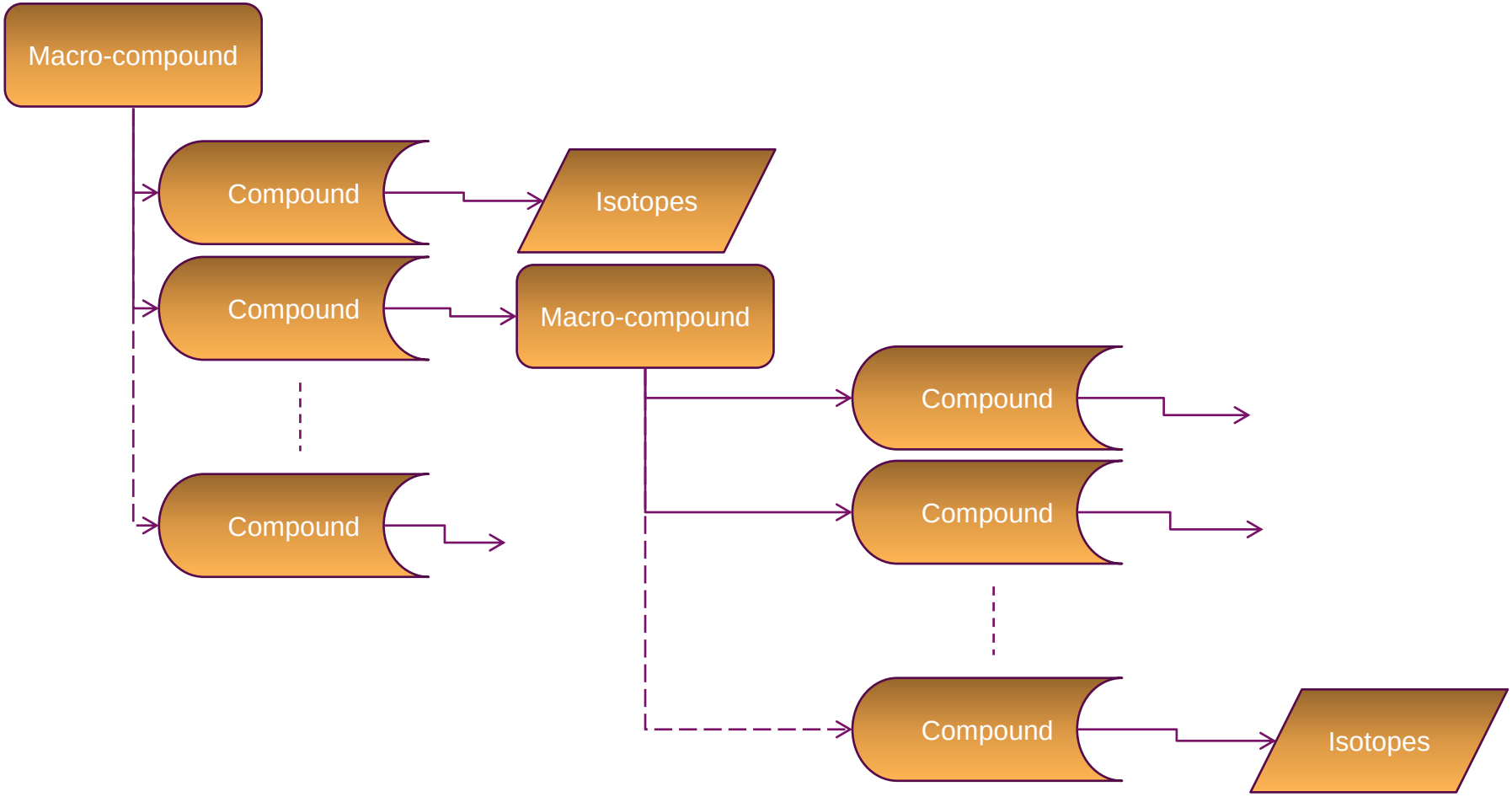
- Study parameters or pertinent parameters of materials may be versatile
- Obtaining a generic analytical relation need all intermediate parameter such as:
  - atom or weight fraction of isotopes
  - molar mass of compounds

Circumvent the problem

- Tree-shaped compound description
- Mix fissile material and moderator tree-shaped compound descriptions
- Density law solver

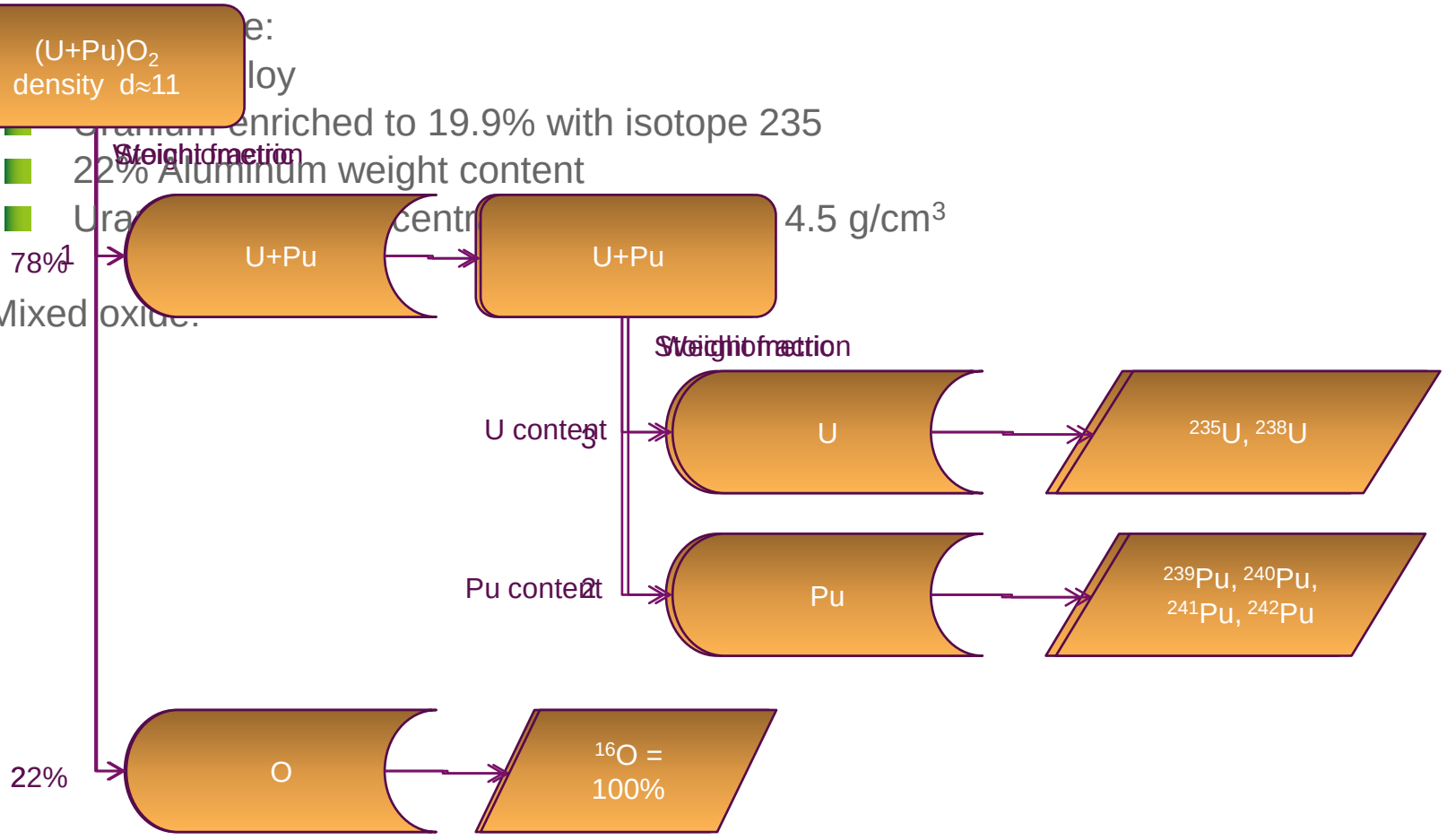
TREE-SHAPED COMPOUND DESCRIPTION

- Split the compound in increasingly smaller sub-compounds, until its isotopic components, keeping each intermediate compound



Illustrative example

- (U+Pu)O_2 density d≈11
  - Uranium enriched to 19.9% with isotope 235
  - 22% Aluminium weight content
  - Ura… centr… 4.5 g/cm^3
- Mixed oxide:



DENSITY LAW RESOLUTION PRINCIPLE

- Density law resolution implies to solve the following equation with a constraint given by the user on the value of a given relation named M (usually moderator to fuel ratio, atomic density of an atom …)

$$\frac{C_{m,\,fuel}}{\rho_{fuel}} + \frac{C_{m,\mathrm{moderator}}}{\rho_{\mathrm{moderator}}} = 1$$

- α variable is introduced:

$$\begin{cases} C_{m,\,fuel} = \alpha\,\rho_{fuel} \\ C_{m,\mathrm{moderator}} = (1-\alpha)\,\rho_{\mathrm{moderator}} \end{cases}$$

- α is searched until M(α) is equal to user input value

CONCLUSIONS

- Tree-shaped description and dilution law solver have been implemented in a tool
  - Input file structure reflects tree-shaped description
  - No difference with CIGALES V3.2 of CRISTAL V1.2 criticality safety package
- Coupling tree-shaped compound description and associated solver with a multi-parameterization tool has increases its power and gives the user more ease and flexibility in the choice of parameters for criticality safety studies
- All user-performed tests have demonstrated the effectiveness and ease to calculate atomic and mass concentrations of any material with any moderator

Thanks for your attention

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