

Efficient Subsurface Radioactive Transport Modeling using yam2ogsprj Python Package

Qian Chen
24.10.2023

Different Scenario models

$$(\underbrace{\phi + \rho K_{d,i}}_{(3)}) \frac{\partial c_i}{\partial t} = \underbrace{\frac{\partial}{\partial x} \left(\phi D_p \frac{\partial c_i}{\partial x} \right)}_{(1)} - \underbrace{q \frac{\partial c_i}{\partial x}}_{(2)} + (\underbrace{\phi + \rho K_{d,i}}_{(3)}) \underbrace{\left(\sum_j \lambda_{j,i}^e c_j - \sum_l \lambda_{i,l}^e c_i \right)}_{(4)}$$

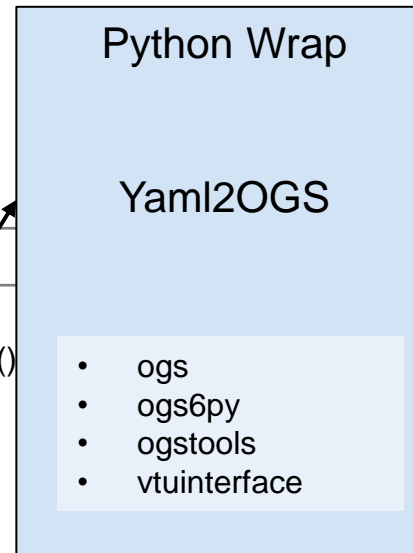
(1) Diffusion; (2) Advection; (3) Absorption; (4) Decay

Scenario	Diffusion	Advection	Absorption	Decay
S_1				√
S_2	√			√
$S_{3,1}$	√	√		√
$S_{3,2}$	√		√	√
S_4	√	√	√	√

decaychain.run_simulation()

Yaml Files:

```
Scenarios(Decay=True,
           Diffusion=True,
           Advection=True,
           Absorption=True)
```



Scenario	Concentration Field	Accumulated Dose
S_1		
S_2		
$S_{3,1}$		
$S_{3,2}$		
S_4		

- Concentration Field for each nuclides (.vtu)
- Accumulated Dose

Examples

Actinium decay chain $A = 4n+3$



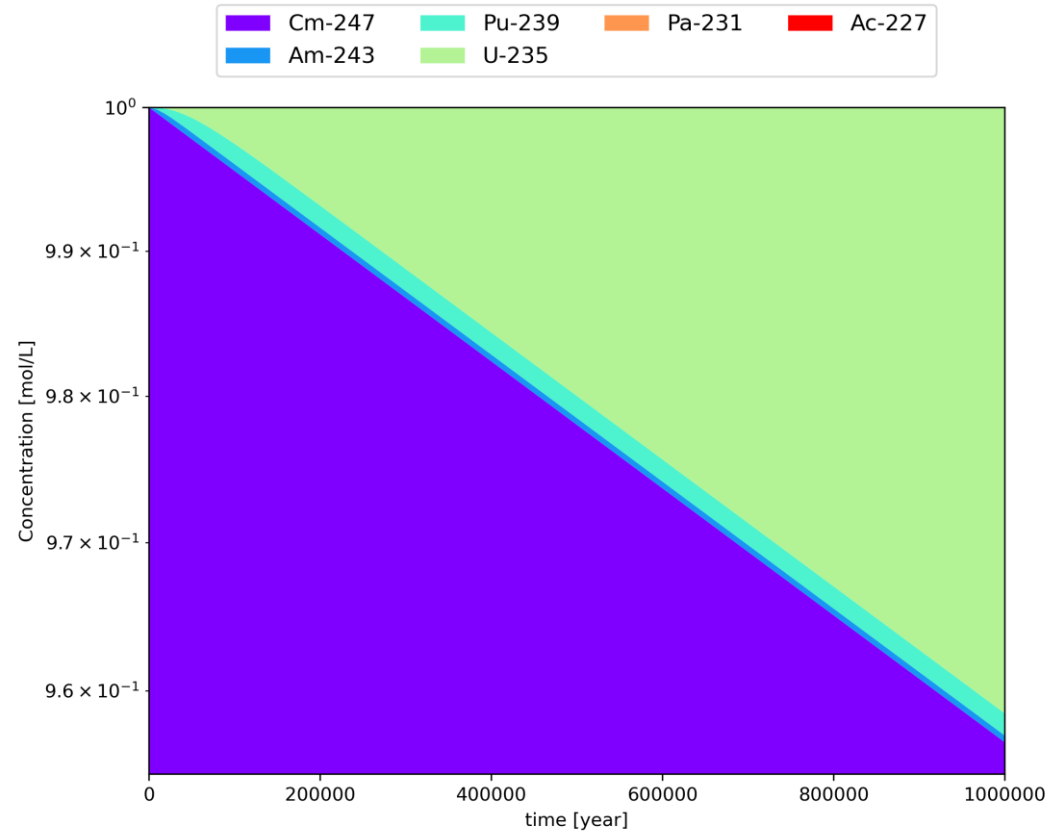
	cm-247	Am-243	Pu-239	U-235	Pa-231	Ac-227
half_life[year]	1.56e7	7.37e3	2.41e4	7.04e8	3.28e4	21.773
init c(x,0)	0	0	0	0	0	0
bc: c(0,t)	1	0	0	0	0	0

Scenario	Diffusion	Advection	Absorption	Decay
S_1				√
$S_{3,2}$	√		√	√
S_4	√	√	√	√

Example: Decay only

	cm-247	Am-243	Pu-239	U-235	Pa-231	Ac-227
half_life[year]	1.56e7	7.37e3	2.41e4	7.04e8	3.28e4	21.773
c(t=0)	1	0	0	0	0	0

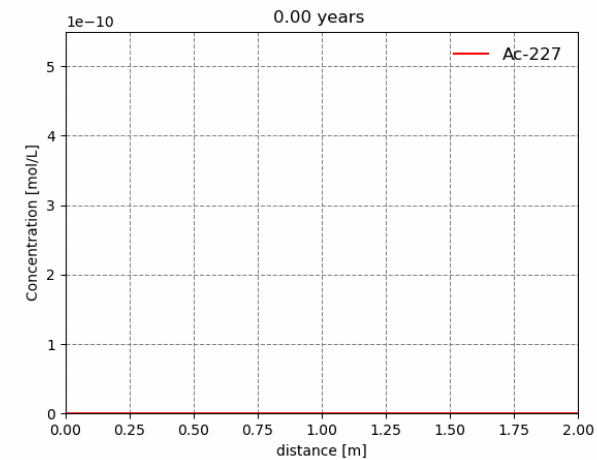
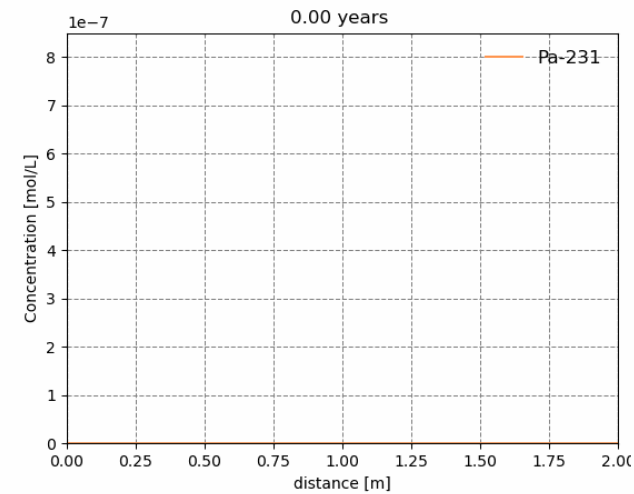
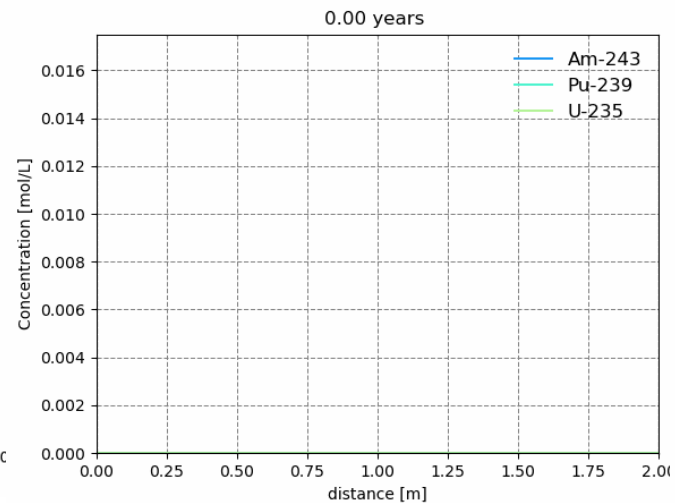
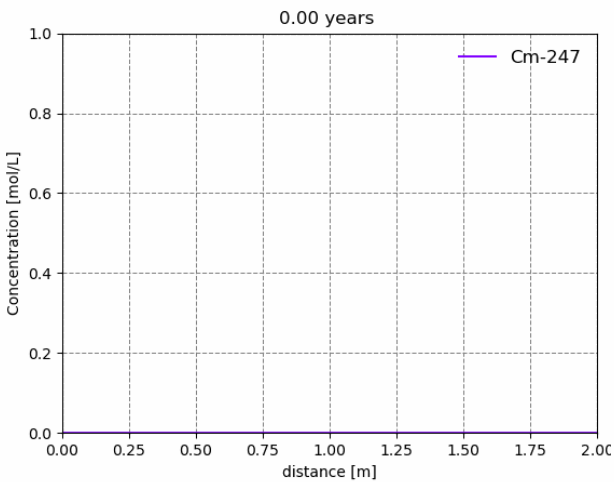
Decay only: Concentration Vs Time



Example: Decay+Diffusion+Sorption

	cm-247	Am-243	Pu-239	U-235	Pa-231	Ac-227
half_life[year]	1.56e7	7.37e3	2.41e4	7.04e8	3.28e4	21.773
bc: c(0,t)	1	0	0	0	0	0

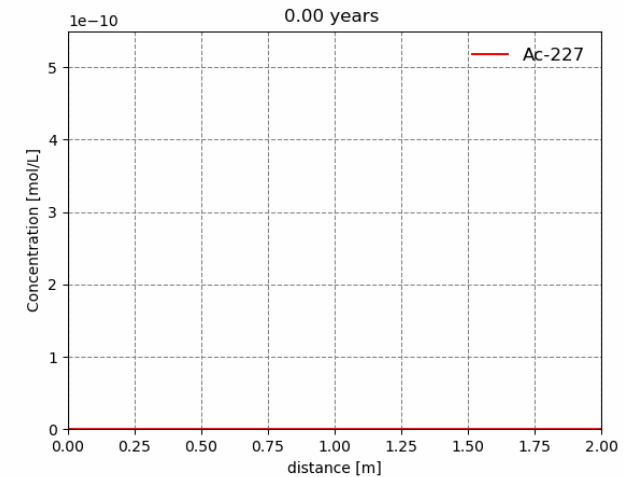
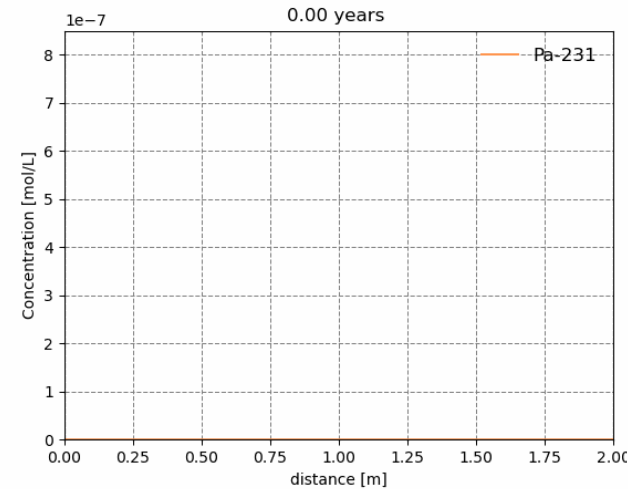
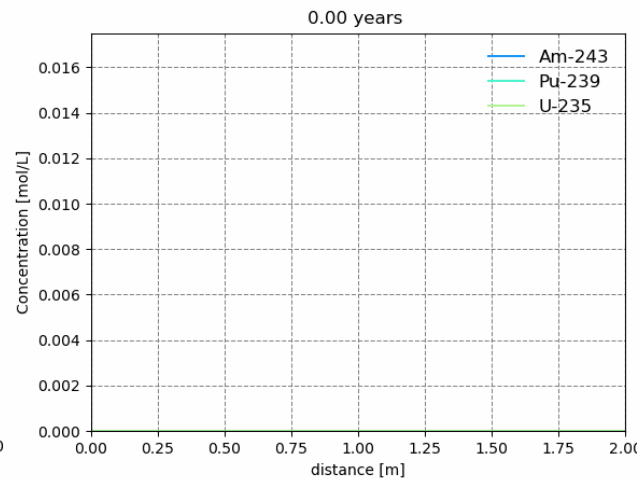
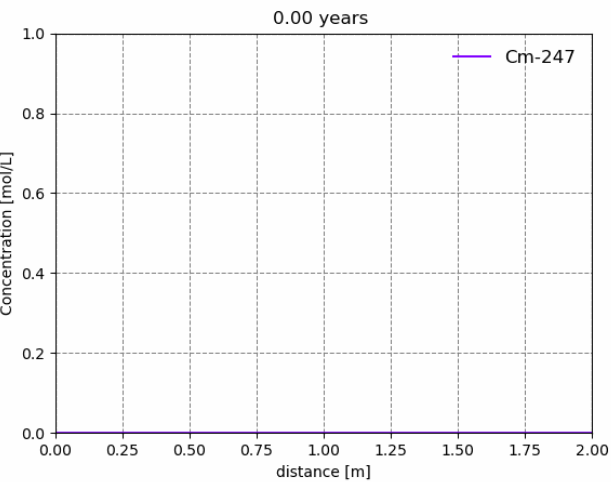
Decay + Diffusion + Sorption(1e-11): Concentration Vs Distance



Example: Decay+Diffusion+Advection+Sorption

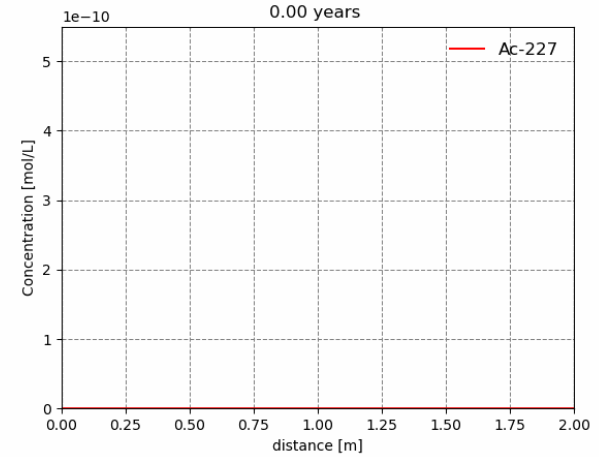
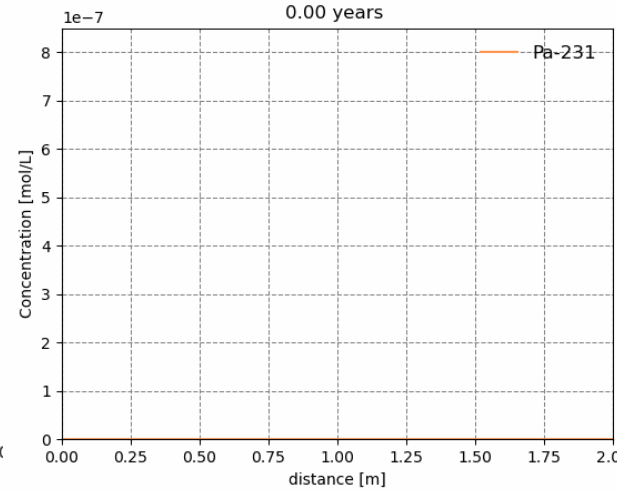
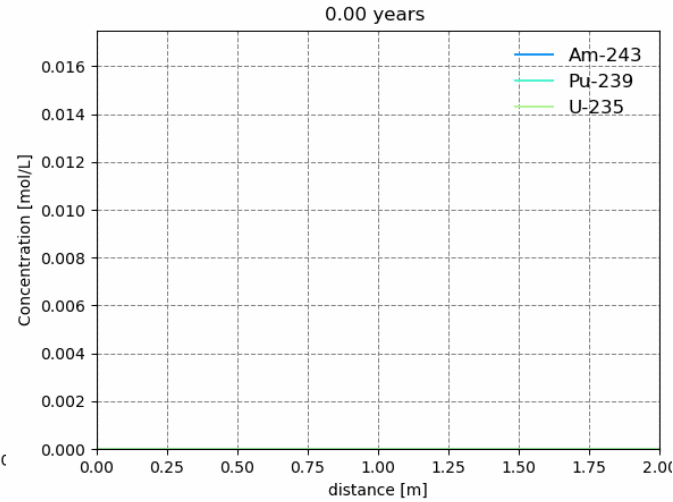
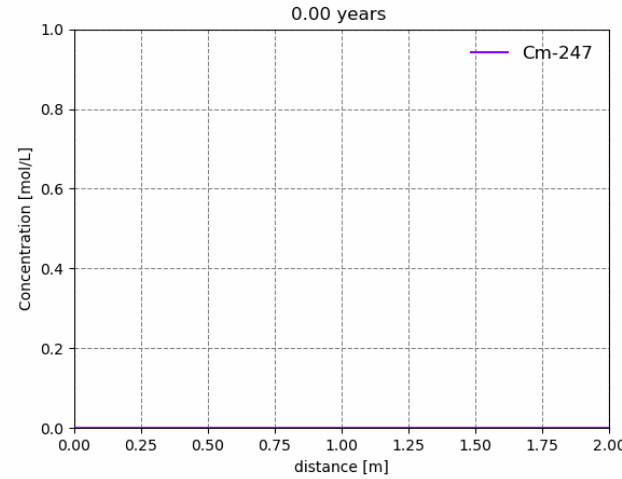
	cm-247	Am-243	Pu-239	U-235	Pa-231	Ac-227
half_life[year]	1.56e7	7.37e3	2.41e4	7.04e8	3.28e4	21.773
bc: c(0,t)	1	0	0	0	0	0

Decay + Diffusion($1e-11$) + Advection($2e-11$)+Sorption(0.5): Concentration Vs Distance

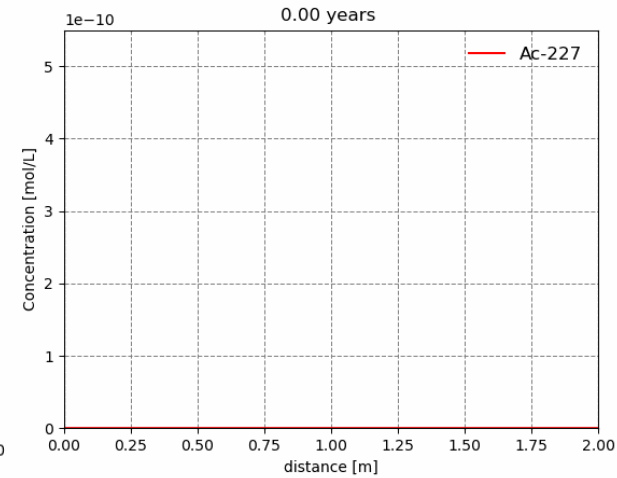
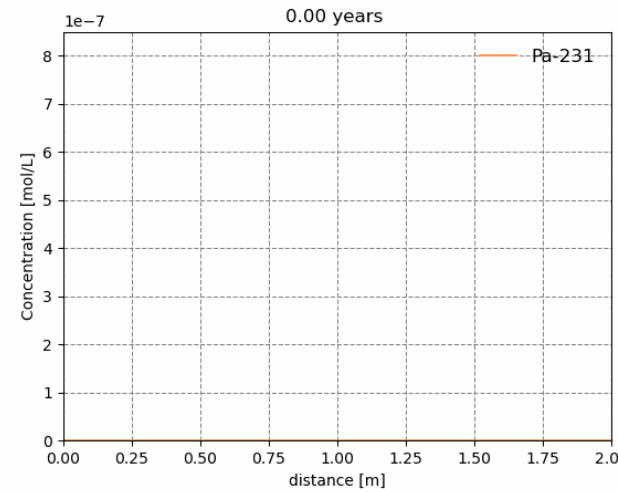
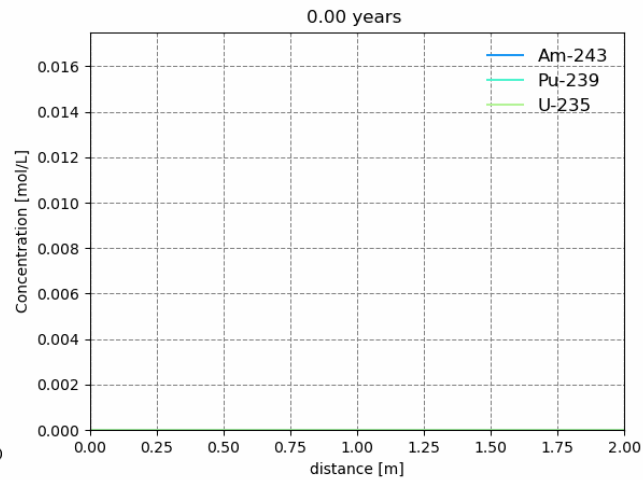
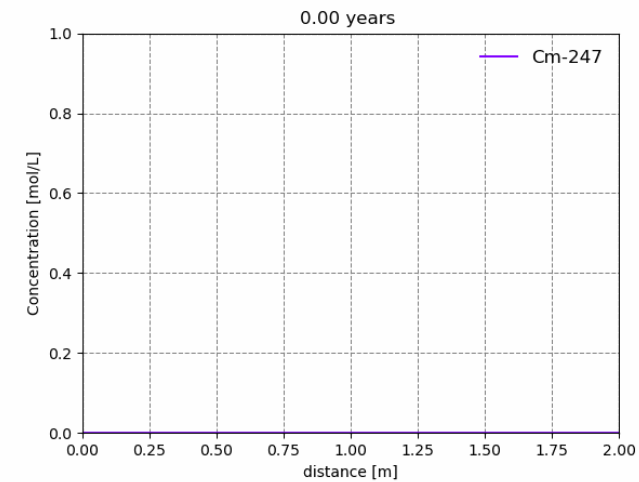


Concentration Vs Distance

Decay + Diffusion($1e-11$)+Sorption(0.5):



Decay + Diffusion($1e-11$) + Advection($2e-11$)+Sorption(0.5):



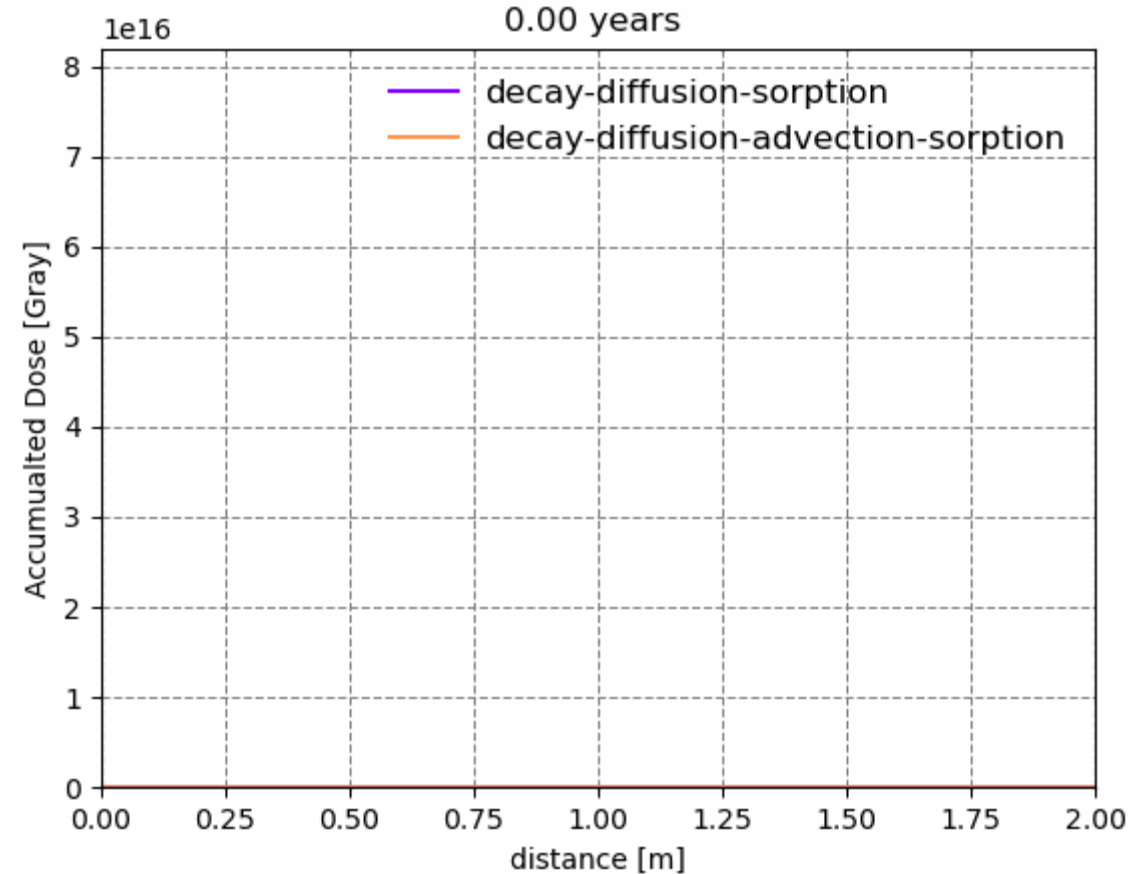
Accumulated Dose

From the evaluation of the absorbed dose (D) (Stabin, 2007):

$$D = \frac{\Delta E}{\Delta m} = \frac{\sum_{i=0}^{N-1} \lambda_i C_i \Delta V_k N_A \Delta t_j \tilde{E}_i}{\rho_k \Delta V_k} = \frac{1}{\rho_k} \sum_{i=0}^{N-1} \lambda_i C_i N_A \Delta t_j \tilde{E}_i$$

- International Commission on Radiological Protection(ICRP)

Z	Element	Nuclide	Half-life	Decay mode	Emitted energy (MeV/nt)			
					Alpha	Electron	Photon	Total
		Cm-240	27 d	ASF	6.3650	0.0108	0.0022	6.3781
		Pu-236	9.9700E-01					
		SF	3.9000E-08					
		Cm-241	32.8 d	ECA	0.0603	0.1342	0.5034	0.6979
		Am-241	9.9000E-01					
		Pu-237	1.0000E-02					
		Cm-242	162.8 d	ASF	6.2041	0.0096	0.0020	6.2156
		Pu-238	1.00					
		SF	6.3700E-08					
		Cm-243	29.1 y	AEC	5.8929	0.1342	0.1353	6.1624
		Pu-239	9.9760E-01					
		Am-243	2.4000E-03					



GUI for Data Hub

Sim Data Hub

Map name: Earth

Datasets: multivariables_test

Overview Map | Data | Plot

Map

North America | Europe | Asia | Africa | Australia

Table

multivariables_test

property	type	value	unit	unit	variabl	variabl	variabl	source
test_case2	expressio	9.31*x + 3...	kg/m ³	[1 -3 0 0 -]	{'x': 'temp'}	{'x': ['0 0-']}	{'x': 'K'}	None
test_case3	expressio	9.31*x + 3...	kg/m ³	[1 -3 0 0 -]	{'x': 'temp'}	{'x': ['0 0-']}	{'x': 'K'}	None

Plot

multivariables_test

Ice-
data-
hub:

Ice Data Hub

Planetary body: Earth

Datasets: Greenland - NorthGRIP

Overview Map | Data | Plot

Greenland - NorthGRIP

75.016667° N, 42.533333° W

URS-
data-
hub

URS Data Hub

Host rock: Claystone

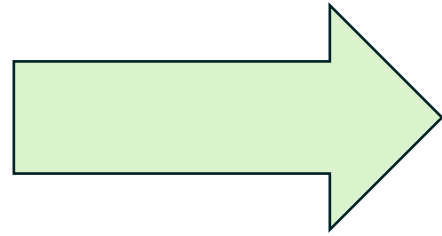
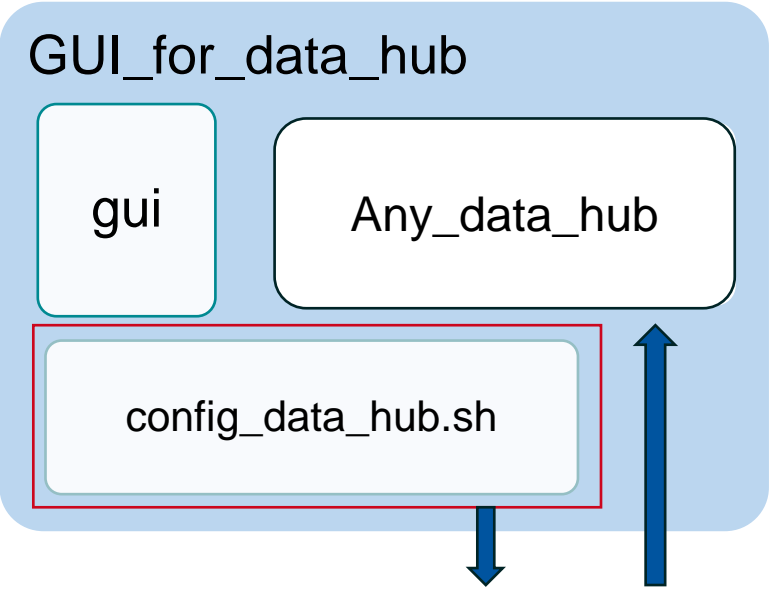
Datasets: Reference Model north, claystone

Overview Map | Data | Plot

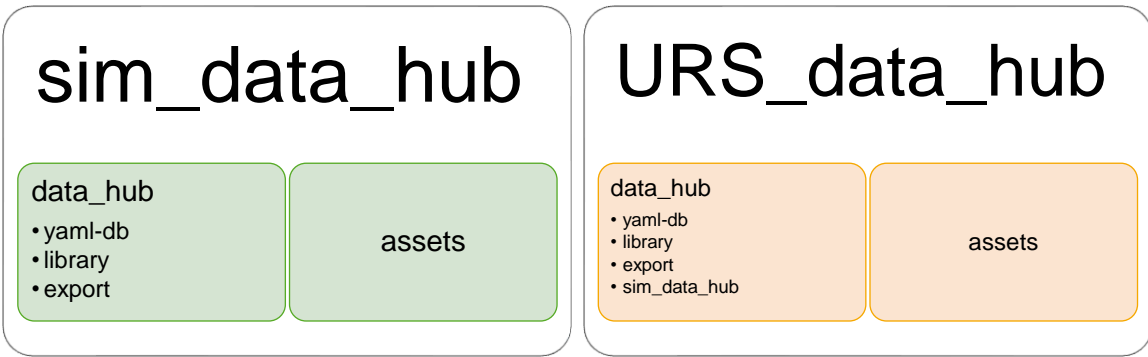
Reference Model north, claystone

GUI for Data Hub

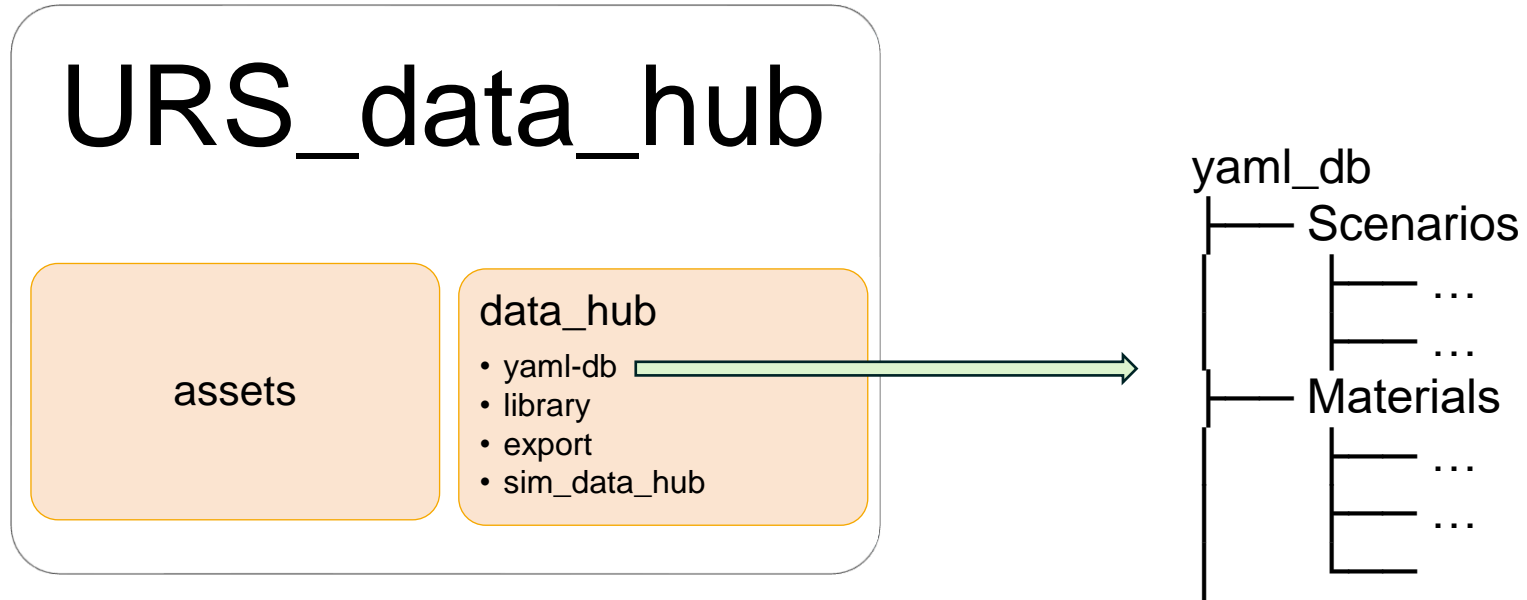
FRONTEND:



BACKEND (Any data_hub):



Yaml-db structure



Thank you for your attention