External Neutrons: Material Properties

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DUNE Backgrounds Mitigation Strategies Workshop

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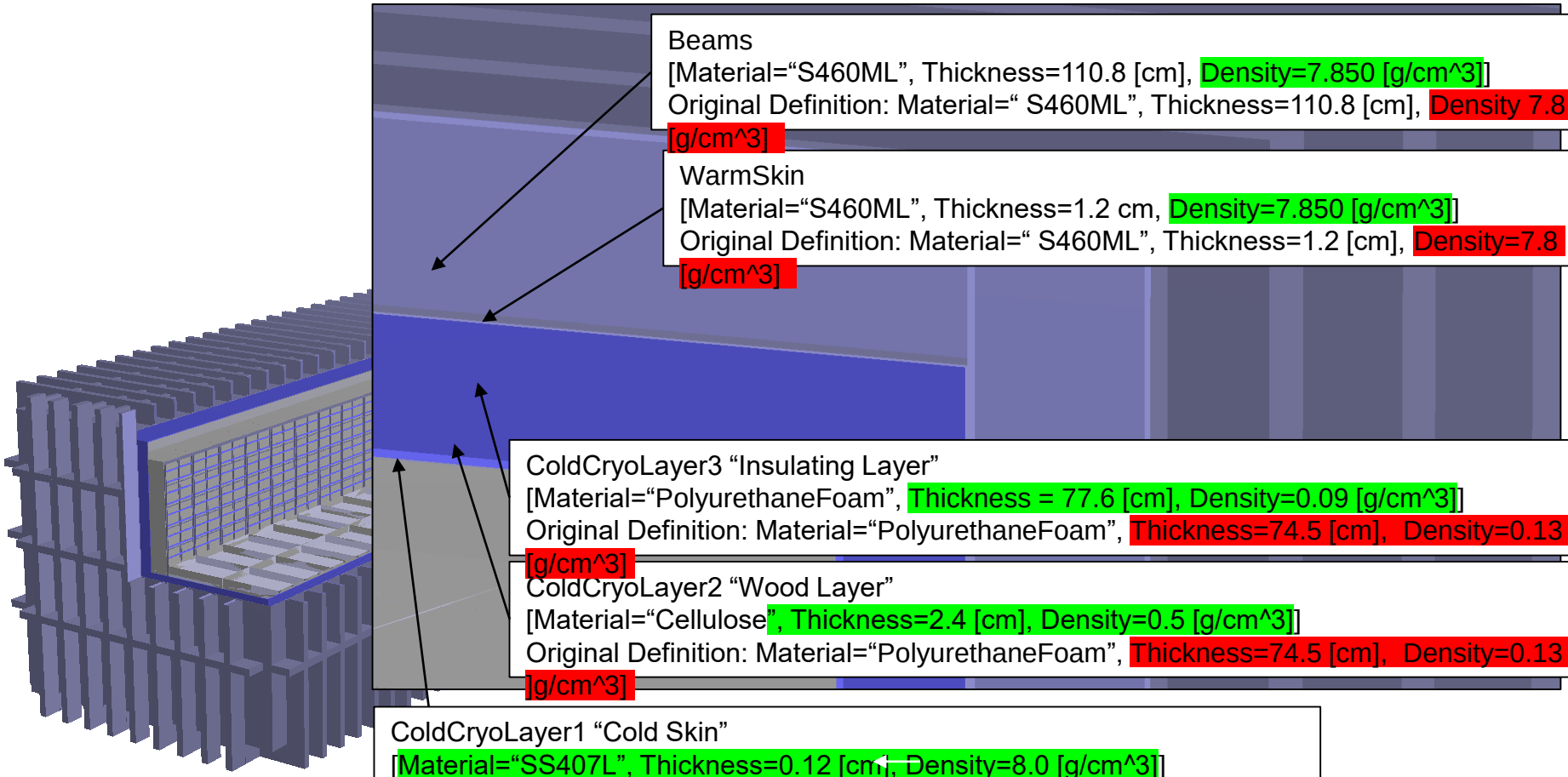
Far Detector Construction and Layers

File Names: larfd.gdml and larfd_nowires.gdml
Files created by Pierre Lasorak, and Aran Borkum



Beams
[Material="S460ML", Thickness=110.8 [cm], Density=7.850 [g/cm^3]]
Original Definition: Material=" S460ML", Thickness=110.8 [cm], Density 7.8 [g/cm^3]

WarmSkin
[Material="S460ML", Thickness=1.2 cm, Density=7.850 [g/cm^3]]
Original Definition: Material=" S460ML", Thickness=1.2 [cm], Density=7.8 [g/cm^3]

ColdCryoLayer3 "Insulating Layer"
[Material="PolyurethaneFoam", Thickness = 77.6 [cm], Density=0.09 [g/cm^3]]
Original Definition: Material="PolyurethaneFoam", Thickness=74.5 [cm], Density=0.13 [g/cm^3]

ColdCryoLayer2 "Wood Layer"
[Material="Cellulose", Thickness=2.4 [cm], Density=0.5 [g/cm^3]]
Original Definition: Material="PolyurethaneFoam", Thickness=74.5 [cm], Density=0.13 [g/cm^3]

ColdCryoLayer1 "Cold Skin"
[Material="SS407L", Thickness=0.12 [cm], Density=8.0 [g/cm^3]]
Original Definition: Material="S460ML" Thickness=0.1 [cm], Density=8.0 [g/cm^3]

Steel Composition Modifications

Default Material		Modified Material	
Structural Steel “S460ML”		Structural Steel “S460ML”	
Density = 7.8 [g/cm^3]		Density = 7.850 [g/cm^3]	
Thickness Beams = 110.8 [cm]		Thickness = 110.8 [cm]	
Thickness WarmSkin = 1.2 [cm]		Thickness WarmSkin = 1.2 [cm]	
Element	**Elemental %**	**Element**	**Elemental %**
Iron (Fe)	96	Iron (Fe)	95.35
Manganese (Mn)	1.8	Manganese (Mn)	1.7
Nickel (Ni)	0.85	Nickel (Ni)	0.80
Silicon (Si)	0.65	Silicon (Si)	0.60
Copper (Cu)	0.6	Copper (Cu)	0.55
Carbon (C)	0.18	Carbon (C)	0.18
		Phosphorus (P)	0.030
		Sulfur (S)	0.025
		Aluminum (Al)	0.0002
		Nitrogen (N)	0.025
		Niobium (Nb)	0.05
		Vanadium (V)	0.12
		Titanium (Ti)	0.05
		Chromium (Cr)	0.30
		Molybdenum (Mo)	0.20

Default value of material changed
Modification to existing materials
New materials added to composition

taken from LBNF Cryostat Warm Structure Requirements - 2018 version 4

Steel Composition Modifications in larfd.gdml and larfd_nowires.gdml

Default Material		Modified Material	
ColdSkin “SS304L” Density = 8.00			
Element	**Mass %**	**Element**	**Num Atoms**
Iron (Fe)	65.045	Iron (Fe)	1219
Carbon (C)	0.03	Carbon (C)	3
Manganese (Mn)	2.0	Manganese (Mn)	36
Phosphorus (P)	0.045	Phosphorus (P)	1
Sulfur (S)	0.03	Sulfur (S)	1
Silicon (Si)	0.75	Silicon (Si)	27
Chromium (Cr)	19	Chromium (Cr)	365
Nickel (Ni)	10	Nickel (Ni)	170
Aluminum (Al)	0.1	Aluminum (Al)	4

This composition of “SS304L” has been created to reflect the actual material used in the cold skin of the cryostat.

https://www.upmet.com/products/stainless-steel/304304l

“PolyurethaneFoam” and “Cellulose”

Default material	Modified Material
Insulation “PolyurethaneFoam”	Insulation “PolyurethaneFoam”
Density = 0.13 [g/cm^3]	Density = 0.09 [g/cm^3]
Thickness = 74.5 [cm]	Thickness = 77.6 [cm]

Element	Num Atoms	Element	Num Atoms
Carbon (C)	54	Carbon (C)	54
Oxygen (O)	15	Oxygen (O)	15
Nitrogen (N)	4	Nitrogen (N)	4
Hydrogen (H)	60	Hydrogen (H)	60

Our CHN chemical analysis

Default Material	Modified Material
Wood layer “Cellulose”	Wood layer “Cellulose”
Density = 0.54591 [g/cm^3]	Density = 0.5 [g/cm^3]
Thickness = 4.5 [cm]	Thickness = 2.4 [cm]

Element	Num Atoms	Element	Num Atoms
Carbon (C)	6	Carbon (C)	50
Oxygen (O)	5	Oxygen (O)	44
Hydrogen (H)	10	Hydrogen (H)	6

Default value of material changed

Modification to existing materials

XRD Measured Weight % of Chemical Compounds: Convert to Atom % (Elemental %)

description	Fe2O3 [w%]	MnO2 [w%]	TiO2 [w%]	CaO [w%]	K2O [w%]	SiO2 [w%]	Al2O3 [w%]	MgO [w%]	Na2O [w%]	N2O [w%]	CO2 [w%]	H2O [w%]	total [w%]	*density [g/cm^3]*	*error*	O [a%]	Fe [a%]	Mn [a%]	Ca [a%]	K [a%]	Si [a%]	Al [a%]	Mg [a%]	Na [a%]	N [a%]	C [a%]	H [a%]	total [a%]
DUNE Ross - #6 Winze	18.0	0.1	0.0	0.0	0.7	40.7	24.8	8.9	0.3	0.0	0.0	6.5	100.0	2.67	0.05	55.3	2.8	0.0	0.0	0.3	13.9	6.0	6.8	0.2	0.0	0.0	14.8	100.0
DUNE Ross - Governor's Corner	3.8	0.3	0.0	0.0	4.4	74.9	12.7	1.4	0.8	0.0	0.0	1.7	100.0	2.65	0.10	62.4	0.6	0.1	0.0	2.0	26.2	3.1	1.1	0.5	0.0	0.0	4.0	100.0
DUNE Ross - Test Blast Site	16.4	0.1	0.0	0.2	0.9	39.3	27.7	8.1	0.2	0.0	0.0	7.1	100.0	2.68	0.10	54.8	2.5	0.0	0.1	0.4	13.3	6.6	6.1	0.1	0.0	0.0	16.0	100.0
DUNE Ross - #4 Winze	0.0	0.0	0.0	0.6	8.0	73.3	15.1	0.0	2.8	0.0	0.0	0.2	100.0	2.60	0.09	62.8	0.0	0.0	0.4	3.7	26.8	3.9	0.0	2.0	0.0	0.0	0.5	100.0
mean DUNE rock	**9.6**	**0.1**	**0.0**	**0.2**	**3.5**	**57.1**	**20.1**	**4.6**	**1.0**	**0.0**	**0.0**	**3.9**	**100.0**	**2.65**	**0.04**	**58.742**	**1.501**	**0.030**	**0.112**	**1.554**	**19.854**	**4.940**	**3.580**	**0.692**	**0.000**	**0.000**	**8.996**	100.000
Serenity's x-check on DUNE rock																58.9	1.5	0.0	0.1	1.6	20.0	4.9	3.5	0.7	0.0	0.0	8.8	100.0
Vitaly/Aran early numbers																59.0	2.3	0.0	0.1	1.4	18.3	7.6	2.2	0.6	0.0	0.0	8.5	100.0
& concrete ingredients:															<XRF>	56.4	4.1	0.05	6.63	3.04	21.32	4.95	2.29					98.78
sand (Cheyenne River, Oral/SD)	0.0	0.0	0.0	0.0	6.1	75.7	9.8	0.0	1.8	0.0	6.5	0.0	100.0	2.56	0.09	64.3	0.0	0.0	0.0	2.7	26.3	2.4	0.0	1.2	0.0	3.1	0.0	100.0
sand (commercial bag)	0.0	0.0	0.0	0.0	5.3	81.1	9.0	0.0	1.6	0.0	3.0	0.0	100.0	2.66	0.10	64.6	0.0	0.0	0.0	2.4	28.3	2.2	0.0	1.1	0.0	1.4	0.0	100.0
sand (Fisher in Nisland/SD)																												
gravel (Rapid City limestone quarry)	0.0	0.0	0.0	55.1	0.0	1.7	0.0	0.0	0.0	0.0	43.2	0.0	100.0	2.57	0.09	58.4	0.0	0.0	24.7	0.0	0.5	0.0	0.0	0.0	0.0	16.4	0.0	100.0
gravel (bag from South America)	0.0	0.0	0.0	0.0	10.9	74.3	13.7	0.0	1.1	0.0	0.0	0.0	100.0	2.49	0.09	63.1	0.0	0.0	0.0	5.1	27.4	3.6	0.0	0.8	0.0	0.0	0.0	100.0
gravel (Rogers Pit, Sundance/WY)														*2.9 cement?*													
Portland cement (Rapid City)	1.4	0.0	0.0	62.4	0.0	21.8	0.5	3.4	0.0	0.7	8.3	1.5	100.0	1.34	0.14	54.1	0.2	0.0	29.9	0.0	6.5	0.1	2.3	0.0	0.6	3.4	3.0	100.0
fly ash (power plant, Hastings/NE)														2.90	0.04	44.1	3.8	0.0	21.1	0.2	14.3	8.8	4.1	0.0	0.0	0.0	0	96.4
water (4850 Davis industrial & sump)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	100.0	1.00	0.01	33.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	66.7	100.0
mean Pete Lien														2.332		**56.538**	**0.132**	**0.001**	**21.061**	**0.283**	**4.173**	**0.514**	**0.382**	**0.120**	**0.067**	**12.005**	**4.724**	100.000
mean TCC														2.501		60.121	0.132	0.001	4.100	3.123	23.129	2.630	0.382	0.717	0.067	0.874	4.724	100.000
mean Croell															<XRF>	53.787	2.737	0.055	28.798	0.550	7.033	1.291	0.359				4.724	99.335
mean combined contractors														2.40	0.10	56.815	1.000	0.019	17.986	1.319	11.445	1.479	0.375	0.279	0.044	4.293	4.724	99.778

Identified 3 Different Potential Suppliers (Collected and Analyzed Detailed Ingredients at SDSMT)

(example Pete Lien & Sons)

Cement:	Type I-II (LA), GCC Dacotah Cement, Rapid City, SD	
Fly Ash:	Class F Modified, Boral Resources, Coal Creek, ND	
Coarse Aggr.:	Crushed Limestone, Pete Lien & Sons, Inc., Rapid City, SD	
Fine Aggr.:	Natural Sand, Pete Lien & Sons, Inc., Oral, SD	
Fine Aggr.:	Fine Limestone, Pete Lien & Sons, Inc., Rapid City, SD	
Admixtures:	BASF Admixtures Co., Air Entraining Agent, MBVR	
	Water Reducing Agent, Polyheed 997 & 322N	
Required Strength:	4000 PSI Comp. @ 28 Days	
Maximum Size Course Aggr.:	3/4 Inch ASTM C-33	
Slump:	4 ± 1 Inch	
Air Content:	4.5 – 7.5%	
Cement (Sp. Gr. 3.15):	452 Lbs.	2.30 CF
Fly Ash: (Sp.Gr. 2.59):	112 Lbs.	0.69 CF
Course Aggr. (Sp. Gr. 2.68):	1745 Lbs.	10.43 CF
Fine Aggr. Oral (Sp. Gr. 2.62):	394 Lbs.	2.41 CF
Fine Aggr. Rapid City (Sp. Gr. 2.66)	917 Lbs.	5.52 CF
Water (@ Maximum Slump):	30.5 Gals. (254 Lbs.)	4.07 CF
MBVR:	3 Ozs. (Approx.)	1.62 CF
997:	12.0 Ozs. (Approx.)	
322N:	12.0 Ozs. (Aprrox.)	
Theoretical Yield @ 6.0% Air		27.04 CF
Water/Cementitious Ratio:	.45	
Percent Fine Aggregate:	43%	
Cementitious Factor:	6.00 Sacks	

⇒ **Goal to realistically simulate external neutron backgrounds**

⇒ **Need to know precise chemical composition**

Chemical Composition (Atom %) & Density of Rock and Shotcrete Materials Measured at SDSMT

sample	description	density [g/cm^3]	error	O [a%]	Fe [a%]	Mn [a%]	Ca [a%]	K [a%]	Si [a%]	Al [a%]	Mg [a%]	Na [a%]	N [a%]	C [a%]	H [a%]
#1	DUNE Ross - #6 Winze	2.67	0.05	55.3	2.8	0.0	0.0	0.3	13.9	6.0	6.8	0.2	0.0	0.0	14.8
#2	DUNE Ross - Governor's Corner	2.65	0.10	62.4	0.6	0.1	0.0	2.0	26.2	3.1	1.1	0.5	0.0	0.0	4.0
#3	DUNE Ross - Test Blast Site	2.68	0.10	54.8	2.5	0.0	0.1	0.4	13.3	6.6	6.1	0.1	0.0	0.0	16.0
#4	DUNE Ross - #4 Winze	2.60	0.09	62.8	0.0	0.0	0.4	3.7	26.8	3.9	0.0	2.0	0.0	0.0	0.5
mean	**mean DUNE rock**	**2.65**	**0.04**	**58.742**	**1.501**	**0.030**	**0.112**	**1.554**	**19.854**	**4.940**	**3.580**	**0.692**	**0.000**	**0.000**	**8.996**
mean	Serenity's x-check on DUNE rock			58.9	1.5	0.0	0.1	1.6	20.0	4.9	3.5	0.7	0.0	0.0	8.8
mean	Vitaly/Aran early numbers			59.0	2.3	0.0	0.1	1.4	18.3	7.6	2.2	0.6	0.0	0.0	8.5
shotcrete	***& concrete ingredients:***		<XRF>	56.4	4.1	0.05	6.63	3.04	21.32	4.95	2.29				
Pete Lien	sand (Cheyenne River, Oral/SD)	2.56	0.09	64.3	0.0	0.0	0.0	2.7	26.3	2.4	0.0	1.2	0.0	3.1	0.0
TCC	sand (commercial bag)	2.66	0.10	64.6	0.0	0.0	0.0	2.4	28.3	2.2	0.0	1.1	0.0	1.4	0.0
Croell	sand (Fisher in Nisland/SD)														
Pete Lien	gravel (Rapid City limestone quarry)	2.57	0.09	58.4	0.0	0.0	24.7	0.0	0.5	0.0	0.0	0.0	0.0	16.4	0.0
TCC	gravel (bag from South America)	2.49	0.09	63.1	0.0	0.0	0.0	5.1	27.4	3.6	0.0	0.8	0.0	0.0	0.0
Croell	gravel (Rogers Pit, Sundance/WY)	*2.9 cement?*													
GCC	Portland cement (Rapid City)	1.34	0.14	54.1	0.2	0.0	29.9	0.0	6.5	0.1	2.3	0.0	0.6	3.4	3.0
Whelan Energy	fly ash (power plant, Hastings/NE)	2.90	0.04	44.1	3.8	0.0	21.1	0.2	14.3	8.8	4.1	0.0	0.0	0.0	0
SURF	water (4850 Davis industrial & sump)	1.00	0.01	33.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	66.7
mean	**mean Pete Lien**	2.332		**56.538**	**0.132**	**0.001**	**21.061**	**0.283**	**4.173**	**0.514**	**0.382**	**0.120**	**0.067**	**12.005**	**4.724**
mean	mean TCC	2.501		60.121	0.132	0.001	4.100	3.123	23.129	2.630	0.382	0.717	0.067	0.874	4.724
mean	mean Croell		<XRF>	53.787	2.737	0.055	28.798	0.550	7.033	1.291	0.359				4.724
mean	mean combined contractors	2.40	0.10	56.815	1.000	0.019	17.986	1.319	11.445	1.479	0.375	0.279	0.044	4.293	4.724

Potential Issues with G4 (Weight Percent vs. Elemental %)

Material: mixture

- Composition of compound materials

```
G4Element* elC  = …;   // define "carbon" element
G4Material* SiO2 = …;  // define "quartz" material
G4Material* H2O = …;   // define "water" material

density = 0.200*g/cm3;
G4Material* Aerog =
   new G4Material("Aerogel",density,ncomponents=3);
Aerog->AddMaterial(SiO2,fractionmass=62.5*perCent);
Aerog->AddMaterial(H2O ,fractionmass=37.4*perCent);
Aerog->AddElement (elC ,fractionmass= 0.1*perCent);
```

Mitigate Potential Issues with G4

Material: molecule

- A Molecule is made of several elements (composition by number of atoms):

```
a = 1.01*g/mole;
G4Element* elH  =
   new G4Element("Hydrogen",symbol="H",z=1.,a);
a = 16.00*g/mole;
G4Element* elO  =
   new G4Element("Oxygen",symbol="O",z=8.,a);
density = 1.000*g/cm3;
G4Material* H2O =
   new G4Material("Water",density,ncomp=2);
H2O->AddElement(elH, natoms=2);
H2O->AddElement(elO, natoms=1);
```

=> Scale our measured elemental %