

Preliminary STS Moderator Thermal Hydraulic Analysis

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Background

- This thermal-hydraulic analyses were performed to demonstrate that the current cylinder and tube moderator designs can meet the following requirements.
- Requirements
 - Pressure drop < 0.05 bar
 - Low pressure drop allows flexibility for CMS design
 - Maximum hydrogen temperature < 32K
 - Hydrogen density starts to change quickly over 32K
 - Average hydrogen density > 72.9 kg/m³
 - This density was assumed by neutronic calculations, but neutronics team thinks small deviations from this value will not cause significant loss of performance
 - Residence time > 0.2s, No regions of much longer residence time
 - Residence time >0.2s indicates the hydrogen will be in the moderator for greater than 3 beam pulses at 15 Hz which helps validate the steady state assumption



Background

- Previous MRA analysis (2020) done by Elvis (Elvis E Dominguez-Ontiveros) applied bounding curves for the heating. Bounding curve is a more conservative method, and the heating was overestimated by about a factor of 2.
- MRA geometry has been updated by Jim Janney and Ken Gawne since 2020.
- New heat sources were obtained from the MCNP energy deposition calculations done by Lukas Zavorka.
- The new MCNP calculations with Attila4MC unstructured mesh provides higher fidelity of heating results.
- Additional heating from 27AI(n,g)28AI reaction is also included in the new MCNP heating calculations.







Steady State Heat Transfer Analysis for Cylinder Moderator, Geometry







Steady State Heat Transfer Analysis for Cylinder Moderator, Mesh Configuration

Cylinder Moderator				
Al				
Mesh Type	Polyhedral mesh			
Base Size (m)	0.001			
Target Surface Size (m)	3.60E-04			
Minimum Surface Size (m)	1.00E-04			
Number of Prism Layers	3			
Prism Layer Stretching	2			
Prism Layer Total Thickness (m)	2.00E-04			
Number of Cells	3.31E+06			
H2				
Mesh Type	Polyhedral mesh			
Base Size (m)	0.001			
Target Surface Size (m)	5.00E-04			
Minimum Surface Size (m)	1.00E-04			
Number of Prism Layers	7			
Prism Layer Stretching	1.5			
Prism Layer Total Thickness (m)	2.00E-04			
Number of Cells	1.74E+06			
Total Cells (Al+H2)	5.04E+06			

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Steady State Heat Transfer Analysis for Tube Moderator, Mesh Configuration





CFD Modeling Details

- Simulation software: Simcenter STAR-CCM+
- Computer resource: Libby cluster at ORNL
 - Compute node:
 - □ Processors: two 16-core Intel Xeon E5-2683v4
 - □ 512 GB RAM
 - ✤ 1-3 nodes used
- Solution time: 2-3 days
- Flow and Energy model: Segregated solver
- Turbulence model: Realizable k-ε
- Wall treatment: Two-layer all y+
- H2 Volumetric flow rate: 0.5 l/s
- Unirradiated material properties
- Steady state simulation
- H2 inlet temperature: 19 K
- H2 outlet pressure: 14.5 bar
- Heat sources: MCNP Neutronics (Lukas Zavorka)

Mesh-Independent Study:

Mesh-independent studies were performed for earlier moderator concepts. The maximum temperature variations for AI and H2 were less than 0.4°C. Similar mesh settings were adopted for the current moderator designs. The wall y+ values in the cylinder and tube moderators are also kept below 5 to ensure the mesh configurations are appropriate for the usage of the two-layer all y+ wall treatment model in the CFD simulations.





Thermal Properties

Material	Thermal Conductivity, k (W/m-K)	Density, ρ (kg/m ³)	Specific Heat, Cp (J/kg-K)
AI (T = 20K)	28.43	2800	8.85
Para-H2	Table(T)	Polynomial in T	Table(T)

Thermal properties of Para-H2 can be found on https://webbook.nist.gov/chemistry/fluid/

Thermal properties of Al6061-T6 can be found on https://trc.nist.gov/cryogenics/materials/6061%20Aluminum/6061_T6Aluminum_rev.htm $\rho_{H_2}(T) = a + bT + cT^2 + dT^3$

 $k_{Al}(T) = 10^{a+b(\log_{10} T)} + c(\log_{10} T)^2 + d(\log_{10} T)^3 + e(\log_{10} T)^4 + f(\log_{10} T)^5 + g(\log_{10} T)^6 + h(\log_{10} T)^7 + i(\log_{10} T)^8$

 $Cp_{Al}(T) = 10^{a+b(\log_{10} T)} + c(\log_{10} T)^2 + d(\log_{10} T)^3 + e(\log_{10} T)^4 + f(\log_{10} T)^5 + g(\log_{10} T)^6 + h(\log_{10} T)^7 + i(\log_{10} T)^8$

Coefficient	$ ho_{H_2}$ (kg/m3)	k _{Al} (W/m-К)	Cp _{Al} (J/kg-K)
a	138.907	0.07918	46.6467
b	-8.23187	1.0957	-314.292
С	0.370104	-0.07277	866.662
d	-0.00621765	0.08084	-1298.3
е		0.02803	1162.27
f		-0.09464	-637.795
g		0.04179	210.351
h		-0.00571	-38.3094
i		0	2.96344



Thermal properties of Al6061-T6 can be found on https://trc.nist.gov/cryogenics/materials/6061%20 Aluminum/6061_T6Aluminum_rev.htm



Thermal Properties of Para-H2@1.45 MPa (14.5 bar)

https://webbook.nist.gov/cgi/fluid.cgi?Action=Load&ID=B5000001&Type=IsoBar&Digits=5&P=1.45&THigh=40&TLow=15&TInc=1&RefState=DEF&TUnit=K&PUnit=K&PUnit=kg%2Fm3&HUnit=kg%2Fm3&HUnit=m%2Fs&VisUnit=Pm*2Fs&VisUnit=N%2Fm

Temperature	Pressure	Density	Volume	Internal Energy	Enthalpy	Entropy	Cv	Ср	Sound Spd.	Joule-Thomson	Viscosity	Therm. Cond.	Phase
(К)	(MPa)	(kg/m3)	(m3/kg)	(kJ/kg)	(kJ/kg)	(J/g*K)	(J/g*K)	(J/g*K)	(m/s)	(K/MPa)	(Pa*s)	(W/m*K)	1 11450
15.000	1.4500	77.241	0.012946	-48.154	-29.382	-2.6918	5.2775	7.0899	1277.6	-1.5529	2.4601e-05	0.092173	liquid
16.000	1.4500	76.451	0.013080	-41.113	-22.146	-2.2249	5.3273	7.3893	1261.2	-1.4699	2.2056e-05	0.095267	liquid
17.000	1.4500	75.618	0.013224	-33.762	-14.587	-1.7667	5.3864	7.7374	1244.7	-1.3801	1.9938e-05	0.097931	liquid
18.000	1.4500	74.738	0.013380	-26.058	-6.6569	-1.3136	5.4585	8.1293	1226.8	-1.2869	1.8140e-05	0.10016	liquid
19.000	1.4500	73.806	0.013549	-17.961	1.6851	-0.86267	5.5415	8.5610	1206.8	-1.1922	1.6595e-05	0.10197	liquid
20.000	1.4500	72.820	0.013733	-9.4346	10.478	-0.41178	5.6311	9.0301	1184.5	-1.0969	1.5250e-05	0.10334	liquid
21.000	1.4500	71.775	0.013932	-0.44422	19.758	0.040913	5.7227	9.5370	1160.1	-1.0008	1.4069e-05	0.10430	liquid
22.000	1.4500	70.665	0.014151	9.0459	29.565	0.49705	5.8123	10.085	1133.5	-0.90325	1.3020e-05	0.10484	liquid
23.000	1.4500	69.483	0.014392	19.076	39.944	0.95832	5.8974	10.682	1104.9	-0.80288	1.2081e-05	0.10498	liquid
24.000	1.4500	68.220	0.014659	29.695	50.950	1.4266	5.9763	11.340	1073.9	-0.69779	1.1232e-05	0.10471	liquid
25.000	1.4500	<mark>6</mark> 6.862	0.014956	40.964	62.651	1.9042	6.0484	12.078	1040.6	-0.58545	1.0454e-05	0.10405	liquid
26.000	1.4500	65.393	0.015292	52.968	75.141	2.3939	6.1136	12.925	1004.5	-0.46250	9.7355e-06	0.10301	liquid
27.000	1.4500	63.789	0.015677	65.820	88.551	2.8999	6.1729	13.926	965.25	-0.32430	9.0613e-06	0.10164	liquid
28.000	1.4500	62.015	0.016125	79.687	103.07	3.4277	6.2284	15.155	921.99	-0.16406	8.4190e-06	0.099862	liquid
29.000	1.4500	60.021	0.016661	94.820	118.98	3.9859	6.2833	16.742	873.63	0.028890	7.7952e-06	0.097672	liquid
30.000	1.4500	57.719	0.017325	111.63	136.76	4.5883	6.3446	18.948	818.36	0.27297	7. 17 32e-06	0.095018	liquid
31.000	1.4500	5 4.952	0.018198	130.89	157.27	5.2609	6.4264	22.384	752.91	0.60440	6.5284e-06	0.091797	liquid
32.000	1.4500	51.35 7	0.019472	154.29	182.52	6.0618	6.5662	28.974	670.52	1.1108	5.8131e-06	0.087785	liquid
33.000	1.4500	45.670	0.021896	187.70	219.45	7.1966	6.9155	50.428	552.16	2.1104	4.8772e-06	0.082744	supercritical
34.000	1.4500	26.227	0.038129	290.76	346.04	10.961	8.2878	154.04	393.52	5.7891	2.7995e-06	0.072017	supercritical
35.000	1.4500	18.615	0.053721	344.62	422.52	13.185	7.5856	45.216	417.49	6.7857	2.3764e-06	0.050051	supercritical
36.000	1.4500	16.043	0.062333	368.49	458.87	14.210	7.1967	30.303	436.27	6.7671	2.3032e-06	0.045324	supercritical
37.000	1.4500	14.475	0.069086	385.70	485.87	14.950	6.9661	24.392	451.59	6.5915	2.2854e-06	0.043362	supercritical
38.000	1.4500	13.346	0.074928	399.88	508.52	15.554	6.8168	21.189	464.92	6.3739	2.2889e-06	0.042386	supercritical
39.000	1.4500	12.466	0.080217	412.32	528.64	16.077	6.7152	19.171	476.92	6.1480	2.3033e-06	0.041886	supercritical
40.000	1.4500	11.747	0.085129	423.64	547.07	16.544	6.6434	17.781	487.97	5.9262	2.3239e-06	0.041658	supercritical



Thermal Properties of Para-H2@1.45 MPa (14.5 bar)

https://webbook.nist.gov/cgi/fluid.cgi?Action=Load&ID=B5000001&Type=IsoBar&Digits=5&P=1.45&THigh=40&TLow=15&TInc=1&RefState=DEF&TUnit=K&PUnit=MPa&DUnit=kg%2Fm3&HUnit=kg%2Fm3&HUnit=m%2Fs&VisUnit=Pm%2Fs

	А	В	С	D	E	F	G	Н	I	J	K	L	М	N
1		original data	Polynomial			1.38907E+02			138.907					
2	Temperature (K)	Density (kg/m3)		error(%)		-8.23187E+00			-8.23187					
3	15	77.241	77.72	-0.48		3.70104E-01			0.370104					
4	16	76.451	76.48	-0.03		-6.21765E-03			-0.00621765					
5	17	75.618	75.38	0.24										
6	18	74.738	74.39	0.35										
7	19	73.806	73.46	0.34				De	nsity (kg	/m3)				
8	20	72.82	72.57	0.25						,,				
9	21	71.775	71.67	0.10		y = -6.21	.765E-	-03x ³ +	3.70104E-	-01x ² -	8.231	87E+00	X +	
10	22	70.665	70.73	-0.07		,			1 200075	02				
11	23	69.483	69.71	-0.23					1.369076+	UΖ				
12	24	68.22	68.57	-0.35	90									
13	25	66.862	67.27	-0.41	80									
14	26	65.393	65.79	-0.39	70	••••••	•••••••							
15	27	63.789	64.07	-0.28	70									
16	28	62.015	62.09	-0.07	2 00 Z							****		
17	29	60.021	59.80	0.22	<u>is</u> 50								····	
18	30	57.719	57.17	0.55	อี 40								-	
19	31	54.952	54.16	0.79	Õ 30									
20	32	51.357	50.73	0.62	20									
21	33	45.67	46.85	-1.18	20									
22					10									
23		Cylinder	Tube		0									
24	m_dot(l/s)	0.5	0.5			15		20	21	_		20		25
25	m_dot(m^3/s)	0.0005	0.0005			CT		20	23)		50		33
26	m_dot(kg/s)	0.0369	0.0369						Tempera	ture()	<)			
27			↑						rempere		`/			

Inlet mass flow rate

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Energy Deposition from Neutronics Calculation (from Lukas Zavorka)

energy deposition data for MRA

Link:

https://ornl.sharepoint.com/sites/sts/targetsystems/Shared%20Documents/Forms/AllItems.aspx?id=%2Fsites%2Fsts%2 Ftargetsystems%2FShared%20Documents%2FS%2E03%2E02%20Target%20Assembly%2F1%5FCALCULATIONS%2FCALC% 2D016%20%2D%20MRA%2FMRA%5FR5%2FNeutronics&viewid=9be9bc88%2D5a13%2D48c7%2D9fff%2Dd22f94ffdeb5

From: Zavorka, Lukas <zavorkal@ornl.gov> Sent: Monday, September 12, 2022 1:28 PM To: Kao, Min-Tsung <<u>kaom@ornl.gov></u> Cc: Janney, Jim <<u>janneyjg@ornl.gov></u> Subject: MRA energy deposition

Min-Tsung,

The energy deposition data for MRA have been uploaded here:

https://ornl.sharepoint.com/sites/sts/targetsystems/Shared%20Documents/Forms/AllItems.aspx?id=%2Fsites%2Fsts%2Ftargetsystems%2FShared%20Documents%2FS%2E03%2E02% 20Target%20Assembly%2F1%5FCALCULATIONS%2FCALC%2D016%20%2D%20MRA%2FMRA%5FR5%2FNeutronics&viewid=9be9bc88%2D5a13%2D48c7%2D9fff%2Dd22f94ffdeb5

Format as usual, i.e.,

X(cm), Y(cm), Z(cm), Energy(J/cc/pulse), Rel.error(neutrons and photons only), Volume(cm3)

in the .csv files for individual materials. This includes both MRA and backbone.

Total heating is also stored in "mra total numbers.xlsx", which gives 30.6 kW for MRA and 30.2 kW for backbone. Please check the total numbers if they match your import.

Please let me know if you have any questions about the data or if you find anything suspicious.

Thanks, Lukas Additional heating in MRA aluminum due to 27Al(n,g)28Al

Additional heating from the **27Al(n,g)28Al** reaction and **b-decay** in MRA hydrogen and reflector vessel.

Link:

https://ornl.sharepoint.com/sites/sts/targetsystems/Shared%20Documents/Forms/AllItems.aspx?id=%2Fsites%2Fsts%2Ftargetsy stems%2FShared%20Documents%2FS%2E03%2E02%20Target%20Assembly%2F1%5FCALCULATIONS%2FCALC%2D016%20%2D%2 0MRA%2FMRA%5FR5%2FNeutronics&viewid=9be9bc88%2D5a13%2D48c7%2D9fff%2Dd22f94ffdeb5

Additional heating in MRA aluminum due to 27Al(ng)28Al



Min-Tsung,

Here:

https://ornl.sharepoint.com/sites/sts/targetsystems/Shared%20Documents/Forms/AllItems.aspx?id=%2Fsites%2Fstargetsystems%2FShared%20Documents%2FS%2E03%2E02% 20Target%20Assembly%2F1%5FCALCULATIONS%2FCALC%2D016%20%2D%20MRA%2FMRA%5FR5%2FNeutronics&viewid=9be9bc88%2D5a13%2D4&c7%2D9fff%2Dd22194ffdeb5

were uploaded 4 files: 001g_Al_NG_20K_hydrogen_cyl.csv 001g_Al_NG_20K_hydrogen_tube.csv 001g_Al_NG_20K_reflector_cyl.csv 001g_Al_NG_200K_reflector_cyl.csv

with the additional heating from the 27Al(n,g)28Al reaction and b- decay in MRA hydrogen and reflector vessel. (4 files are for tube and cylinder moderator and hydrogen and reflector vessel, as the names indicate). This refers to Igor's note: AI-27 (n, gamma) AI-28 \rightarrow decay with e- emission with average energy of ~ 1.247 MeV.

This additional energy deposition is in the format as usual:

X(cm), Y(cm), Z(cm), Energy(J/cc/pulse), Rel.error(neutrons and photons only), Volume(cm3)

and shall be added to the original data for energy deposition in Aluminum. The calculations used the same UM model, meaning that the UM cell coordinates and volumes are the same, and adding the data to the previous set should be straightforward.

This heating in CYL hydrogen vessel is 36.37 W, which is additional 18.97% of the heating. (Agrees well with Igor's ~20% prediction) This heating in CYL reflector vessel is 164.73 W, which is additional 3.42% of the heating. This heating in TUBE hydrogen vessel is 34.73 W, which is additional 3.97% of the heating. (Agrees well with Igor's ~20% prediction) This heating in TUBE reflector vessel is 182.93 W, which is additional 3.97% of the heating.

Please let me know if this format is good for you or if you want me to combine this additional heating with the original numbers.

Thank you,

Lukas

Heat Sources for CFD calculations were obtained by multiplying the energy deposition by 15Hz.

https://ornl.sharepoint.com/sites/sts/targetsystems/Shared%20Documents/Forms/AllItems.aspx?id=%2Fsts%2Ftargetsystems%2FShared%20Documents%2FS%2E02%20Target%20Assembly%2F99%5FSANDBOX%2FKAO%2F2022%2F0%5FCFD%5FSTS% 5FMRA%2FMin%2DTsung%20Kao%5FSTS%5FMRA%5F2022%5F10%5F11%5FCylinder%5Fand%5FTube%5FModerators&viewid=9be9bc88%2D5a13%2D48c7%2D9fff%2Dd22f94ffdeb5



Energy Deposition from Neutronics Calculation (from Lukas Zavorka)

The energy deposition on AI vessel is not symmetric.



From Lukas:

Energy deposition is quite uniform in hydrogen volume, which means that we are in the optimal X position along the beam axis for cold neutron generation.

On the other hand, an **increased energy deposition in aluminum** at the **rear side** of the vessel most probably comes from **slow** and **thermal neutrons** that are generated in the rear portion of the tungsten target (as the proton beam slows down and neutron energy spectrum changes). This can also be seen on the outer/reflector aluminum body – see below.

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Results of Upper (Cylinder) H₂ Moderator



Steady State Heat Transfer Analysis for Cylinder Moderator, Heat Source



Steady State Heat Transfer Analysis for Cylinder Moderator, Pressure

 $\Delta P_{inlet-outlet} = 0.023$ bar (= 2.3 kPa = 0.33 psi = 0.023 atm)



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Steady State Heat Transfer Analysis for Cylinder Moderator, Density of H₂



Cylinder (upper) Moderator					
H ₂ Density at 19 K (kg/m^3)	73.806				
Average H_2 Density (kg/m^3)	72.569				
Variation (%)	1.68				



Steady State Heat Transfer Analysis for Cylinder Moderator, Temperature of H₂





Steady State Heat Transfer Analysis for Cylinder Moderator, Temperature of Al





Steady State Heat Transfer Analysis for Cylinder Moderator, Temperature for Interfaces between Al & H₂





Steady State Heat Transfer Analysis for Cylinder Moderator, Velocity of H₂





Steady State Heat Transfer Analysis for Cylinder Moderator, Streamlines





Steady State Heat Transfer Analysis for Cylinder Moderator, Streamline Animation



Streamlines and Temperature of H₂



Steady State Heat Transfer Analysis for Cylinder Moderator



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Steady State Heat Transfer Analysis for Cylinder Moderator

Average Heat Transfer Coefficient = 3,691 W/m^2-K





Steady State Heat Transfer Analysis for Cylinder Moderator





Results of Lower (Tube) H₂ Moderator



Heat source link Steady State Heat Transfer Analysis for Tube Moderator, Heat Source



Steady State Heat Transfer Analysis for Tube Moderator, Pressure

 $\Delta P_{inlet-outlet} = 0.0106 \text{ bar} (= 1.06 \text{ kPa} = 0.15 \text{ psi} = 0.0105 \text{ atm})$

High pressure due to stagnation point

Steady State Heat Transfer Analysis for Tube Moderator, Density of H₂

Tube (lower) Moderator	
H ₂ Density at 19 K (kg/m^3)	73.806
Average H_2 Density (kg/m^3)	72.832
Variation (%)	1.32

Steady State Heat Transfer Analysis for Tube Moderator, Temperature of H₂

Steady State Heat Transfer Analysis for Tube Moderator, Temperature of Al

Peak heating location is not where the peak temperature occurs.

Steady State Heat Transfer Analysis for Tube Moderator, Temperature & Velocity

Steady State Heat Transfer Analysis for Cylinder Moderator, Temperature for Interfaces between Al & H₂

Steady State Heat Transfer Analysis for Tube Moderator, Streamlines

Steady State Heat Transfer Analysis for Tube Moderator, Streamline Animation

Steady State Heat Transfer Analysis for Tube Moderator, Location of Peak Al Temperature

Steady State Heat Transfer Analysis for Tube Moderator, Location of Peak Al Temperature

Swirling flow (good for mixing and cooling); The mainstream reaches the AI wall.

Steady State Heat Transfer Analysis for Tube Moderator

Average Heat Transfer Coefficient = 2309 W/m^2-K

Steady State Heat Transfer Analysis for Tube Moderator Residence Time

Comparison between Requirements and CFD Results

	Doquiromont	CFD Re	sult
	kequiremeni	Cylinder Moderator	Tube Moderator
Pressure drop (bar)	< 0.05	0.023	0.0106
Maximum hydrogen temperature (K)	< 32	22.9	24.1
Average hydrogen density (kg/m ³)	> 72.9	72.569	72.832
Residence time (s)	> 0.2	0.64	0.93

- Except for average hydrogen density, all requirements are met with at least a factor of 2 margin
 - High confidence that margins are greater than uncertainties
- Neutronics will evaluate sensitivity to hydrogen density in order to develop a new hydrogen density requirement. We expect that the current results will give acceptable neutronic performance and the requirement will be updated.

Summary

- Most requirements are met except for the average hydrogen density (72.9 kg/m³).
 - All other requirements are met with at least a factor of 2 margin
- Neutronics will evaluate sensitivity to hydrogen density and will update hydrogen density requirement
- Final moderator analysis will include additional details
 - Moderator inlet temperatures updated based on single loop in series CMS design
 - Inclusion of moderator weld backer geometry
 - Inclusion of cylinder moderator transition to concentric flow geometry

