4th International Workshop on Sample Environment at Neutron Scattering Facilities

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Spreadsheet Calculations for Sample Environment Problems

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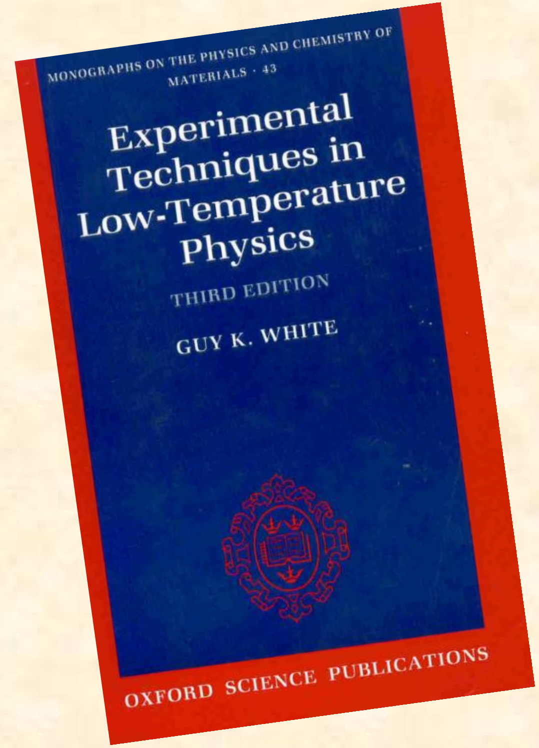
Motivation

- **Learn**
  - **How to apply fundamental principles to sample environment problems**
  - **How to obtain useful quantitative models**

- **Work smarter**
  - **Evaluate concepts before cutting metal**
  - **Compare observed and calculated data to better understand system behavior**

Starting Point

- **Classic reference guide**
  - **Simple examples**
  - **Useful tables**



- **Setup companion spreadsheets**

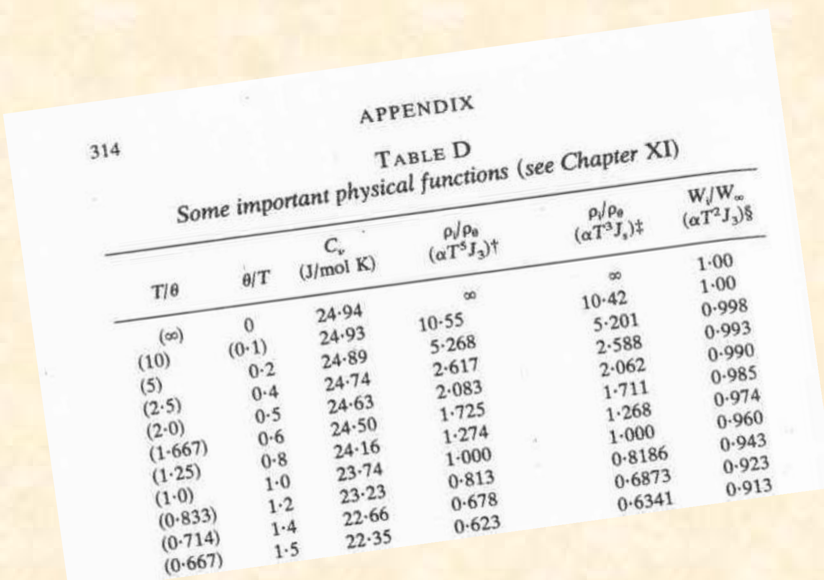


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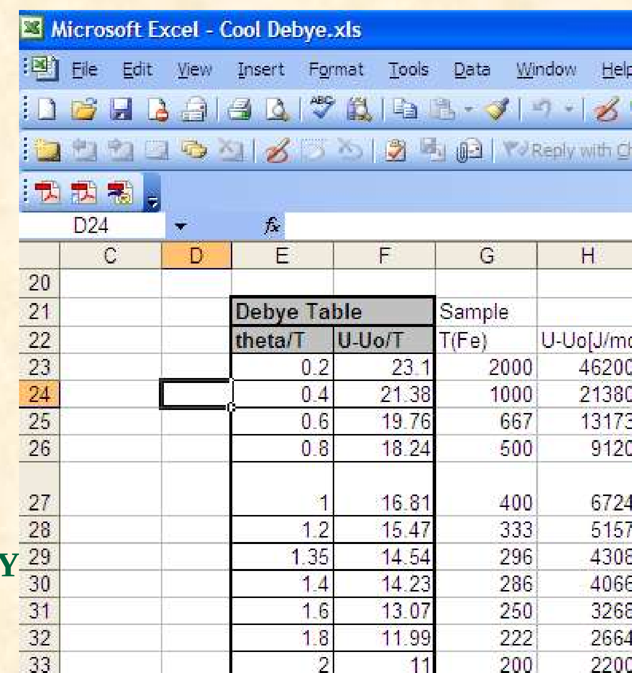
TABLE D

Some important physical functions (see Chapter XI)

T/θ	θ/T	C_v (J/mol K)	ρ_i/ρ_θ $(\alpha T^5 J_5)$†	ρ_i/ρ_θ $(\alpha T^3 J_3)$‡	W_i/W_∞ $(\alpha T^2 J_3)$§
(∞)	0	24·94	∞	∞	1·00
(10)	(0·1)	24·93	10·55	10·42	1·00
(5)	0·2	24·89	5·268	5·201	0·998
(2·5)	0·4	24·74	2·617	2·588	0·993
(2·0)	0·5	24·63	2·083	2·062	0·990
(1·667)	0·6	24·50	1·725	1·711	0·985
(1·25)	0·8	24·16	1·274	1·268	0·974
(1·0)	1·0	23·74	1·000	1·000	0·960
(0·833)	1·2	23·23	0·813	0·8186	0·943
(0·714)	1·4	22·66	0·678	0·6873	0·923
(0·667)	1·5	22·35	0·623	0·6341	0·913



Problem 1: Cooling with Liquid Nitrogen and Helium

- **Need to cool a 10kg hunk of iron**
  - **Initially at 293K**
- **How much liquid helium required …**
  - **to cool to 4.2 K?**
  - **If pre-cooled to 77K with LN2?**

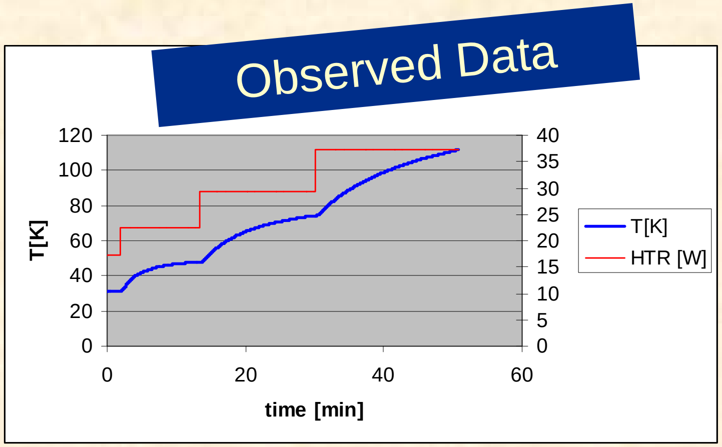
Problem 1: Cooling with Liquid Nitrogen and Helium

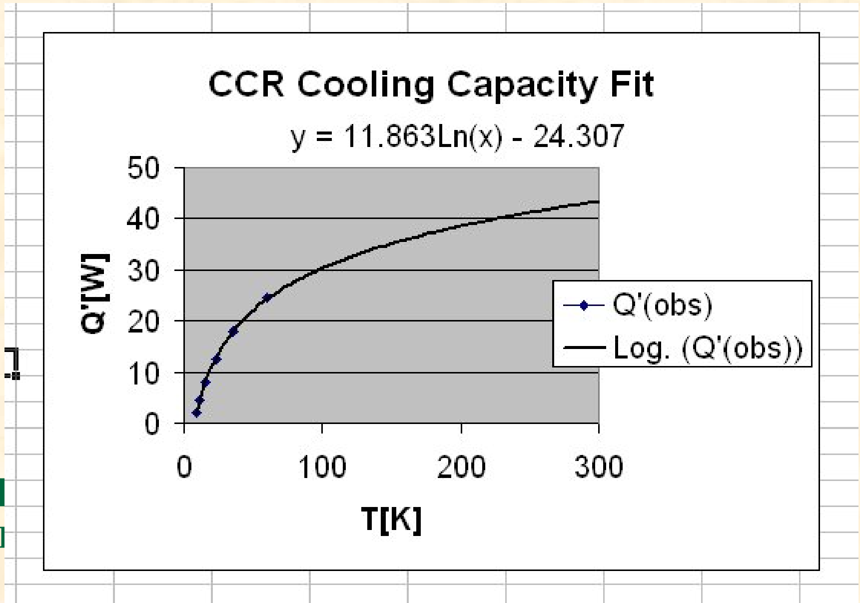
- **Need to cool a 10kg hunk of iron**
  - **Initially at 293K**
- **How much liquid helium required …**
  - **to cool to 4.2 K? 490 liters**
  - **If pre-cooled to 77K with LN2?**
    - **6 liters LN2**
    - **125 liters LHe**

	A	B	C	D	E	F	G	H	I
1	Cryogen Consumption Calculator								
2							Debye Table		
3	Material Spec			Calculate			theta/T	U-Uo/T	
4	mass [g]	10000					0.2	23.1	
5	Debye Temp	400		How many liters?			0.4	21.38	
6	molar mass	55.9		493.2			0.6	19.76	
7	Temperatures						0.8	18.24	
8	T(initial)	293					1	16.81	
9	T(final)	4.2					1.2	15.47	
10							1.35	14.54	
11	Cryogen spec						1.4	14.23	
12	latent heat	2.6					1.6	13.07	
13							1.8	11.99	
14	Reference						2	11	
15	Latent Heat of Vap [J/ml]						2.2	10.08	
16	Helium	2.6					2.4	9.23	
17	Nitrogen	161					2.6	8.44	
18	Debye Temperatures [K]		g/mol				2.8	7.73	
19	Copper	310	63.5				3	7.07	
20	Aluminum	380	27				3.5	5.66	
21	Iron	400	55.9				4	4.53	

Problem 2: Cooling with CCR

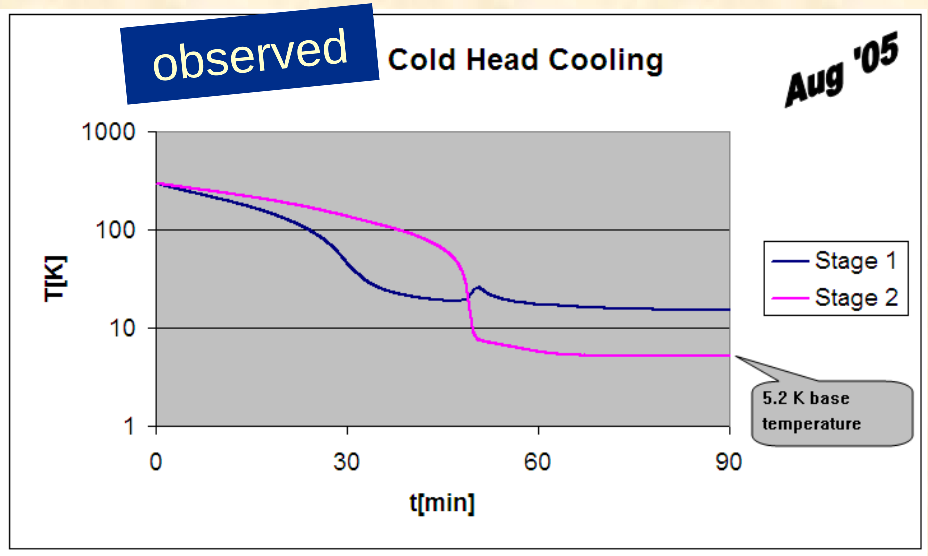
- **2a: What is CCR cooling capacity?**
  - Temperature dependent
  - Vendor info limited
  - We need to measure it ourselves
  - Fit to function





Problem 2b

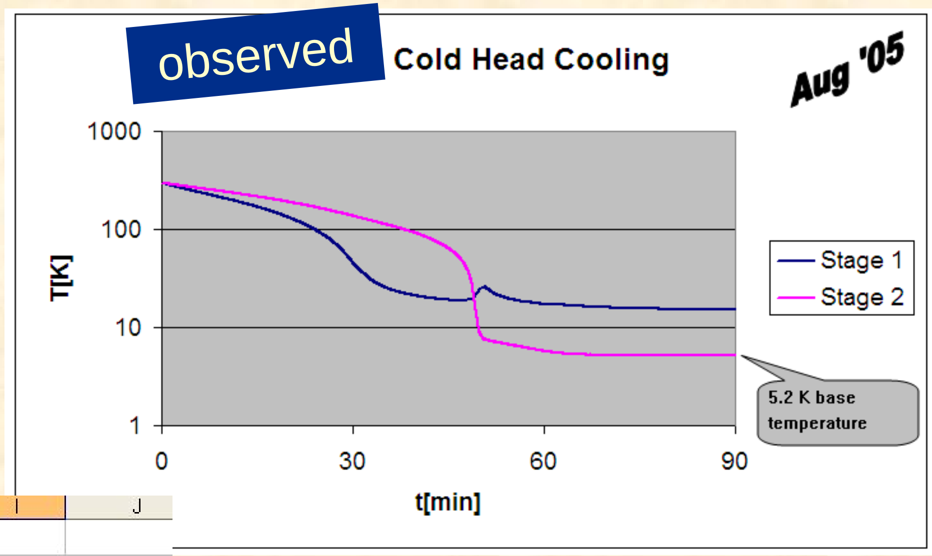
- **How long for the CCR to cool itself?**



Problem 2b

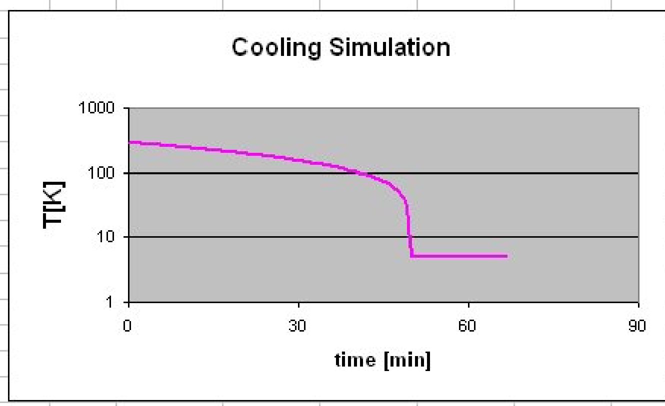
- **How long for the CCR to cool itself?**

observed



	A	B	C	E	F	G
1	Cooling CCR + Load					
2	Using fitted cooling capacity					
3	Debye heat capacity					
4						
5	23.27878261					
6	Material Spec					
7	Debye Temperature [K]	345				
8	Molar mass [g]	63.54				
9	Load mass [g]	0				
10	Self mass [g] est.	1500				
11	Fitted Cooling Capacity [W]					
12	Q'=A*ln(T) - B					
13	A	12				
14	B	24				
15						
16	Calculation Parameters					
17	Start Temperature	293				
18	time step [sec]	40.00				
19	Base temperature	5				
20						
21				*ref G. White*	[J/mol*K]	
22				theta/T	Cv	T
23				0.2	24.89	1725
24				0.4	24.74	863
25				0.6	24.5	575
26	Reference			0.8	24.16	431
27	Material	Debye	molar mass	1	23.74	345
28	Aluminium	426 K	26.97	1.2	23.23	288
29	Cadmium	186 K	112	1.4	22.66	246
30	Chromium	610 K	52	1.6	22.02	216
31	Copper	344.5 K	63.54	1.8	21.33	192

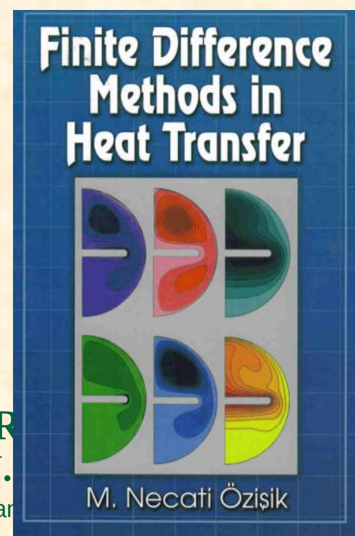
Calculate

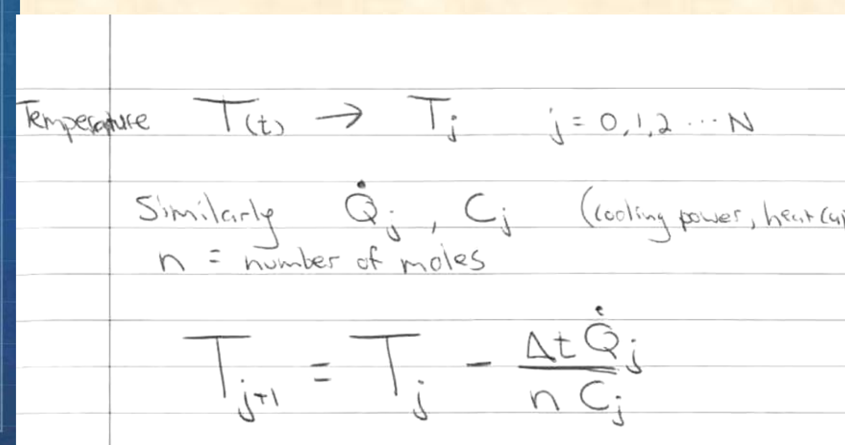


calculated

Calculation Notes

- **Finite difference approximation (FDA)**
- **First order differential equation**
- **Lots of shortcuts**
  - **Using Cv from Debye table**
    - **Need Cp, but Cv is close and easy**
  - **Least accurate (1st order) FDA**
- **Good reference**





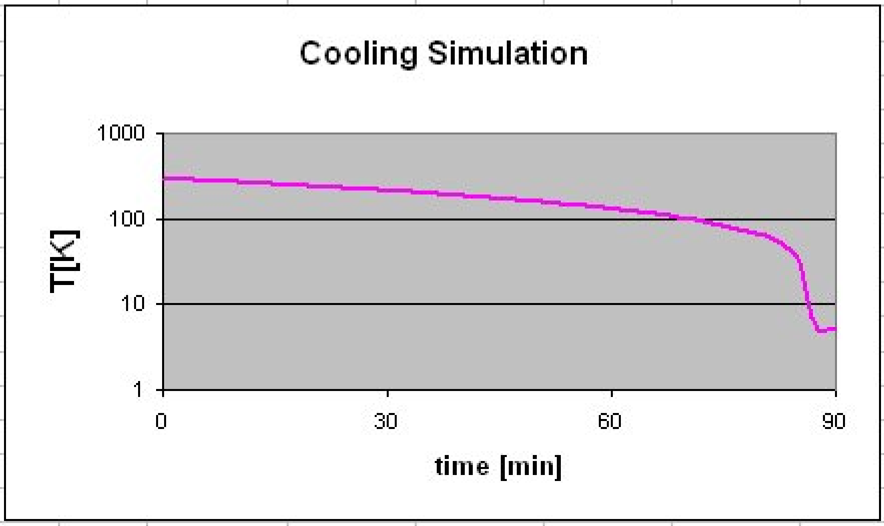
Problem 2c

- **Now attach a load to CCR**
  - **3 pounds of copper**
  - **Simulate “SMASH rig” cold link**

Calculation predicts 90 minute cool down

Row	A	B
1	Cooling CCR + Load	
2	Using fitted cooling capacity	
3	Debye heat capacity	
4		
5	23.27878261	
6	Material Spec	
7	Debye Temperature [K]	345
8	Molar mass [g]	63.54
9	Load mass [g]	1100
10	Self mass [g] est.	1500
11	Fitted Cooling Capacity [W]	
12	Q'=A*ln(T) - B	
13	A	12
14	B	24
15		
16	Calculation Parameters	
17	Start Temperature	293
18	time step [sec]	70.00
19	Base temperature	5

Calculate

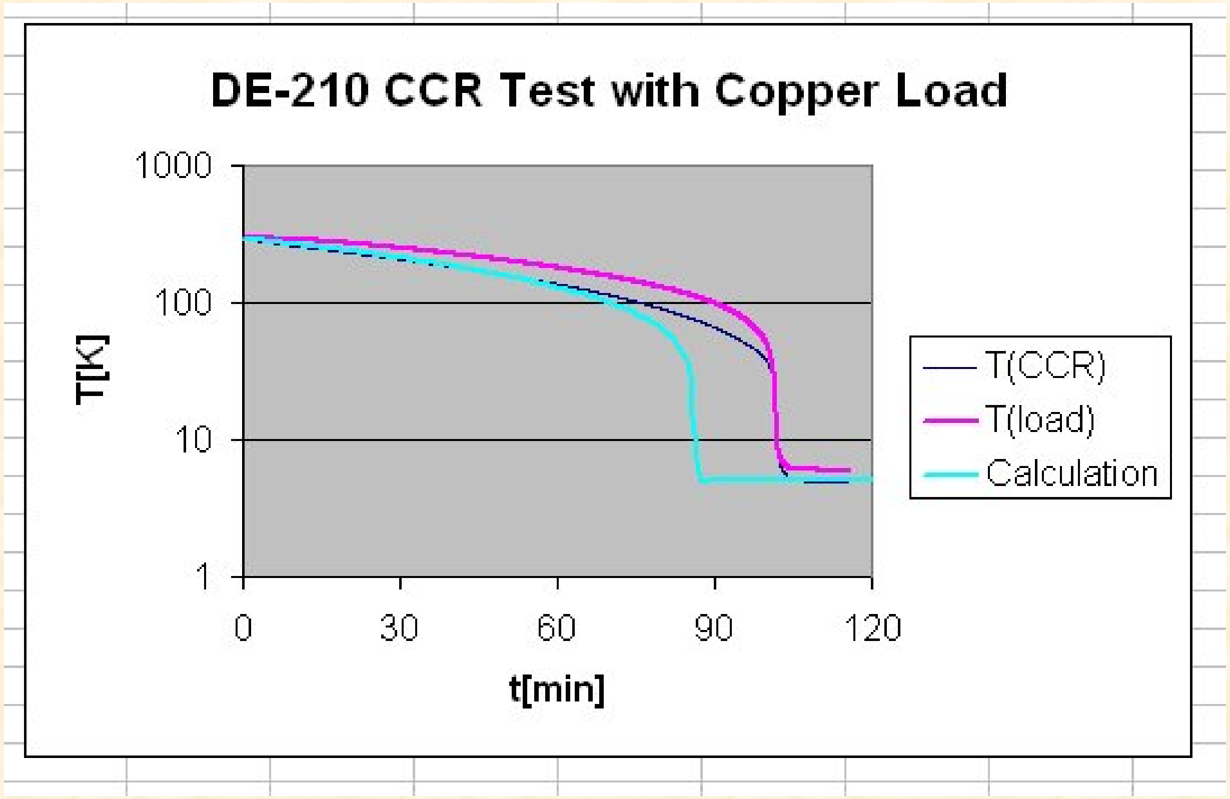


ref G. White theta/T	[J/mol*K] Cv	T
0.2	24.89	1725
0.4	24.74	863

UT-BATTELLE

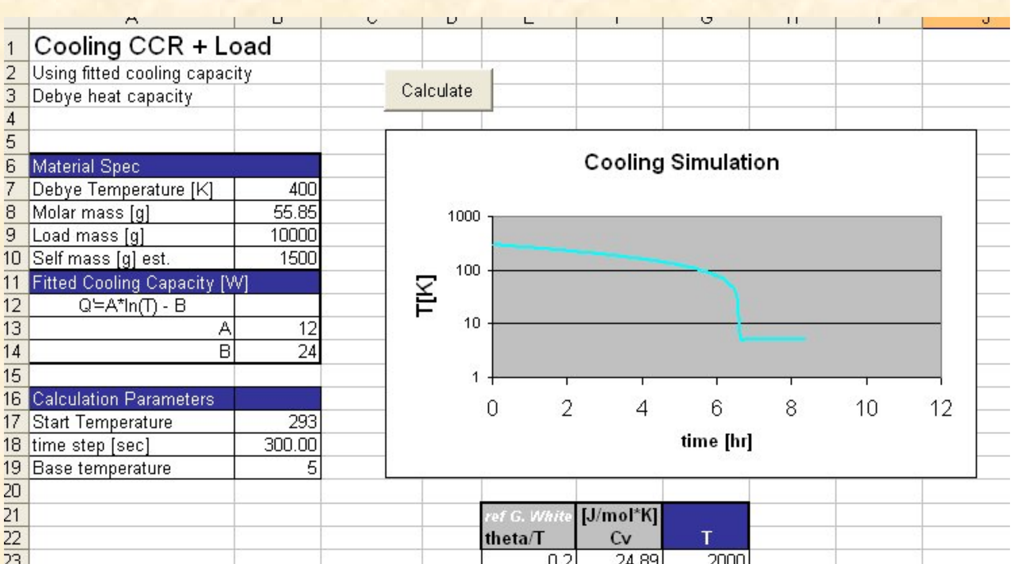
Problem 2c

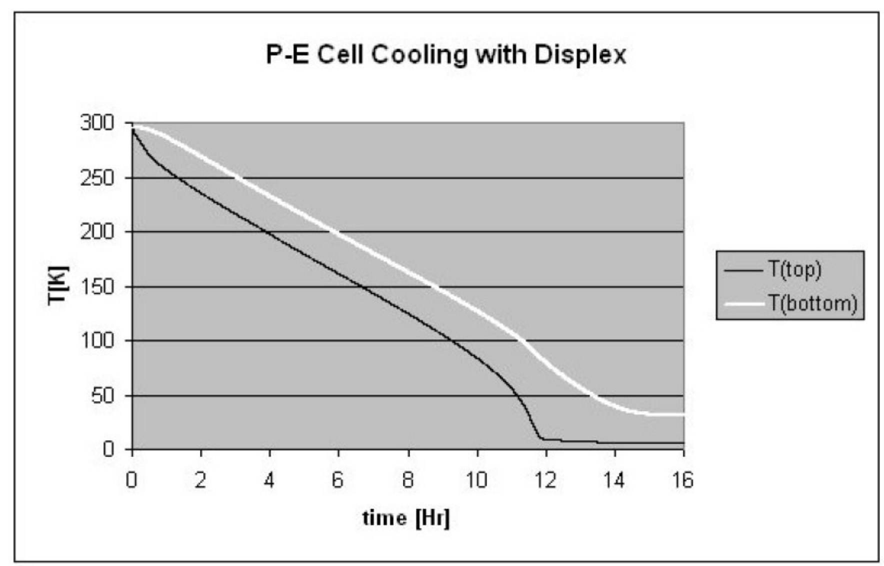
- **Test result gives 100 minutes**



Problem 2d: Cool Something Bigger

- **Massive anvil pressure cell**
  - **Paris-Edinburg Cell (model VX-2)**
  - **25-pound hunk of steel!**
- **Is it feasible to cool using CCR?**
  - **Within a day**
  - **To 77K or lower**





Problem 2d

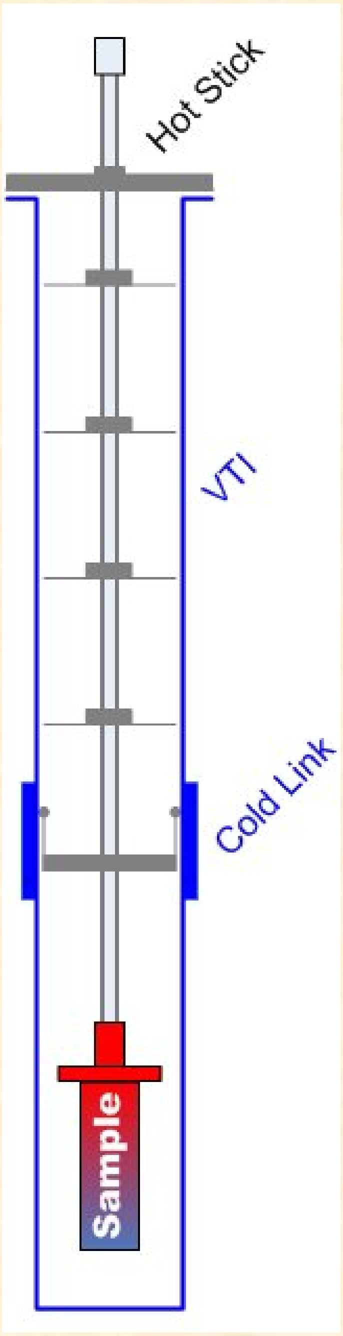
- **Factor of two discrepancy between calculated and observed**
- **But calculation gave the right answer**
  - **Yes, it is feasible**

Problem 3: Hot Stick

- **Top-loading cryostat**
  - **VTI range: 2 to 300 K**

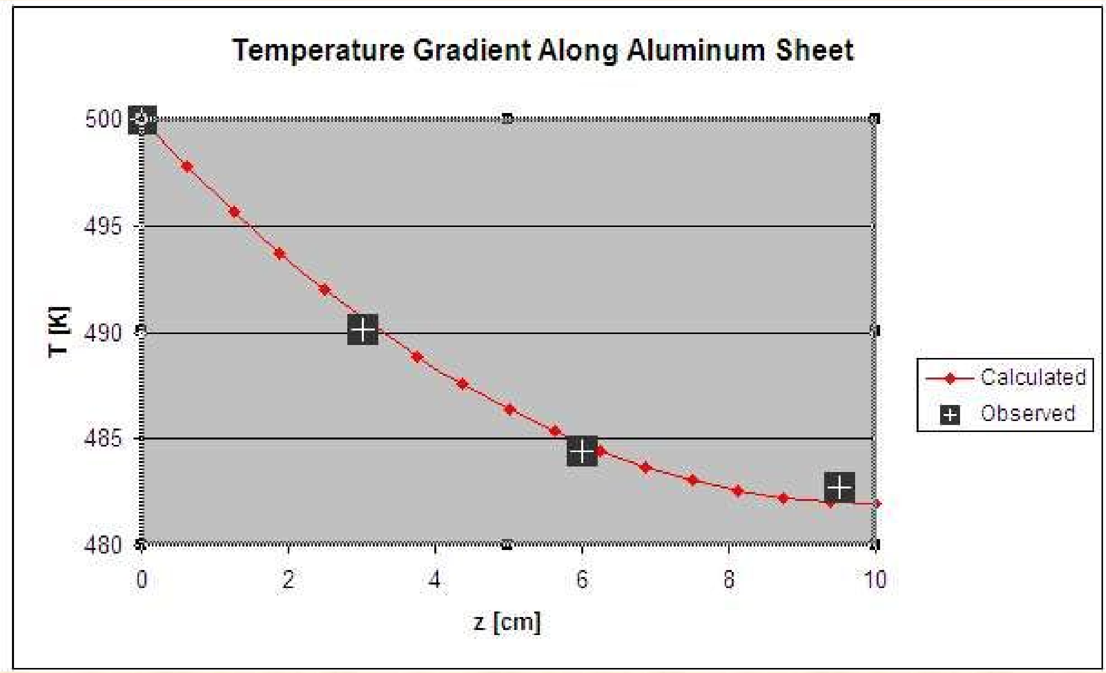
- **Hot stick reaches 600 K**
  - **Different high and low temperature operating modes**
    - **Exchange gas for low temperature**
    - **Evacuated VTI for high temperature**

- **We are concerned about temperature gradients in high temperature mode**



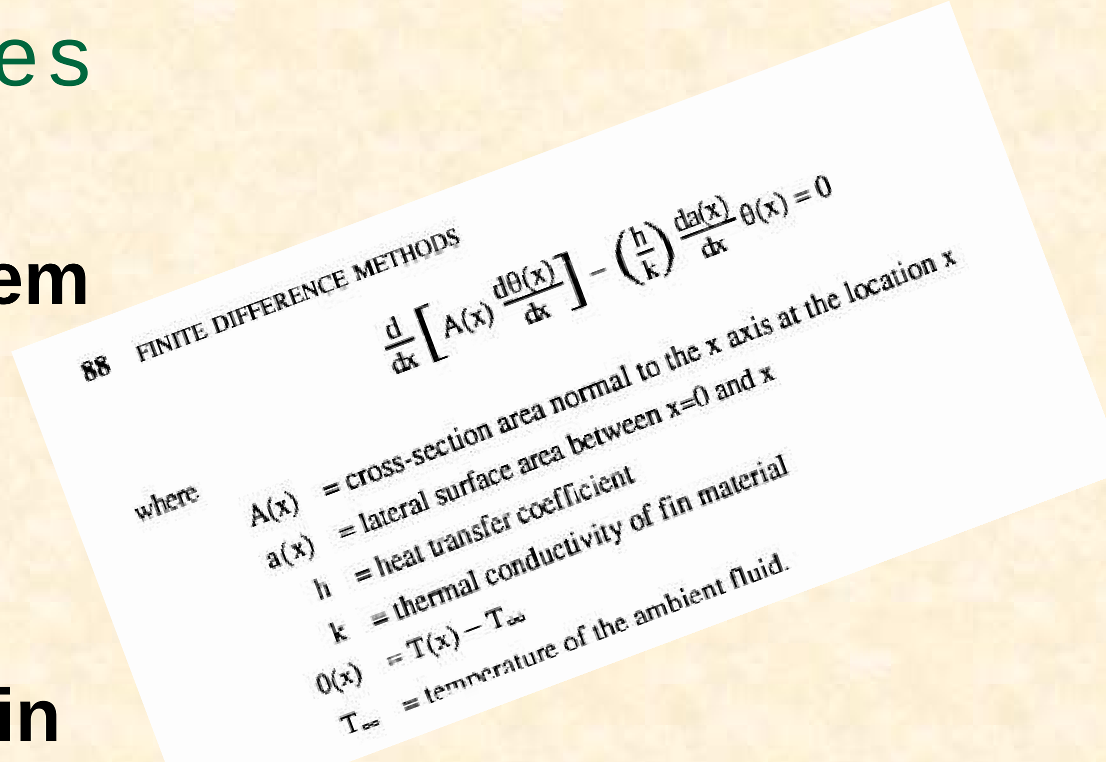
Calculate Gradient

- **Simplified scenario**
  - **Flat sheet of aluminum**
- **Setup comparable test**
- **Use results as a guide**



Calculation Notes

- **Setup like fin problem**
  - **T-dependent “h”**
  - **Iterate, update h**



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$$\frac{d}{dx}\left[A(x)\frac{d\theta(x)}{dx}\right] - \left(\frac{h}{k}\right)\frac{da(x)}{dx}\theta(x) = 0$$

where

$A(x)$ = cross-section area normal to the x axis at the location x

$a(x)$ = lateral surface area between x=0 and x

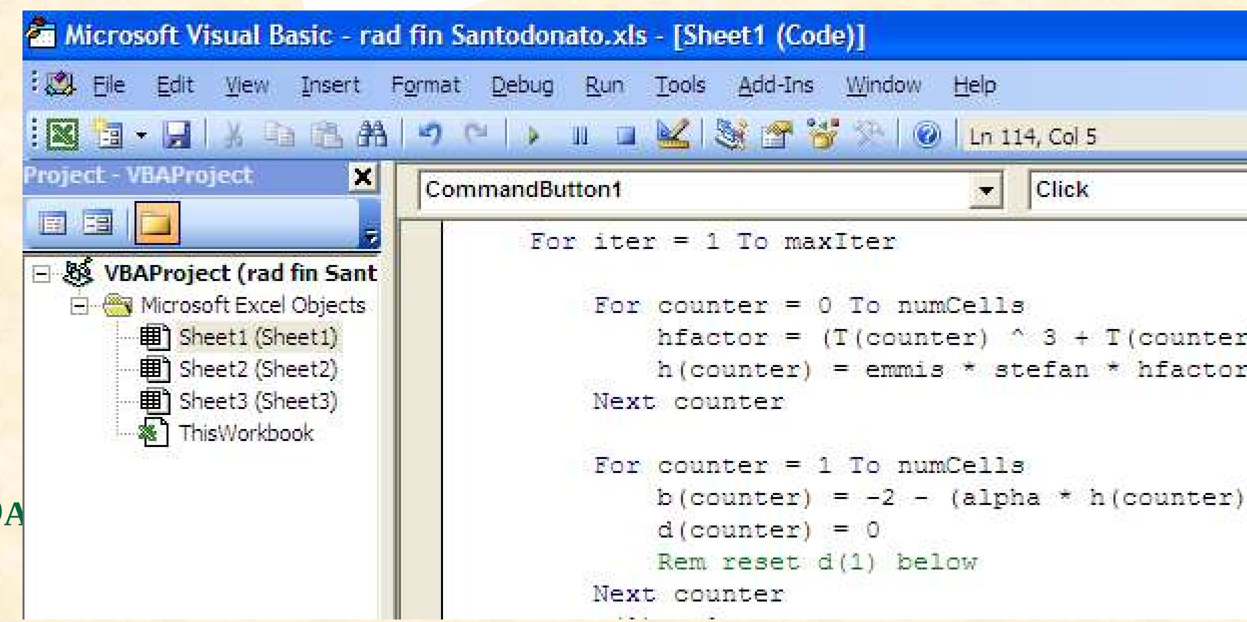
h = heat transfer coefficient

k = thermal conductivity of fin material

$\theta(x)$ = $T(x) - T_\infty$

T_∞ = temperature of the ambient fluid.

- **Use “VBA” routine in spreadsheet**



Summary

- **Rough calculations sometimes roughly agree with observed data**
  - **No need for exact match**
  - **Just looking for guidelines**
- **Gain a better understanding of sample environments by implementing <u>both</u> …**
  - **Rigorous equipment testing**
  - **Quantitative analysis**

Acknowledgements

- **SNS Student Intern**
  - **Rachel Morris**
- **SNS Sample Environment Team**
  - **L. Walker, B. Hill, J. Wenzel & R. McPherson**

- **References**

  - **Guy K. White, "Experimental Techniques in Low Temperature Physics", Oxford University Press**
  - **M. Necati Ozisik, "Finite Difference Methods in Heat Transfer", CRC Press (1994)**