

*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



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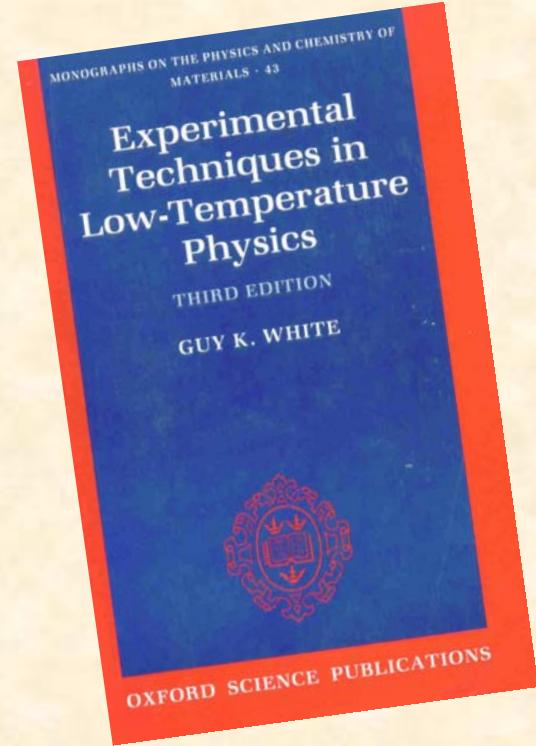
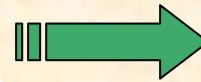
Starting Point

- Classic reference guide
 - Simple examples
 - Useful tables
- Setup companion spreadsheets

314 APPENDIX

TABLE D
Some important physical functions (see Chapter XI)

T/θ	θ/T	C _v (J/mol K)	ρ_1/ρ_0 ($\alpha T^5 J_3$) [†]	ρ_1/ρ_0 ($\alpha T^3 J_3$) [‡]	W_1/W_∞ ($\alpha T^2 J_3$) [§]
(∞)	0	24.94	∞	10.42	1.00
(10)	(0.1)	24.93	10.55	5.201	0.998
(5)	0.2	24.89	5.268	2.588	0.993
(2.5)	0.4	24.74	2.617	2.062	0.990
(2.0)	0.5	24.63	2.083	1.711	0.985
(1.667)	0.6	24.50	1.725	1.268	0.974
(1.25)	0.8	24.16	1.274	1.000	0.960
(1.0)	1.0	23.74	1.000	0.8186	0.943
(0.833)	1.2	23.23	0.813	0.6873	0.923
(0.714)	1.4	22.66	0.678	0.6341	0.913
(0.667)	1.5	22.35	0.623		



Microsoft Excel - Cool Debye.xls

	D24	fx			
20					
21			Debye Table	Sample	
22			theta/T	U-Uo/T	T(Fe) U-Uo[J/mol]
23			0.2	23.1	2000 46200
24			0.4	21.38	1000 21380
25			0.6	19.76	667 13173
26			0.8	18.24	500 9120
27			1	16.81	400 6724
28			1.2	15.47	333 5157
29			1.35	14.54	296 4308
30			1.4	14.23	286 4066
31			1.6	13.07	250 3268
32			1.8	11.99	222 2664
33			2	11	200 2200

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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?



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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								
3	Material Spec			Calculate				
4	mass [g]	10000						
5	Debye Temp	400		How many liters?				
6	molar mass	55.9		493.2				
7	Temperatures							
8	T(initial)	293						
9	T(final)	4.2						
10								
11	Cryogen spec							
12	latent heat	2.6						
13								
14	Reference							
15	Latent Heat of Vap [J/ml]							
16	Helium	2.6						
17	Nitrogen	161						
18	Debye Temperatures [K]	g/mol						
19	Copper	310	63.5					
20	Aluminum	380	27					
21	Iron	400	55.9					
22								

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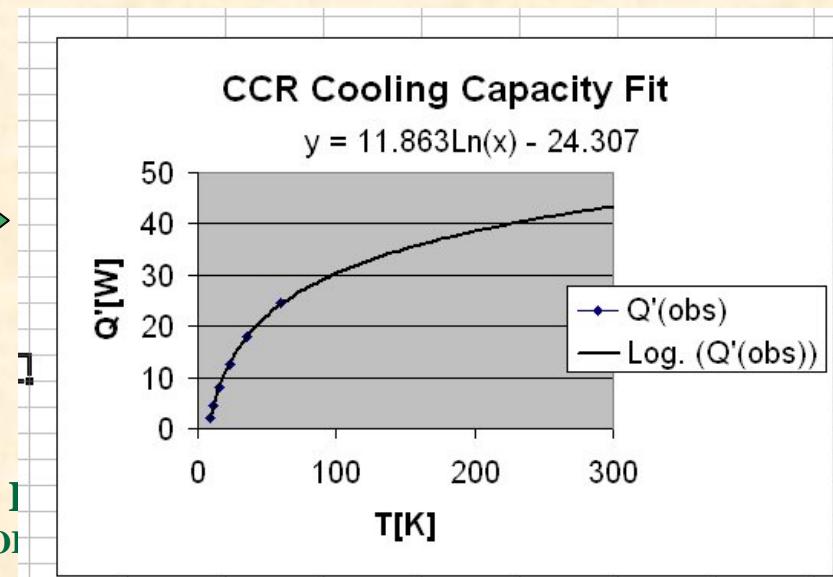
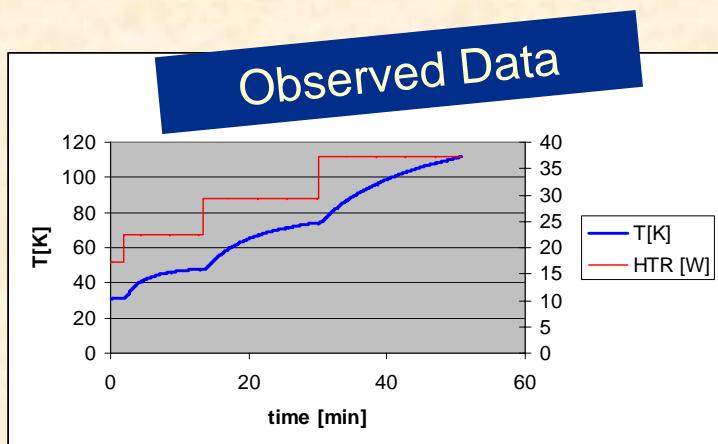
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Problem 2: Cooling with CCR



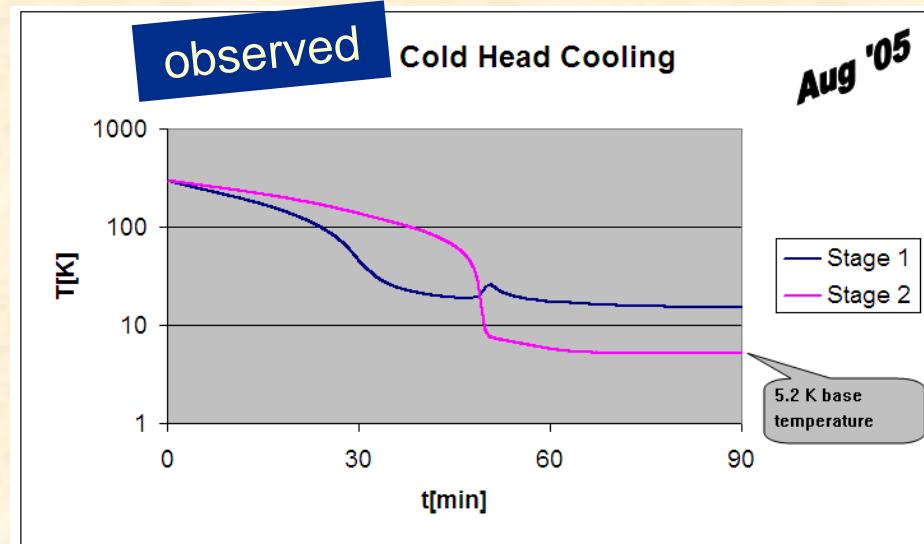
- **2a: What is CCR cooling capacity?**

- Temperature dependent
- Vendor info limited
- We need to measure it ourselves
- Fit to function



Problem 2b

- How long for the CCR to cool itself?



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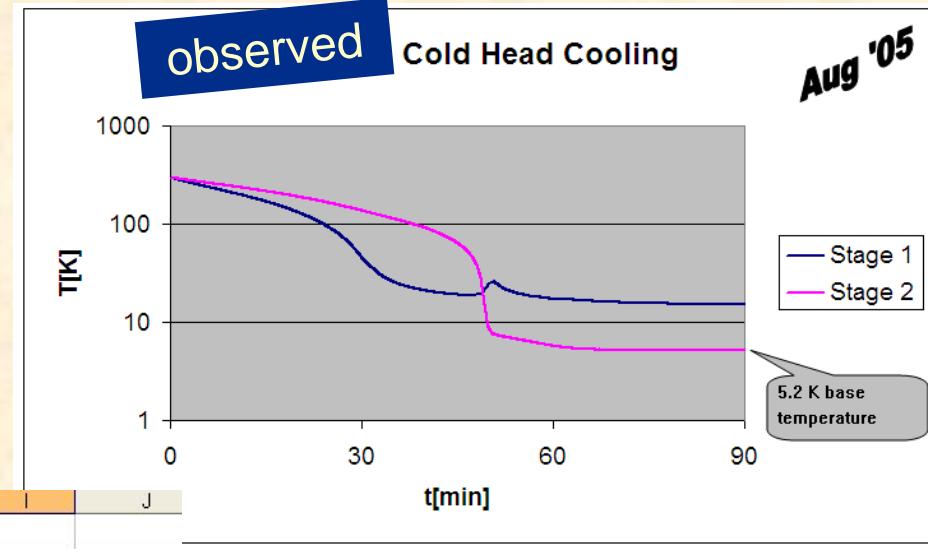
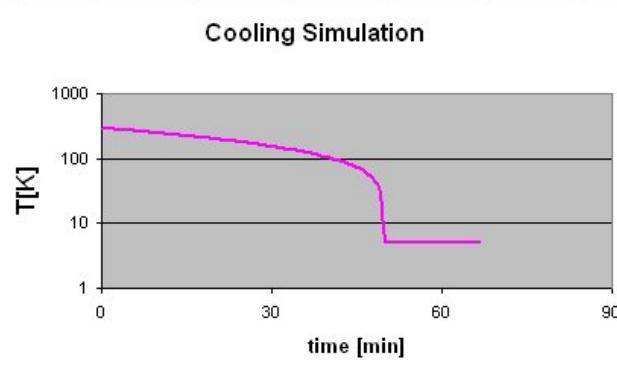
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Problem 2b

- How long for the CCR to cool itself?

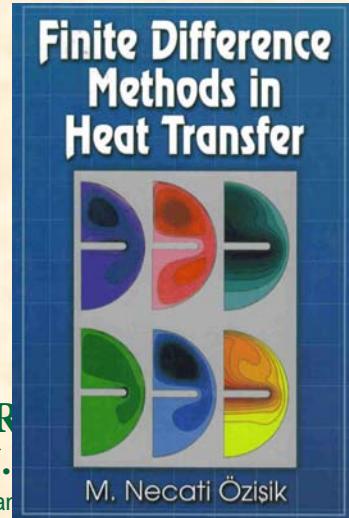
	A	B	C	D	E	F	G	H	I	J
1	Cooling CCR + Load									
2	Using fitted cooling capacity									
3	Debye heat capacity									
4										
5	23.27878261									
6	Material Spec									
7	Debye Temperature [K]	345								
8	Molar mass [g]	63.54								
9	Load mass [g]	0								
10	Self mass [g] est.	1500								
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										
22										
23										
24										
25										
26	Reference									
27	Material	Debye	molar mass							
28	Aluminium	426 K	26.97							
29	Cadmium	186 K	112							
30	Chromium	610 K	52							
31	Copper	344.5 K	63.54							



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



Temperature $T(t) \rightarrow T_j \quad j = 0, 1, 2 \dots N$

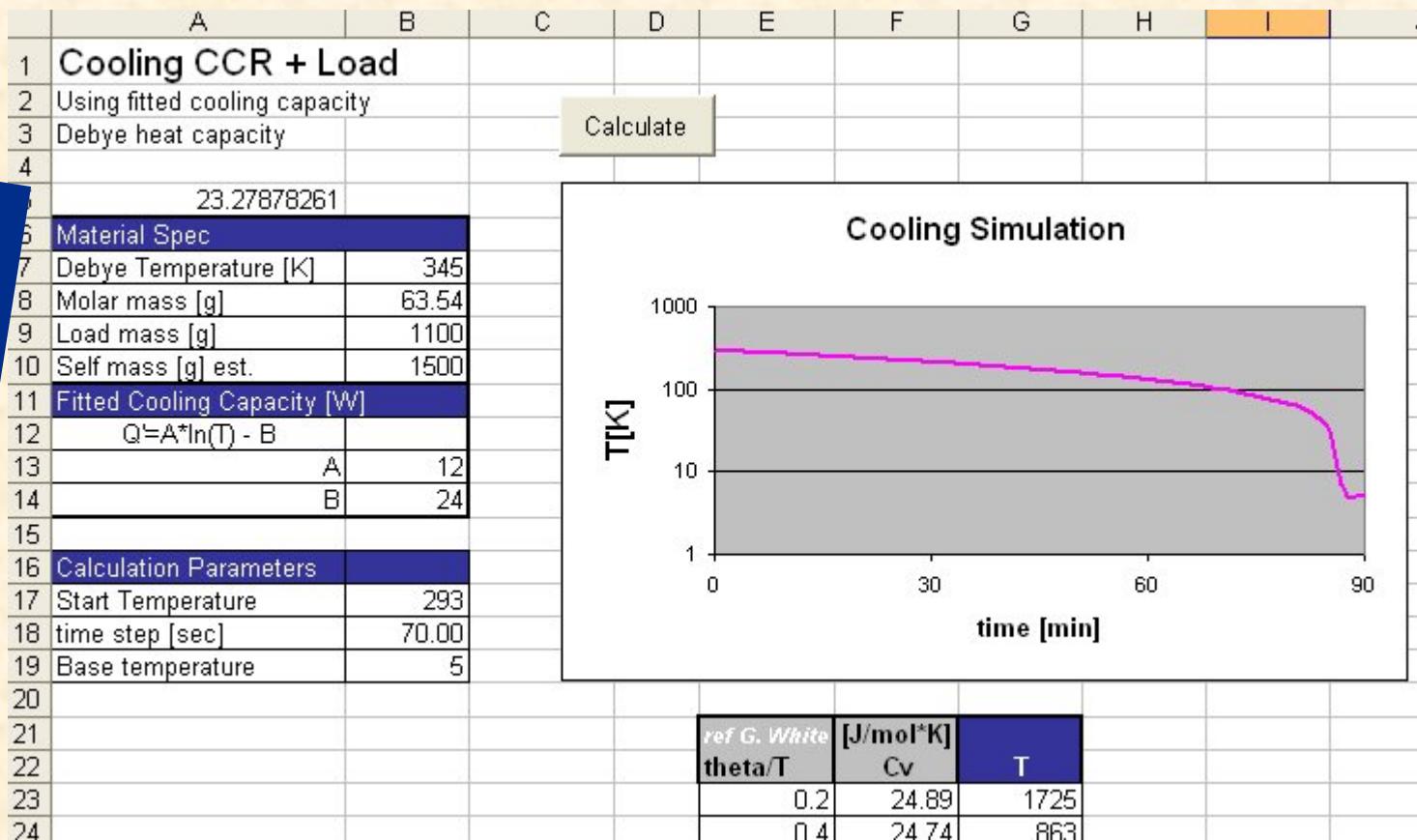
Similarly \dot{Q}_j, C_j (cooling power, heat capacity)
 n = number of moles

$$T_{j+1} = T_j - \frac{\Delta t \dot{Q}_j}{n C_j}$$

Problem 2c

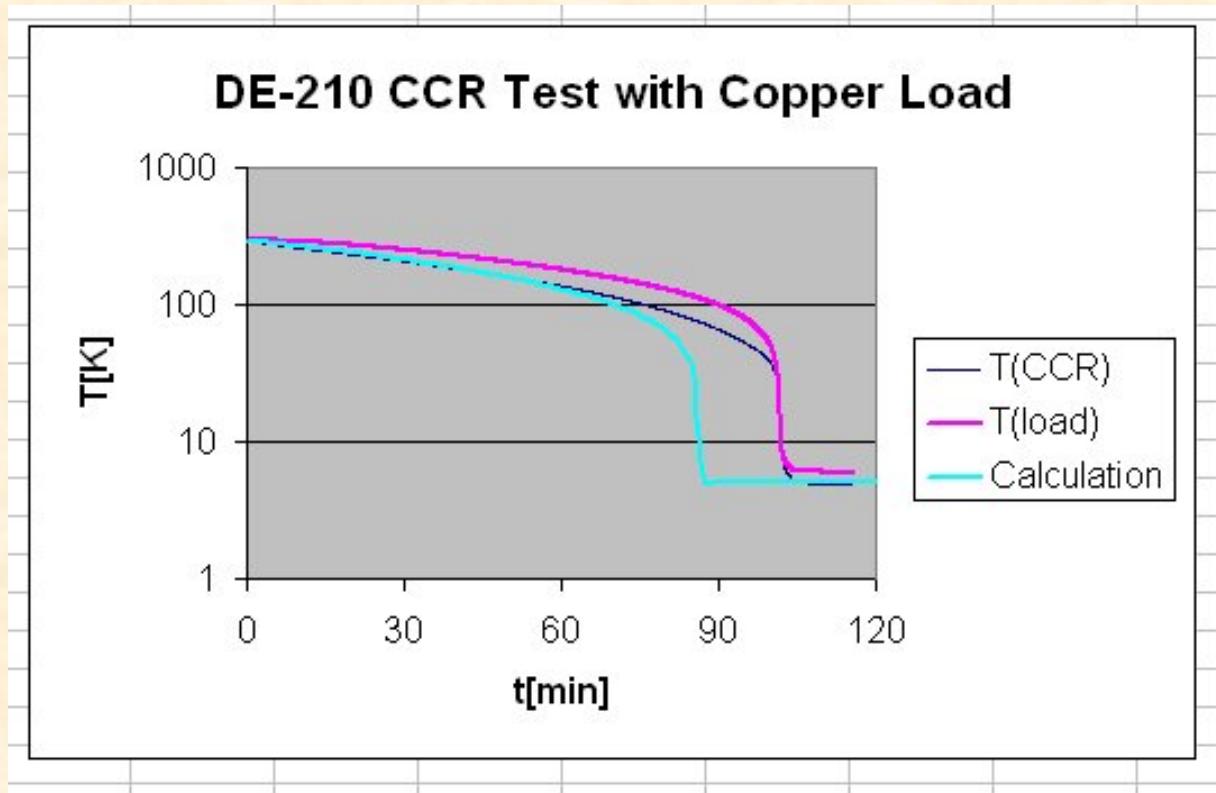
- Now attach a load to CCR
 - 3 pounds of copper
 - Simulate “SMASH rig” cold link

Calculation
predicts 90
minute cool
down



Problem 2c

- Test result gives 100 minutes



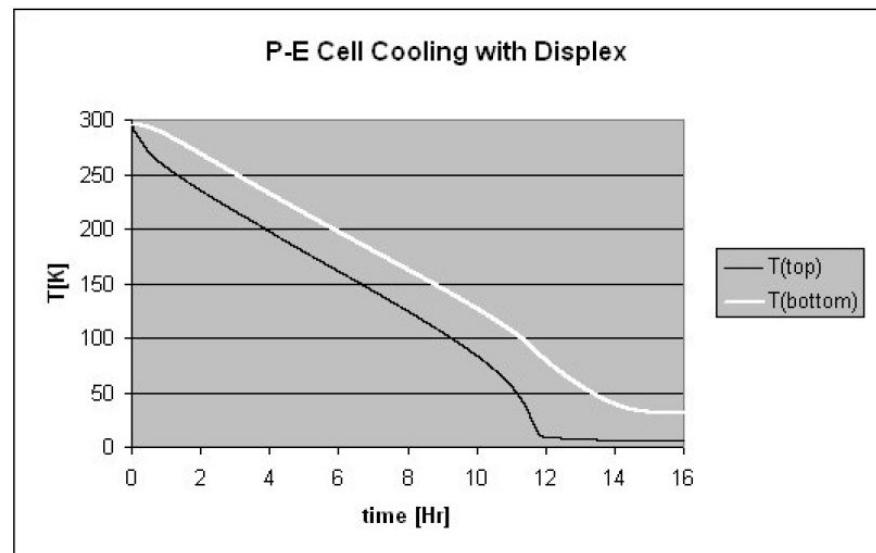
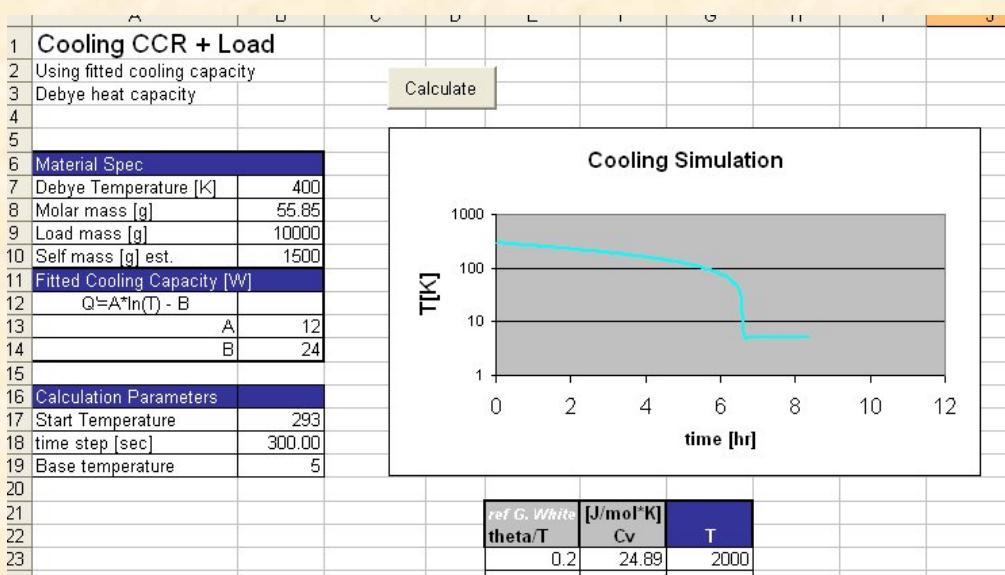
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Problem 2d: Cool Something Bigger

- 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



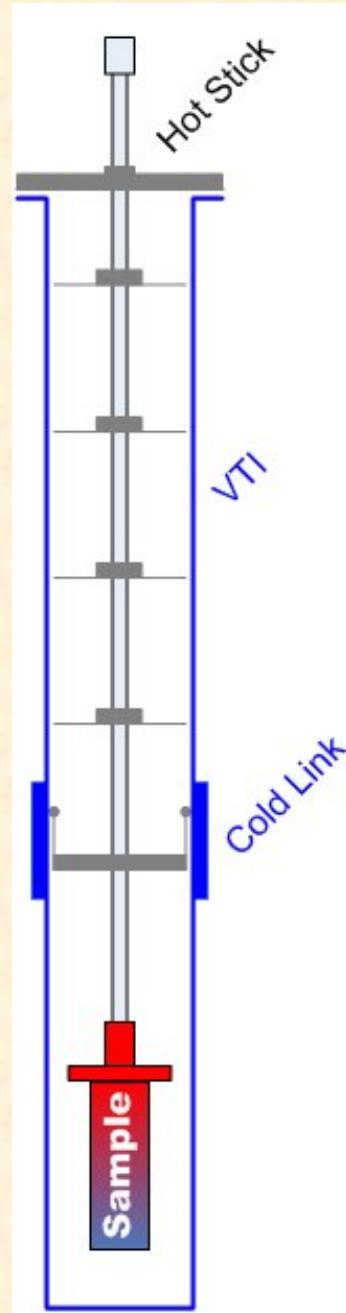
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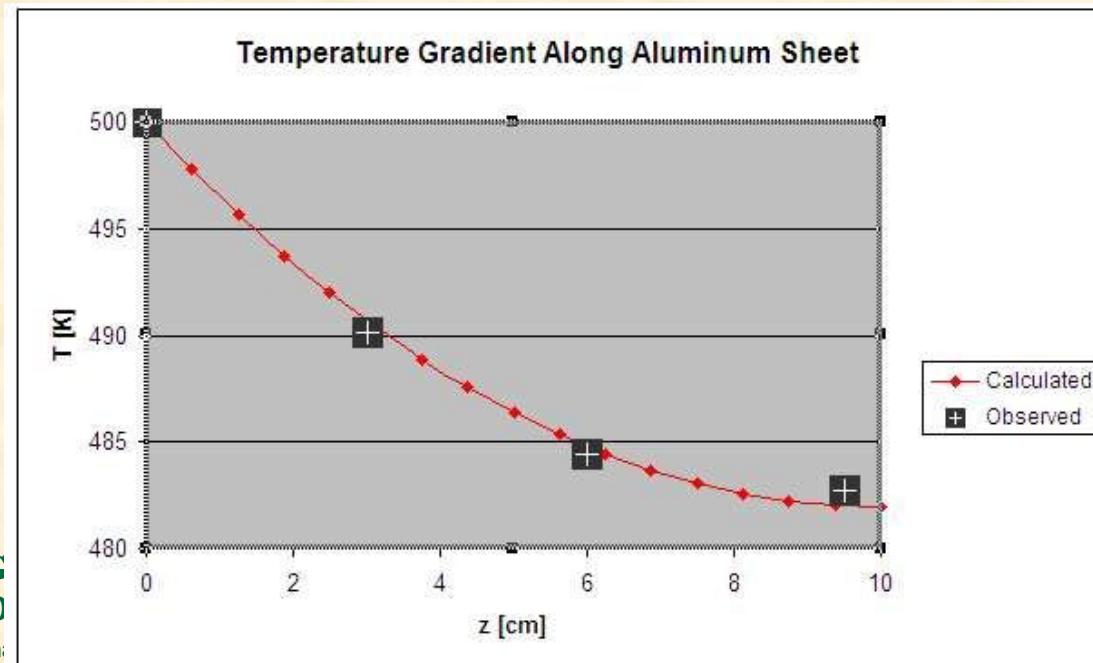
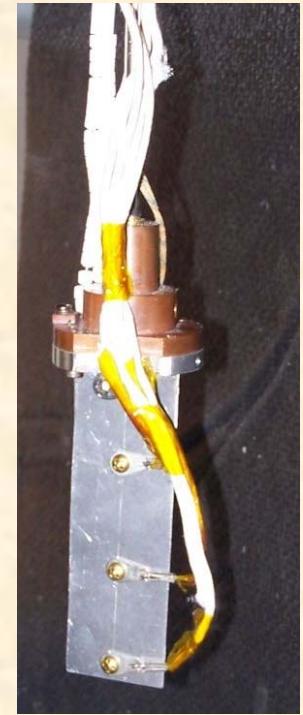
Problem 3: Hot Stick

- 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

88 FINITE DIFFERENCE METHODS

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

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

The screenshot shows the Microsoft Visual Basic Editor interface. The title bar reads "Microsoft Visual Basic - rad fin Santodonato.xls - [Sheet1 (Code)]". The menu bar includes File, Edit, View, Insert, Format, Debug, Run, Tools, Add-Ins, Window, and Help. The toolbar below has various icons for file operations. The Project Explorer window on the left shows a VBAProject named "VBAProject (rad fin Sant)". It contains a Microsoft Excel Objects folder with "Sheet1 (Sheet1)", "Sheet2 (Sheet2)", "Sheet3 (Sheet3)", and "ThisWorkbook". The code editor window on the right is titled "CommandButton1 Click". The code is as follows:

```
For iter = 1 To maxIter
    For counter = 0 To numCells
        hfactor = (T(counter)) ^ 3 + T(counter)
        h(counter) = emmis * stefan * hfactor
    Next counter

    For counter = 1 To numCells
        b(counter) = -2 - (alpha * h(counter))
        d(counter) = 0
        Rem reset d(1) below
    Next counter
```

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 both ...
 - Rigorous equipment testing
 - Quantitative analysis



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Acknowledgements

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- **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)



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