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APPENDICES

Appendix A Estimating volume of sample holder.

For example: in the purified $NaAlH_4$ experiment

Table A1 Pressure data for calculate volume space of the sample holder

Run No.	Pressure (atm)			
	Manifold		Sample holder	
	Initial	Final	Initial	Final
1	138.2500	26.8155	1.0000	26.4101
2	138.0010	47.4479	26.4101	46.8930
3	137.1560	64.1930	46.8930	63.8385
4	138.1510	77.9978	63.8385	77.3433
5	139.7480	89.6597	77.3433	88.9043
6	138.7010	98.9320	88.9043	98.1253
7	139.7460	106.6540	98.1253	105.8000
8	139.4960	112.8340	105.8000	112.0300
9	137.9020	117.5680	112.0300	116.8140
10	138.4320	121.5550	116.8140	120.7510

At given $V_1 = 4.14\ cm^3$, mol of gas in sample holder is calculated by substitution all measurement value into Equation (3.4) and estimate the compressibility factor from Equation (3.5).

Table A2 Mol balance of two states

Run No.	mol in $V_{1,initial}$	mol in $V_{1,final}$	mol in $V_{2,final}$
1	0.02246	0.00455	0.01791
2	0.02242	0.00798	0.01444
3	0.02229	0.01073	0.01156
4	0.02242	0.01297	0.00945
5	0.02269	0.01484	0.00785
6	0.02253	0.01632	0.00621
7	0.02269	0.01752	0.00517
8	0.02262	0.01849	0.00413
9	0.02238	0.01923	0.00315
10	0.02246	0.01985	0.00261

Table A3 Volume of sample holder

$P_{2,\ final}$(atm)	V_2
26.4101	17.2939
46.8930	17.6101
63.8385	17.6046
77.3433	17.5595
88.9043	17.5931
98.1253	17.5042
105.8000	17.6083
112.0300	17.5516
116.8140	17.4811
120.7510	17.6600
Average	17.5466

Appendix B Desorbed and absorbed hydrogen calculation.

Desorbed hydrogen calculation

For example: at 6 mol% $ZrCl_4$–added sample (V_2 is given in Table 4.2)

Use equation of state for estimating mol of hydrogen in the sample holder and this relation:

$$\text{wt\%} = \frac{\text{weight of released hydrogen}}{\text{weight of } NaAlH_4\text{(not include doped metal)}}$$

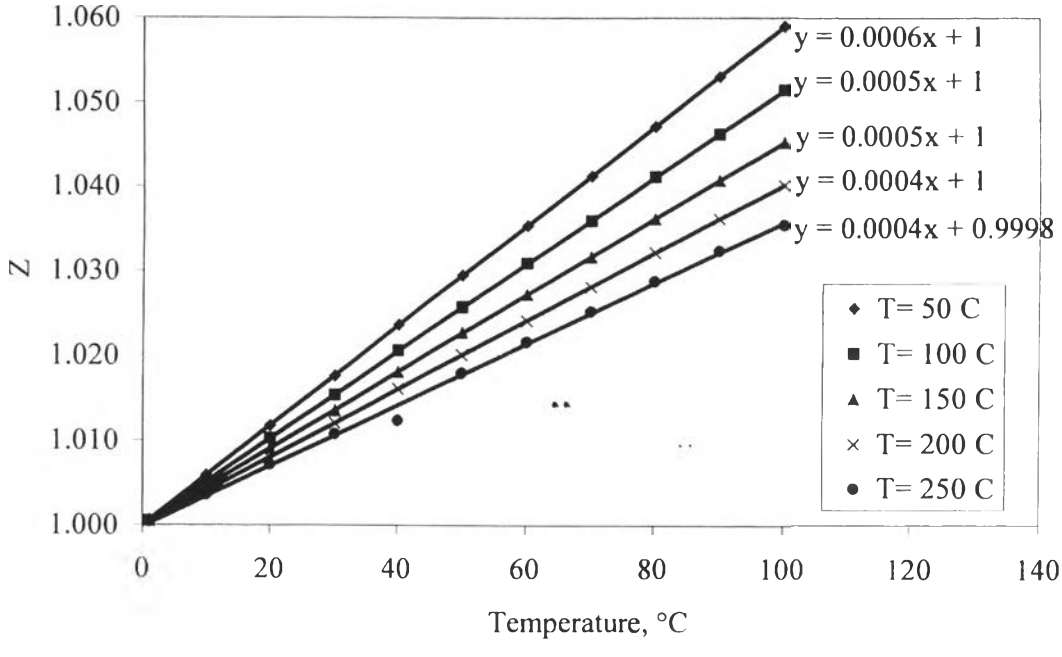

Figure B1 Approximated Z value at different temperature ranges.

Table B1 Calculated capacity from Equation of State with compressibility factor

Temperature (°C)	P (atm)	mol	Z	wt%
80	0.131432	0.000078	1.000066	0.015575
85	0.161946	0.000095	1.000081	0.018940
90	0.176498	0.000102	1.000088	0.020316
95	0.191058	0.000108	1.000096	0.021649
100	0.182531	0.000102	1.000091	0.020466
105	0.180959	0.000100	1.000090	0.019924
110	0.200832	0.000109	1.000100	0.021803
115	0.213428	0.000115	1.000107	0.023021
120	0.233015	0.000124	1.000117	0.024819
125	0.240578	0.000127	1.000120	0.025408
130	0.283687	0.000147	1.000142	0.029427
135	0.330160	0.000170	1.000165	0.033945
140	0.444386	0.000225	1.000220	0.045050
145	0.569253	0.000285	1.000285	0.057011
150	0.644282	0.000319	1.000322	0.063755
155	0.769148	0.000376	1.000385	0.075213
160	0.844178	0.000408	1.000422	0.081588
165	6.755432	0.003220	1.003378	0.644032
170	7.622529	0.003588	1.003811	0.717551
175	7.747396	0.003605	1.003874	0.721077
180	7.877582	0.003628	1.003909	0.725587
185	8.102122	0.003690	1.004051	0.737990
190	9.472906	0.004264	1.004736	0.852893
195	16.918466	0.007501	1.008459	1.500169
200	28.162252	0.012328	1.011265	2.465647
205	34.616389	0.014956	1.013847	2.991194
210	35.737997	0.015273	1.014295	3.054609
215	36.510734	0.015438	1.014604	3.087560
220	37.228321	0.015565	1.014891	3.112986
225	37.801725	0.015635	1.015103	3.128336
230	38.181095	0.015650	1.015272	3.129938
235	38.699335	0.015691	1.015480	3.138167
240	39.003115	0.015711	1.015600	3.142222
245	39.511557	0.015730	1.015804	3.146000
250	40.020832	0.015752	1.015908	3.150492

Absorbed hydrogen calculation

For example: at 6 mol% $ZrCl_4$ doped sample

Table B2 Absorbed mol of H_2

Time (min)	P (atm)	mol	Δmol
initial	141.6327	0.072281	0.000000
2	141.9816	0.072171	0.000110
4	142.4800	0.072063	0.000218
6	142.8786	0.071978	0.000303
8	143.1777	0.071847	0.000434
10	143.4767	0.071784	0.000497
12	144.0748	0.071526	0.000755
14	144.8223	0.071273	0.001008
16	145.1213	0.071148	0.001133
18	145.4203	0.070958	0.001323
20	145.1213	0.070888	0.001393
22	144.9213	0.070806	0.001475
24	145.8688	0.070709	0.001572
26	146.7659	0.070282	0.001999
28	145.9685	0.070245	0.002036
30	145.0216	0.070395	0.001886
32	144.8223	0.070306	0.001975
34	144.6229	0.070280	0.002001
36	144.6229	0.070217	0.002064
38	144.5233	0.070109	0.002172
40	144.3738	0.070042	0.002239
42	144.3239	0.069893	0.002388
44	144.2242	0.069826	0.002455
46	144.0747	0.069782	0.002499
48	144.0249	0.069675	0.002606
50	143.8754	0.069608	0.002673
52	143.6760	0.069542	0.002739
54	143.6262	0.069457	0.002824
56	143.4767	0.069412	0.002869
58	143.3770	0.069346	0.002935
60	143.2275	0.069301	0.002980

Table B3 Calculated capacity from pressure drop

Time (hr)	P (atm)	mol	wt%
initial	141.6327	0.000000	0.000000
1	143.2275	0.069301	0.845814
2	140.2373	0.067884	1.137367
3	138.0445	0.067024	1.309283
4	136.4996	0.066271	1.459903
5	135.4031	0.065720	1.570211
6	134.4064	0.065272	1.659747
7	133.7087	0.064958	1.706286
8	133.1107	0.064689	1.776290
9	132.5624	0.064500	1.814033
10	132.0641	0.064276	1.858971
11	131.6155	0.064073	1.899435
12	131.2667	0.063916	1.926422
13	131.9178	0.063701	1.930922
14	131.6188	0.063632	1.982429

Appendix C Amount of doped metal (per 1 g of $NaAlH_4$).

Table C1 Weight of activated species

Doped metal	mol%	weight(g)
$ZrCl_4$	2	0.088132
	4	0.179938
	6	0.275374
	9	0.427106
$TiCl_3$	4	0.119135
$HfCl_4$	4	0.247299

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