Qut #	B.P.	S.G.	MW	Kenaler-lee	Pénn-State	Mathur	Cavett	ASPEN
411C	409.6	0.8160	110	3255.0	3269.6	4602.7	2966.3	3287.47
5HC	433.2	0.8827	116	3475.5	3490.7	4374.2	3318.0	3633.58
6HC	467.6	0.9507	127	3528.0	3516.4	4003.0	3512.46	3833.89
7HCB	492.6	0.9672	141	3310.1	3252.7	3613.4	3318.0	3702.08
BHC	519,3	0.9718	158	2999.0	2905.8	3232.4	2984.5	3484.77
1 OHCB	572.1	1.0021	188	2623.7	2511.3	2726.5	2565.5	3254.83
1 1HC	612.6	1.0359	202	2451.5	2327.4	2541.4	2342.5	3133.18
1 5HC	632.1	1.083	220	2561.5	2417.2	2337.6	2429.7	3109.18
1 6HC	658.7	1.091	237	2374.4	2237.5	2173.3	2199.2	2971,999
1711C	692.6	1.1204	258	2263.8	2127.9	2000.0	2035.9	2797.19
1 SHCB	741.5	1.176	293	2191.2	2049,1	1765.8	1879.9	2452.13
1 9HCA	776.5	1.1792	315	1965.0	1853,8	1645.0	1673.7	2342.28
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## Table III-13: Estimation of Critical Pressure from Available Correlations\*

\*BP(K), SG and HW data for coal liquid to calculate the critical pressure (kPa) were taken from Gray and Holder (1982).

# Table III-14: Experimental Vapor Pressure and Percent Relative Deviation from Various Correlations for Heart Cuts of SRC-II Liquid

Heart Cut: 4HC

 $T_c = 601.7 \text{ K}$  $P_c \approx 2895.79 \text{ kPa}$  $T_b = 409.6 \text{ K}$  $\omega \approx 0.3306$ 

### Vapor Pressures (kPa)

T(K)	Experimental	Linear	Riedel	Wilson	Starling	Mobil
324.8	5.17	6.51	4.947	5.52	4.60	4.88
339.0	9,65	11.35	9.275	10,08	8.81	9,19
367.1	28.27	29.99	27.72	28,49	26,73	27.12
395.4	68-88	69.39	67.13	68.71	67,55	67.12
423.7	146.17	143.55	143.67	145.08	147.12	143.93
452.1	284.75	271.68	275,52	275.70	285.68	276.33
480.4	496.42	475,96	482.61	482,27	507.98	484.15
508.9	815.65	785.99	791.23	789.71	842.96	793,54
533.2	1187.27	1155.50	1154.45	1153.01	1242.79	1157.18
537.5	1266.56	1232.56	1229.97	1229.31	1327.16	1232.73
561.2	1713.34	1728.35	1716.83	1718.32	1870.68	1719,40
589.3	2564.84	2491.24	2479.59	2482.91	2723.75	2480.87
603.4	3109.52	2954.72	2957.12	2957.74	3109.52	2957.16
608.9	3301.89	3151,31	3163.83	3163.22	3301.88	3163.26

Heart Cut: 4HC

## Relative % Deviation

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T(K)	Linear	Riedel	Wilson	Starling	Mobil
324.8	25.919	-4.313	6.770	-11.025	-5.519
339.0	17.617	-3.886	4.456	-8.705	-4-576
367.1	6.084	-1.946	0.778	-5.447	-4.085
395.4	0.740	-2,541	-0.247	-1.931	-2.560
423.7	-1.792	-1.712	-0.746	0.650	-1.531
452.1	-4.590	-3.241	-3,178	0.327	-2.958
480.4	-4.122	-2.782	-2.850	2.329	-2.470
508,9	-3.636	-2.994	-3,180	3.348	-2.710
533.2	-2.676	-2.764	-2.886	4.676	-2.534
537.5	-2.684	-2.889	2,586	4.785	-2.671
561.2	0.876	0.204	0.291	9.183	0.354
589.3	-2.870	-3.324	-3.194	6.196	-3.274
603.4	-4.978	-4.901	-4.881	0.0	-4,900
608.9	-1.560	-4.181	-4.200	0.0	-4.199
AAD%	17.376	2.977	2.875	4.186	3.167

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III-79

Heart Cut: 5HC

Vapor Pressure (kPa)

T(K)	Experimental	Linear	Reidel	Wilson	Starling	Mobil
3/4 8	7.24	8.14	6.286	7.02	6.02	6.21
366 5	13.31	14.78	12.314	13.38	12.04	12.21
300.3	32.27	35.67	32.54	34.19	32.57	32.43
574.5 100 0	71 84	77-03	74.44	76.49	75.66	74.41
422.J 440 7	149 62	149.10	148.765	150.86	152.92	148.98
447 <b>.</b> /	143002	267 63	270.80	271.93	280.35	271.49
4//.1	273012 105 79	450 60	466.25	466.18	487.05	467.63
505.0	473+73 779 91	736 96	743.755	473.70	785.34	745.89
533.4	1160.25	1106 79	1106 63	1106.54	1179.29	1109.35
559.8	1109.35	1670 75	1572 32	1572.45	1690.02	1575.21
585.4	1682.31	13/9./3	1671 04	1671 60	1799.36	1674-80
590.1	1/92.63	1081.29	10/1.74	2200 /0	2/96 17	2298.52
615.4	2613.10	2313.00	2290.32	2277047	2420017	3228 45
644.3	3461.16	3229.30	3228,28	342/.01	3401017 9600 73	3220.45
645.7	3509.42	3279.45	3280.52	3281.19	3309 <b>.</b> 42	5200 <sub>0</sub> 54

Heart Cut: 5HC

Relative % Deviation

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T(K)	Linear	Riede1	Wilson	Starling	Mobil
349.8	12.43	-13.17	-3,028	-16,776	-14,194
366.5	11.04	-7.483	0.532	-9.543	
394.3	10.54	0.859	5,969	0.948	0 406
422.3	7.279	3.626	6-462	5.312	2 575
449.7	-0.348	-0.571	0.834	2,209	-0 420
477.1	-8,883	-7.801	-7-416	-4.550	-7 570
505.6	-7.270	-5,946	-5.961	-1 751	-5 660°
533.4	-4.565	-3.685	-3,692	1 701	
559.7	-5.527	-5.363	-5.371	0.850	-5 101
590.1	-6.211	-6.732	-6.752	0.376	-4 E73
585.4	-6.096	-6.538	-6.531	0 4 5 9	-0.373
615.4	-11.484	-12,12	-12.002	-4 475	-0.300
644.3	-6.694	-6.728	-6.748		-12.039
645.7	-6.553	-6,525	-6.503	0.0	-0.724
·			•••••		0.0066
AAD%	7.495	6.225	5.557	3.496	6.210

Heart Cut: 6HC

T_	11	698.3	ĸ	$P_{a} = 3578.36 \text{ kPa}$
TB	<b>-R</b>	467.6	ĸ	ω= 0,3447

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Vapor	Pressure	(kPa)
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T(K)	Experimental	Linear	Riede1	Wilson	Starling	Mobil
367.1	3.31	5.276	3.774	4.30	3.72	3.69
395.4	10.00	14.10	11.582	12.60	11.66	11 41
423.7	28.89	33.07	29.838	31.45	30.36	20 56
452.1	67.57	69.90	67.034	68.95	68-31	66 71
480.4	139.27	134.92	134.176	136.25	173.04	133 93
508.9	262,69	242.97	246,122	247.31	250 96	26 16
537.5	453.67	411.83	4149.30	419.43	427,99	419 99
561.2	693.61	612.24	622.236	621.32	636.30	623 36
566.1	740.49	661.80	671,970	670,75	687.40	673 22
589.3	1045.24	940.04	948,909	947.35	974.07	950 74
617.5	1559.59	1389.93	1391.624	1389.81	1435.38	1303 00
645.7	2206.31	1986.12	1976.279	1975.03	2050.98	1078 71
673.9	3161.23	2754.50	2738.275	2740.39	3161.23	2730 04
682.4	3385.31	3023.80	3009,689	3011.76	3385 31	3010 02
685.6	3585.26	3130.00	3117.511	3116.41	3585.26	3118,55

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Heart Cut: 6HC

Relative % Deviation

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T(K)	Linear	Riede1	Wilson	Starling	Mobil
367.1	59,396	14.018	29,959	12,488	11,360
395.4	41.000	15.820	26.027	16,600	14.055
423.7	14.469	3.281	8,873	5,109	2,329
452.1	3.448	-0.793	2.049	1,101	-1.276
480.4	-3,123	-3,658	-2.169	-1.602	-3.835
508.9	-7,507	-6.307	-5.854	-4.466	-6.293
537.5	-9.223	-7.547	-7.548	-5.662	-7.425
561.2	-11.731	-10.291	-10.422	-8,262	-10 120
566.1	-10.627	-9.253	-9,419	-7.170	-9 085
589.3	-33,105	-32,687	-9.366	-6.810	-9 041
617.5	10.879	-10,770	-10.886	-7.964	-10.618
645.7	-9,980	-10,426	-10-483	-7.040	-10.316
673.9	12.866	-13.379	-10.313	0_0	-13,327
682.4	-10.679	-11.096	-11.035	0.0	-11.059
685.6	-12.698	-13.046	-13.077	0.0	-13.017
AAD%	16.715	10,825	11.165	5.618	8.878

Heart Cut: 7HC-B

$T_{B} \stackrel{i}{=} T_{B}$	728.9 492.6	К К	P <sub>c</sub> ω	33 32	3385.31 0.3615	kPa
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Vapor	Pressure	(kPa)	)
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T(K)	Experimental	Linear	Riede1	Wilson	Starling	Mobil
395.4	4.69	7.06	5.314	5.92	5.17	5.20
423.7	13.79	17.39	14.737	15.80	14.70	14.54
452.1	34.54	38.36	35,270	36.72	35.54	34.99
480.4	75.43	76.87	74,516	76.29	75.71	74.22
508.9	146.86	143.15	143,217	144.58	145.72	143.05
537.5	269.58	250.02	254,021	254.55	259.00	254.18
561.2	429.54	380.17	387.721	387.33	396.28	388.32
566.1	452.98	412.76	420,973	420.28	430.41	421.68
589.3	673.62	598,12	608,456	606.94	624.19	609.72
617.5	958.26	904.26	913,53	910,95	941.34	915.45
645.7	1447.89	1318.63	1321.36	1318,59	1369.91	1323.83
673.9	2068.42	1863.12	1855,29	1855.63	1940.57	1857.80
702.3	2819.94	2565.87	2551.34	2551.96	2819.94	2553.12
720.0	3523.21	3092.54	3083.84	2085.08	3523.21	3084.63

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Heart Cut: 7HC-B

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T(K)	Linear	Riedel	Wilson	Starling	Wilson
395.4	50,533	13,305	26.196	10.312	10 947
423.7	26,106	6.867	14,616	6 502	5 436
452.1	11.060	2.113	6.304	2 800	J 430
480.4	1,909	-1.212	1,136	2.099 A 30A	1.001
508.9	-2.526	-2.481	-1 5/0	-0 773	-1.001
537.5	-7.256	-5.772	-5 570		-2.395
561.2	-11.494	-9.736	-0.007	-3.941	-5./11
566.1	-8.879	-7 066	-7 110	-/./44	-9,596
589.3	-11 208		-/.220	-4.984	-6.909
617.5		-9.074 4.600	-9.899	-7.337	-9.486
6/5 7		-4.008	-1.542	-4.457	-4.463
04J./	-8.927	-8./39	-8,931	-5.386	-8,568
0/3.9	-9.925	-10.304	-10.287	-6.181	-10.184
702.3	-9.010	-9,525	-9.503	0.0	-9.462
720.0	-12.224	-12.471	-12.436	0.0	-12.448
AAD %	12,621	7.424	9.359	4.355	7.051

**TTT-85** 

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Heart Cut: 8 HC

$T_{B} = 756.7 \text{ K}$ $T_{B} = 519.8 \text{ K}$	$P_{c} = 3047.47 \text{ kPa}$ $\omega = 0.3901$	
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Vapor Pressure (kPA)

T(K)	Experimental	Linear	Riede1	Wilson	Starling	Mobil
421.4	5.86	7.89	6.185	6.76	5,81	6.06
453.2	17.24	20,46	17.866	18,77	17.36	17.66
479.9	36.96	40.96	38,273	39.43	37.99	38.02
505.7	74.43	74.72	72,93	73.91	73.11	72.70
533.2	138.58	133.01	133,56	134.13	135.25	133.48
561.1	241-32	225.34	229,54	228.82	233.79	229.80
589.3	406.79	364.95	373.13	371.05	382.84	373.92
588.7	386.10	361.40	369,50	367.72	379.33	370.28
616.5	620,53	557.26	567.90	564.64	586 <b>.99</b>	569.33
644.3	924,58	827.75	837,51	833.26	872.43	839,61
672.1	1325.86	1189.92	1194.13	1190.67	1255.71	1196,70
699.8	1865.72	1660.04	1655.12	1653.81	1759.03	1657.71
727.6	2535.19	2260.32	2248,66	2249.31	2535 <b>.19</b>	2250 <b>.5</b> 6
737.7	2847.52	2514.03	2503.01	2503,15	2847.52	2502,56
745.4	3192.26	2721.14	2712,70	2715.23	3192.26	2713.65
748.5	3240,52	2807.97	2801.23	2802.52	3240.52	2301.97

### Heart Cut: 8HC

### Relative % Deviation

T(K)	Linear	Riede1	Wilson	Starling	Mobill
421.4	34.642	5,546	15,267	-0.822	3.498
453.2	18,677	3,631	8.874	0.713	2.437
479.9	10.823	3,552	6.696	2.787	2.860
505.7	1,757	-0.681	0.654	-0.432	-2.327
533.2	-4.019	-3,622	-3.216	-2.405	-3.680
561.1	-6.622	-4.881	-5,179	-3.117	-4.775
588.7	-6.397	-4.299	-4.762	-1.755	-4.297
589.3	-10,285	-8.275	-8,786	-5.888	-8.080
616.5	-10,196	-8,481	-9.007	-5,405	-8,251
644.3	-10.473	-9.417	-9.877	-5.640	-9.190
672.1	-10.253	-9.935	-10.196	-5.290	-9.742·
699.8	-11.024	-11.288	-11.358	-5.718	-11.149
727.6	-10,842	-11.302	-11.277	0.0	-11.227
737.7	-11,712	-12.099	-12.094	0.0	-12.049
745.4	-14,758	-12.247	-14.943	0.0	-14.993
748.5	-13.348	-13,556	-13.516	0.0	-13.533
AAD %	11.614	7.676	9.106	2.498	7.618

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Heart Cut: 10 HC-B

 $T_c = 815.6 \text{ K}$  $P_c = 2792.37 \text{ kPa}$  $T_B = 572.1 \text{ K}$  $\omega = 0.4502$ 

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T(K)	Experimental	Linear	Riede1	Wilson	Starling	Mobil
466.2	6.21	8.10	6.36	6.84	5.86	6.24
480.4	9,79	12,13	10.07	10.65	9.46	9.91
508,9	22.75	25.45	23.03	23.73	22.24	22.82
537.5	47.50	49.49	47.49	48.12	46.78	47.29
566.1	90.32	89,95	89.64	89.82	89.47	89.56
589.3	144.79	139,97	142.06	141.55	142.94	142,18
617.5	236.49	229,08	235.01	233.10	238,17	135.57
645.7	378,52	359,14	369.00	365.34	376.54	370.16
673.9	559.16	542.24	554,55	550.03	570.86	556.43
702.3	823.23	794.07	805,62	799.83	835,69	808.18
730.7	1163.83	1128.90	1135.34	1129.82	1184.33	1138.34
759.1	1651.29	1563,20	1561.24	1557.29	1655.07	1564.17
787.6	2381.44	2116.54	2108.22	2106.80	2381.44	2110.26



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Heart Cut: 10 HC-B

			Relative % De	viation	
T(K)	Linear	Riedel	Wilson	Starling	Mobil
466.2	30.435	2,415	10,152	-5-564	0.535
480.4	23,902	2.860	8.790	-3.382	1.263
508.9	11.868	1,231	4.312	-2,241	0.313
537.5	4.189	-0.021	1.304	-1.517	-0.445
566.1	-0.410	-0.753	-0,555	-0.939	-0.847
589.3	-3,329	-1,885	-2.238	-1.278	-1.802
617.5	-3.133	-0.626	-1.432	0.711	-0.388
645.7	-5,120	-2,515	-3,481	-5.524	-2,208
673.9	-3.026	-0.824	-1.634	2,092	-0.488
702.3	-3,542	-2,139	-2.843	1,513	-1.828
730.7	-3.001	-2.448	-2,922	2,191	-2.190
759.1	-5.335	-5,453	-5,692	0.229	-5.276
787.6	-11.086	-11.436	-11.532	0.0	-11.387
AAD %	8.337	2.662	4.376	2.091	2.228
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**III-89** 

Heart Cut: 11 HC

т	32	865.6	K	P_ =	2688,95	kPa
TB	13	612.6	ĸ	ພັ=	0.4776	

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## Vapor Pressure (kPa)

T(K)	Experimental	Linear	Riedel .	Wilson	Starling	Mobil
506.9	8.14	9,17	7.90	8.34	7.22	7.77
533.7	17.17	18.44	17.01	17.54	16.07	16.83
561.0	34.54	35.09	33.91	34.35	32.79	33.71
588.7	61-36	63.41	63.05	63.14	62.04	62,45
589.1	65.71	63.92	63.58	63.58	62.49	63.91
616.5	102.73	108.83	109.71	108.99	109.24	109.77
644.3	174.44	178.32	180,14	178.13	181.02	180.54
672.1	289.58	280.46	281.52	277.83	285.18	282.44
699.8	437.82	424.90	421.30	416.39	430.75	422.87
727 6	644.66	624.51	609.42	603.15	628.28	611.69
755 4	897.00	892.24	855.67	848.78	890.47	858,56
783.2	1413.42	1242.88	1172.13	1165.67	1233.44	1175,32

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## Relative % Deviation

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<b>T(K)</b>	Linear	Riede1	Wilson	Starling	Mobil
506.9	12.654	-2,948	2,552	-11.225	-4.532
533.7	7.397	-0,932	2.176	-6.386	-1.960
561.0	1.592	-1.824	-0.547	-5.068	-2.390
588 <b>.</b> 7	3.341	2.754	2.899	1.102	2,526
589.1	-2.724	-3.242	-3.237	-4.893	-3.439
616.5	5.948	6.795	6.093	6,337	6.851
644.3	2.224	3.268	2.116	3.773	3.499
672.1	-3.149	-2.783	-4.056	-1.520	-2,466
699.8	-2.951	-3.773	-4.894	-1.615	-3.416
727.6	-3.065	-5,466	-6,438	-2,540	-5.114
755.4	-0.531	-4.605	-5.376	-0.729	-4.286
783.2	-12.066	-17.071	-17,528	-12.734	-16.846
AAD %	4.804	4.622	4.826	4.827	4.777

**III-91** 

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Heart Cut: 15 HC-B

T	3	901.7	ĸ	$P_{a} = 28$	368.21	kPa
т <sub>В</sub>	=	632.1	К	ü≖0,	4589	

## Vapor Pressure (kPa)

T(K)	Experimental	Linear	Riedel	Wilson	Starling	Mobil
508.9	4.83	6.74	5,13	5,56	4.69	5.02
537.5	11.72	14.13	11.92	12,54	11.30	11.75
561.2	23.72	24.63	22.15	22.89	21.46	21.95
566.1	25.44	27.46	24,98	25.73	24.28	24.77
589.3	41.58	44.91	42.72	43.44	42.09	42.51
594.8	49.30	50.18	48.15	48.83	47.57	47.94
617.5	72.05	77.68	76.76	77.10	76.43	76.62
645.7	121.35	128.08	129,59	129,13	129.98	129,67
673.9	210.29	202.53	207.48	206,10	209.68	207.93
702.3	314.40	309,56	318,40	315.34	323.25	319.37
730.7	465.39	457.80	469,85	465.23	479.89	471.48
759.1	717.05	657.51	670.71	664.85	689.88	673.03
787.6	1112.12	921.03	932.08	925 80	967.03	934.99

Heart Cut: 15HC-B

## Relative % Deviation

T(K)	Linear	Riede1	Wilson	Starling	Mobil
508.9	39.545	6.211	15,125	-2.850	4 0.28
537.5	20,563	1.706	6.972	-3.615	A 279
561.2	3.836	-6.619	-3.481	-9.536	-7 475
566.1	7,940	-1.808	1,124	-4 582	-1.475
589.3	8.009	2.742	4.482	1 2/4	-4.022
594.8	1.785	-2.333	-0.942		2.24
617.5	7.814	6.537	7 016	-3.510	-2./31
645.7	5.546	6.790	6 413		0.340
673.9	-3,690	-1.336	-1 000	/ • L L / 	0.853
702.3	-1.539	1,272	0.200	-0.291	-1.123
730.7	-1.631	1 447 4 A 458	-0 036	2.010	1.582
759.1	-8,303	-6 463	-7 201	3.113	1.309
787.6	-17,182	_16 100	-/ +401 16 751	-3./89	-6.138
	1/1102	-10.109	-10./54	-13.047	-15,927
AAD %	9.799	4.690	5,532	4.738	4.512

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Heart Cut: 16 HC

T-	2	930.6	К	P	Ξ	2647.58	kPa
тв	-	658 <b>.</b> 7	K	ŝ	=	0.4713	

## Vapor Pressure (kPa)

T(K)	Experimental	Linear	Riedel	Wilson	Starling	Mobil
560.9	11,51	14.42	12.24	12.83	11.17	12.17
588.7	23.10	26.80	24.42	25.06	23.06	24.35
616.5	44•47	47.10	45.18	45.62	43.74	45.13
644.3	76.53	78.83	78.35	78.19	77.23	78.34
672.1	129.62	126.45	128.52	127.24	128,49	128,55
699.8	204.47	195.05	200,68	198.02	203.31	200.70
727.6	313.02	291,50	301.27	296.46	308.43	301.15
755.4	472.29	422.96	436.63	429.25	451.56	436.10

### Relative % Deviation

T(K)	Linear	Riedel	Wilson	Starling	Mobil
560.9	25.282	6.342	11.431	-2,985	5.741
588.7	16.017	5.714	8,483	-0.144	5.422
616.5	5.914	1.597	2.573	-1.649	1.487
644.3	3.005	2.378	2,162	0,916	2,360
672.1	-2.446	-0.849	-1.834	-0.873	-0.828
699.8	-4.607	-1.854	-3.300	-0.716	-1.842
727.6	-6.875	-3,754	-5,292	-1.468	-3.791
755.4	-10.445	-7.550	-9.113	-4.390	-7.662
AAD %	9.324	3.755	5,524	1.643	3.642

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Heart Cut: 17 HC

 $T_c = 969.4 \text{ K}$  $P_c = 2523.47 \text{ kPa}$  $T_B = 692.6 \text{ K}$  $\omega = 0.4973$ 

## Vapor Pressure (kPa)

T(K)	Experimental	Linear	Riede1	Wilson	Starling	Mobil
616.5	21.99	25.19	23.01	23.44	21.49	22.92
644.3	41.30	43.49	41.78	41.94	40.03	41.70
672.1	67.02	71.77	71.39	70.91	69.72	71.36
699.8	113.76	113.63	115.60	114.19	114.78	115.63
727.6	180.64	173.97	179.26	176.27	180.16	179.33
755.4	284.06	258.14	267.33	262.26	271.57	267.37

## Relative % Deviation

T(K)	Linear	Riedel	Wilson	Starling	Mobil
616.5	14.552	4.638	6.594	-2.276	4.242
672.1	<b>5</b> ,303 <b>7</b> ,087	1.162	1.546	-3.079	0.974
699.8	-0.114	1.617	0.379	4.037	6.473 1.643
727.6	-3.692	-0.764	-2.419	-0.267	-0.725
/22.4	-9.125	-5.890	-7.674	-4.398	-5.875
AAD %	6.646	3.430	4.071	2.492	3.322

Heart Cut: 18 HC-B

 $T_c = 1032.6 \text{ K}$  $P_c = 2675.16 \text{ kPa}$  $T_B = 741.5 \text{ K}$  $\omega = 0.5520$ 

## Vapor Pressure (kPa)

T(K)	Experimental	Linear	Riedel	Wilson	Starling	Mobil
589.3	4.48	5.34	3.72	4.25	3,50	3.63
617.5	<b>'8</b> ,89	10.27	8.03	8,80	7.73	7,90
645.7	15,79	18.66	15.97	16.90	15.58	15.81
673.9	31.51	32.72	29.60	30.53	29.14	29.43
702.3	49.92	53,58	51.79	52.20	51.06	51.69
730.7	86.18	85.51	85.87	85.07	84.65	85,93
759.1	130.31	131.79	135.87	132,85	133.73	136.23
787.6	189.61	197.14	206.70	200.13	203,14	207.51

### Relative % Deviation

T(K)	Linear	Riedel	Wilson	Starling	Mobil
589,3	19.196	-16,964	-5.120	-21.869	-18,995
617.5	15,523	-9.674	-1.100	-13.085	-11.162
645.7	18,176	1.140	7.039	-1.303	0,105
673.9	3.840	-6.062	-3.113	-7.510	-6.589
702.3	7.332	3.746	4.569	2,291	3,546
730.7	-0.777	-0.360	-1.288	-1.781	-0.285
759.1	1,136	4.267	1.946	2.626	4.542
787.6	3.971	9.013	5,552	7.136	9.439
AAD %	8.744	6.403	3.716	7.200	6.833

.

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Table 1 4 Concluded

Heart Cut: 19HC-A

## Vapor Pressure (kPa)

T(K)	Experimental	Linear	Riede1	Wilson	Starling	Mobil
644.3	7.03	9.31	7.61	7.88	6.86	7.49
672.1	13.03	16.63	14.67	14.90	13.62	14.53
699.8	26.34	28.30	26.48	26.53	25.13	26.34
727.6	40.27	46.32	45.26	44.82	43.58	45.19

T(K)	Linear	Riede1	Wilson	Starling	Mobil
644.3 672.1 699.8 727.6	32.43 27.63 7.44 15.02	8.25 12.59 0.53 12.39	12.081 14.329 0.711 11.318	-2.418 4.520 -4.568 8.222	6.510 11.494 0 12.212
AAD %	20.630	8.440	9.610	4.939	7,554

## Relative % Deviation

# COMPARISON OF $\mathrm{T_c}$ CORRELATIONS



Figure III-5

## COMPARISON OF P<sub>c</sub> CORRELATIONS



Figure III-6

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HEART CUT: 4HC









Figure III-8





HEART CUT: 7HC-B



Figure III-10

HEART CUT: 8HC



Figure III-11

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HEART CUT: 10HC-B



Figure III-12





HEART CUT: 15HC-B



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## HEART CUT: 16HC









Figure III-16



HEART CUT: 18HC-B



HEART CUT: 19HC-A

Figure III-18

ERROR BETWEEN LINEAR CORRELATION AND EXPT. DATA




# DEVIATION BETWEEN RIEDEL CORRELATION AND EXPT. DATA



Deviation Between Starling Correlation and Expt. Data

Figure III-21

# Deviation Between Mobil Correlation and Expt. Data





# Wilson Correlation

Linear Correlation



# **Riedel Correlation**



Figure III-25







# Mobil Correlation

Figure III-27

#### HEAT OF REACTION FOR DIRECT COAL LIQUEFACTION PRODUCTS

### Introduction

A coal liquefaction process can be represented as: coal + solvent +  $H_2 \rightarrow$  liquid products + solid residue + hydrocarbon gases

The conversion of coal to distillable liquids is generally accepted as occurring essentially in two stages: dissolution followed by hydrogenation. During the dissolution process, the reactive molecular fragments formed by the breakup of the macromolecular structure of coal are either stabilized by the solvent or undergo retrogressive reactions. Subsequently, these coal derived products are further liquefied by hydrogen, derived not only from molecular hydrogen but more frequently by hydrogen provided by a donor solvent, by cracking and by removal of functional groups. Reduction of the average molecular weight leads to distillable coal derived products. Actually, the solvent can be considered as a reactant in a complex series of reactions which involves coal and hydrogen.

The rational design of a coal liquefaction reactor requires fundmental information about the kinetics and thermodynamics of the reactions, the hydrodynamics of the reactor, and the thermal behavior of the reactor. In the recent past, considerable information has been published in the literature (Shah, 1979, Kelkar et al., 1983) about the kinetics and hydrodynamics of the reactor. Information on bench-scale or pilot scale studies on the heat of reaction or thermal behavior of a coal liquefacton reactors is scarce, however. The objective of this report is to summarize the existing information available in the literature on the heat of reaction of a coal liquefaction reactor and to present an approximate alternative method for the estimation of heat of reaction of a coal liquefaction reactor.

#### Literature Review

The basic reason for the scarcity of data on heat of reaction is the fact that it is very difficult to design and operate a bench-scale adiabatic coal liquefaction reactor. In a commercial scale reactor, the surface area to volume ratio is small and therefore the heat losses to the surroundings are very small compared to the total amount of heat generated in the reactor. The reverse is true, however, for a bench-scale reactor and special designs (Fredrickson et al., 1978, Stephenson, 1981, Shah and Carr, 1981) have to be utilized to produce adiabatic conditions and measure the total amount of heat generated in the reactor.

Fredrickson et al. (1978) reported the design and construction of a calorimeter to determine the heat of reaction for solvation and hydrogenation of coal slurries characteristic of those occurring in coal liquefaction processes. The unit was designed for operating temperatures up to 475° C and pressures up to 28 MPa. Basically, the calorimeter was a constant heat flow reactor which at thermal equilibrium maintains a constant temperature differential between the reaction vessel and its jacket. A heater located in the calorimeter body is used to maintain this temperature difference. The power for this heater is controlled and measured very accurately throughout the experiment. When a reaction occurs in the pressure vessel, the heat released or absorbed changes the temperature differential between the vessel and the jacket. The control system counteracts this thermal change by varying the power applied to the temperature maintenance heater in the calorimeter. This change in power applied to the heater integrated over the time interval of the experiment, equals the amount of heat released or absorbed by the reaction. The gaseous products and unreacted hydrogen were passed from the calorimeter through an analytical train where the gaseous products which

include  $H_2$ ,  $CH_4$ ,  $H_2S$ , and  $NH_3$  and heavier hydrocarbons were removed (with the exception of  $H_2$  and  $CH_4$ ) in a liquid nitrogen trap maintained at 77 K. A large number of calibration runs are presented in this report. For calibration purposes, an accurately measured amount of power is supplied to a calibration heater and the automatically integrated response of the calorimeter circuitry is observed and a calibration factor is calculated in terms of arbitrary units (energy counts/unit energy released by the heater). The calorimeter temperature was maintained at 462  $\pm$  10° C for all runs. The gas in the calorimeter was either helium or hydrogen at pressures ranging from ambient to approximately 9.7 MPa (1400 psig). A number of experimental runs were carried out with coal slurries and liquids in the calorimeter but unfortunately, severe mechanical and electronic control problems prevented the acquisition of any meaningful data.

Subsequently, a second attempt was made by a joint collaboration between The University of Pittsburgh and Gulf Research and Development Corporation to design and operate an adiabatic bench-scale coal liquefaction reactor. The reactor was supported vertically in a rectangular aluminum case which contained electrical heaters and insulating Vermiculite packing. During operation, the heaters were controlled automatically to limit the temperature differential between the dissolver skin thermocouples and the corresponding thermocouples on the clam shell to  $5^{\circ}$  C. The purpose of this instrumentation was to eliminate radial heat losses from the reactor and assure adiabatic operation. A detailed heat survey was done on the dissolver unit and it was estimated that for a typical run at 4.25% hydrogen consumption the net heat loss from the system was 363.8 Btu/hr which was quite small (1.7%) when compared with the total rate of heat generation (21420 Btu/hr). When Powhatan No.5 Mine Coal was run, an exothermic heat of reaction was

observed. The data showed a trend of decreasing heat of reaction with increased hydrogen consumption and Stephenson (1981) correlated all the data as a function of weight percent hydrogen consumed by reaction. The correlation is given by:

 $\Delta H$  reaction = 1.0-0.1140(wt % H<sub>2</sub>), cal/scc of H<sub>2</sub> consumed (1)

standard deviation = 0.026 cal/scc of hydrogen

and a plot of exothermic heat of reaction, plotted as a function of hydrogen consumption, is shown in Figure III-28. The decreasing trend of exothermic heat of reaction with increased hydrogen consumption was explained by the author as due to the fact that the hydrogenation reactions in the coal liquefaction process are mainly due to the saturation of aromatic rings (approximately 0.684 cal/scc at standard conditions estimated from heat of formation data). Stephenson concludes that this saturation of aromatic rings is more representative of the coal liquefaction process and not the hydrocracking reactions, which are much less exothermic (approximately 0.089 cal/scc at Standard Conditions). It is possible that the net heat of reaction thus decreases with hydrogen consumption as additional hydrogen is consumed in hydrocracking reactions. Stephenson also calculated the heat of reaction by the CHAMP Program (a property data base utilized by Gulf) and predicted a value of 0.528 cal/scc at 4.25 weight percent hydrogen consumption.

### Present Work

In the absence of any reliable data on heat of reaction for coal liquefaction reactions, an attempt was made by the present authors to estimate the heat of reaction from the heat of combustion data for the reactants and products of the hydrogenation reaction. Let us represent the coal liquefaction reaction as:

 $coal + H_2 \rightarrow (aA + bB + cC + - - - -) + solid$ 

Thus the heat of reaction can be represented as:

$$\Delta H_{R} = (a\Delta H_{a} + b\Delta H_{R} + c\Delta H_{C} + - - -) - (\Delta H_{coal} + \Delta H_{H_{c}})$$

+ correction for sensible heat of the reactants and products

where  $\Delta H_R$  = Heat of reaction at standard conditions  $\Delta H_i$  = Heat of combustion for the products and reactants at standard conditions

The heat of combustion data for coal is calculated from the elemental analysis of the coal and from Dulong's formula (Perry and Chilton, 1973) which is given by:

$$\Delta H_{c} = 145.55C + 620 (H - \frac{0}{8}) + 41S - 92.7 H$$
(2)

 $\Delta H_{c}$  = Heating value of the coal (Btu/1b)

C = Weight percent of carbon

H = Weight percent of hydrogen

0 = Weight percent of oxygen

S = Weight percent of sulfur

N = Weight percent of nitrogen

This equation gives an average deviation of 2% for coals containing up to 10% of oxygen on a dry ash-free basis.

The heat of combustion data of coal derived liquids were estimated by the following equation (Venturino, 1978).

$$\Delta H_{c} = 151.2 C + 499.7 H + 27.0 N + 45.05 S - 47.7 0$$
(3)

Material balances and elemental analyses for three typical coal liquefaction reactions are given in Table III-15, and Table III-16 (Gray, 1981) and equations (2) and (3) were used to estimate the heat of combustion of the coal and coal derived liquids and these results are given in Table III-17. The heat of combustion data for the other hydrocarbons (viz.  $C_1-C_4$ ) and NH<sub>3</sub>, H<sub>2</sub>S, CO and CO<sub>2</sub> were calculated from the heat of formation data which are readily available (Perry and Chilton, 1973) and are given in Table III-18. Since no measure of the specific amounts of  $C_1-C_4$  or the other inorganic gases was given, an average value was used for their contribution.

#### Results and Discussion

The material and energy balances for three different runs are shown in Tables III-19, III-20, and III-21. We can see that among the reactants the total heat contributed by coal is almost 85-90% of the total whereas among the products the contribution by different fractions of the hydrocarbons are comparable. Sensible heat carried by either the reactants or the products are always within 5% of the corresponding heat of combustion. The net heat of reaction calculated for Run #55, 56 and 66 from material and energy balances are 0.668, 0.248 and 0.824 Cal/scc H<sub>2</sub> while those calculated from equation (1) for these runs are 0.544, 0.521 and 0.624 Cal/scc of H<sub>2</sub> respectively. The deviation for these three cases are 22.79%, -52.4% and 32.05% respectively. Such large deviations between the experimental value and that calculated from energy balances can be attributed primarily to the following reasons:

. Direct coal liquefaction produces a variety of products which are grouped as different cuts of liquids. It is very difficult to make an accurate material balance for such a process.

. Each cut of liquid consists of a wide range of hydrocarbons having varying degrees of heat of combustion. In the present analysis, the heat of combustion for each cut of liquid is determined on the basis of elemental analysis and equation (3), which might introduce considerable error in the energy balance.

. The overall energy balance is highly sensitive to the heat of combustion of the coal used for liquefaction. Heat of combustion of coal is again determined from its elemental analysis and Dulong's formula (equation 2) which is supposed to represent a wide spectrum of coals. However, we think more experimental data on the heat of combustion of coal may enable one to develop a superior empirical prediction relationship.

• The property data base e.g. specific heat data for coal derived liquids is very limited at the present time. Sensible heat for products have very little influence on the overall energy balance, however.

The present study was undertaken to make an energy balance around the dissolver and to check the validity of equation (1) to be used in our simulator program. However, we think that the energy balance approach is difficult to apply and equation (1) derived from actual experimental data should be used for simulation of any coal liquefaction reactor. Conclusions

Significant progress has been made in the past decade to understand the chemistry, kinetics and hydrodynamics of a direct coal liquefaction reactor. However, experimental data on the heat of reaction studies are still scarce because of the difficulty in building a prototype bench-scale adiabatic coal liquefaction reactor. The estimation of heat of reaction from the material and energy balances given in this report is only approximate and very sensitive to the heat of combustion data of the coal and the heavier liquids formed during the reation. Further, the heat capacity data of the coal derived liquids at the reaction temperature are limited. They were obtained from one of our earlier reports (Albal et al., 1983). More experimental data on the actual heat of reaction of coal liquefaction reactions, heat of combustion data of the coal derived liquids, and specific heat data of the products of liquefaction reaction at or near the reaction conditions are urgently needed for any rational design and thermal control of an actual industrial scale reactor.

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## PDU P-99 OPERATING CONDITIONS AND YIELDS DURING PRODUCTION OF COAL DISTILLATES USED IN PROCESS SOLVENT-DEBUTANIZER BOTTOMS BLEND

Run No., P99-	<u>55*</u>	56**	66***
Operating Conditions			
Temperature, <sup>O</sup> F	851	851	855
Pressure, psig	2000	2000	<b>20</b> 00
Residence Time, hr	1.0	1.0	1.0
Coal in Feed Slurry, wt %	30	30	30
Recycle Solids, wt %	16	14	12
Gas Rate, 10 <sup>3</sup> SCF/Ton of coal	52.9	58.8	54.0
Outlet H <sub>2</sub> Part. Press., psia	1350	1290	1510
Yields, wt % Moisture Free Coal			
Hydrogen	-4.0	-4.2	-3.3
C <sub>1</sub> -C <sub>4</sub> 15.9	16.0	13.2	
$NH_3$ , $H_2S$ , CO, CO <sub>2</sub>	3.2	3.6	3.1
Water 7.2	6 • 5	5.7	
C <sub>5</sub> -380 <sup>o</sup> F	6.9	7.2	6.8
380–550°F	14,5	15.1	12.8
550–900 <sup>0</sup> F	13.9	13.8	10.8
Total C <sub>5</sub> -900°F	35.3	36.1	30.4
900°F+Pyridine Sol.	24.1	23.6	32.6
IOM 7.4	7.0	9.3	
Ash 10.9	12.4	9.0	
Total 900°F+	42.4	42.0	50 <b>.9</b>

<sup>\*</sup> Powhatan No. 5 Mine Coal, LR-25844
\*\* Powhatan No. 5 Mine Coal, LR-29682
\*\*\*Powhatan No. 5 Mine Coal, LR-27383

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## ANALYSES OF POWHATAN NO. 5 MINE COALS USED FOR PRODUCTION OF COAL LIQUID STOCKS

Run P99- 55 Sample NO., LR-	56 25844(2nd Batch)	62 and 66 26982	27383
Elemental Analyses			
Wt % of Moisture-Free Coal			
Carbon	71.62	70.18	74.26
Hydrogen	5.26	4.99	5.17
Pyritic Sulfur	0.88	1.68	1.00
Organic Sulfur	1.63	1.69	1,50
Sulfate Sulfur	• 0.20	0.15	0.04
Total Sulfur	2.71	3,52	2.54
Nitrogen	1.27	1.23	1.40
	13.16	13.41	11.64
Matale	5.93	6.63	4.91
Iron	0.81	1.62	0.94
W/C Atomic Batio	0.86	0.85	0.84
Moleture Content.	1.7	1.2	0.7
Why 7 of Ac-Repaired Cost			
We hold a Mar 7 of	34, 5	36.5	39.2
Volatile, wt % of	0.00		
ASTRECEIVED Wals	10-8	12.4	9.1
Ash, WE & OF MOISture-Free Coal	10.0		
Analysis of Coal Substance,	a 14		
Wt % Moisture Mineral-Free	Coal#	13 6	13 9
Volatile	39.5	42.0 01 0	4J.0
Carbon	61.6	01.Y E 0	01.7
Hydrogen	6.0	<b>D</b> •ŏ	J.O 1 6
Nitrogen	1.4	1.4	0 O
Oxygen**	. 9.0	8°A .	0.0
Sulfur	2.0	2.0	±, • /

\* Mineral Matter = 1.08 x ash content + 0.55 x pyritic sulfur content \*\*By difference

## Heat of Combustion for Goal and Coal Derived Liquids Calculated from Equations (2) and (3)

Elemental Analysis						
Material	<u>c</u>	H	<u>0</u>	N	<u>s</u>	ΔHc (kCal/gm) From eq. (2)
Coal (sample #55)	71.62	5.26	13.16	1.27	2.71	-6.82
Coal (sample #56)	70.18	4.99	13.41	1.23	3.52	-6.63
Coal (sample # 61)	<b>7</b> 4 <b>.</b> 26	5.17	11.64	1.40	2.54	-7.07
Coal Liquids						ΔH <sub>c</sub> (kCal/gm)
						From Eq.(3)
с <sub>5</sub> –380 <sup>о</sup> ғ	85.51	9.14	2.3	1.28	0.27	-9.685
380-550 <sup>0</sup> F	87.20	9.31	1.3	0.99	0.27	<b>~9.</b> 88
550-900 <sup>0</sup> F	88.60	7.30	2 .3	-	-	-9.41
900 <sup>+</sup> °F	88.02	7.02	<b>ata</b>	-		-9.34

## Heat of Combustion Data for Light Hydrocarbon and Inorganic Gases (Perry and Chilton, 1973)

Heat of Combustion (kcal/gm) (Standard Conditions)
-28.6
-11.95 )
-11.34 (Average = - 11.33
-11.07
-10.99
- 5.37
- 3.95
- 2.41
0.0
0.0
0.0
0.0

## Complete Material and Energy Balance for Run #55

Component	Yield, wt % of moisture free coal	Total heat of combustion of products (kcal)	Total Heat of combustion of reactants (kcal)	Sensible heat of products (kcal)	Sensible heat of reactants (kcal)
Coal	100.0*		682.0		12.9
<sup>H</sup> 2	4.0*		114.4		6.0
c <sub>1</sub> -c <sub>4</sub>	15.9	180.14		2.87	
NH3,H2S,CO, CO2	3.2	7.48		0.57	
Water	7.2	0.0		1.23	
с <sub>5</sub> –380 <sup>о</sup> ғ	6.9	66.79		2.96	
380-550°F	14.5	143.26		6.24	
550 <b>-900<sup>0</sup>F</b>	13.9	130.79		5.97	
900 <sup>0</sup> F +Pyridine	24.1	225.14		10.36	
IOM	7.4	0.0		0.63	
Ash	10.9	0.0		0.94	
		753.60	796.40	31.77	18.9

Net Heat of Reaction (kcal) = 29.93Heat of Reaction (cal/scc of H<sub>2</sub>) = 0.668

\*Consumed by reaction

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## Complete Material and Energy Balance for Run #56

Component	Yield, wt % of moisture free coal	Total heat of combustion of products (kcal)	Total heat of combustion of reactants (kcal)	Sensible heat of products (kcal)	Sensible heat of reactants (kcal)
Coal	100.0*		663.5		12.9
H <sub>2</sub>	4.2*		120.12		.6.32
c <sub>1</sub> -c <sub>4</sub>	16.0	181.2		2.89	
NH3, H2S, CO, CO2	3.6	8.42		0.65	
Water	6.5	0.0		1.23	,
с <sub>5</sub> –380 <sup>о</sup> г	7.2	69,69		3.09	
380 <b>5</b> 50 <sup>0</sup> F	15.1	149.18		6.49	
550–900 <sup>0</sup> F	13.8	129.85		5.93	
900 <sup>0</sup> F +Pyridine	23.6	220.42		10.14	
IOM	7.0	0.0		0.6	
Ash	12.4	0.0		1.06	
		758.76	783.27	32.08	19.22

Net Heat of Reaction (kcal) = 11.65Heat of Reaction (Cal/scc of H<sub>2</sub>) = 0.248

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## Complete Material and Energy Balance for Run #66

Component	Yield, wt% of moisture free_coal	Total heat of combustion of products (kcal)	Total heat of combustion of reactants (kcal)	Sensible heat of products (kcal)	Sensible heat of reactants (kcal)
Coal	100.0*		707.1		12.96
H <sub>2</sub>	3.3*		94.38		4.98
c <sub>1</sub> -c <sub>4</sub>	13.2	149.55		2.39	
NH3, H2S, CO, CO2	3.1	7.25		1.31	
Water	5.7	0.0		1.08	
с <sub>5</sub> -380°ғ	6.8	65.82		2,94	
380–550 <sup>0</sup> F	12.8	126.46		5,53	
500 <b>-9</b> 00 <sup>0</sup> F	10.8	101.62		4.66	
900 <sup>0</sup> F +Pyridine	32.6	304.54		,14.08	
IOM	9.3	0.0		0.92	
Ash	9.0	0.0		0.85	
		755.24	801.48	33.76	17.94

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Net Heat of Reaction (kcal) = 30.42Heat of Reaction (Cal/scc of H<sub>2</sub>) = 0.824

<sup>\*</sup>Consumed by reaction



Figure III-28 Exothermic Heats of Reaction for PDU-P-99 Runs Near Demonstration Plant Design Conditions

## SURFACE TENSION OF COAL LIQUIDS

### Introduction

Like liquid density and viscosity, surface tension is an important physical property of coal liquids essential for the design of coal liquefaction reactors, fractionating towers and other process equipment. Bubble size and rate of coalescence in a coal liquefaction dissolver are directly related to the surface tension of coal liquids used in making the feed slurry and unfortunately little is known about this property under actual reaction conditions. Limited data are available today, at somewhat lower temperatures, for paraffinic liquids typical of petroleum refinery process streams. These paraffinic liquids are mainly straight chain hydrocarbons in contrast to coal liquids derived from typical direct coal liquefaction processes, which are more aromatic in nature. One measure of the extent of aromaticity for coal liquids is given by the Watson characterization factor

$$K_{w} = \frac{(T_{b})^{1/3}}{SG}$$
where  $T_{b}$  = normal boiling point  
SG = specific gravity

Crude oils and heavy paraffins have a  $K_w$  12-13 while aromatic fractions such as coal liquids in general, have  $K_w < 11$ . Because of this difference in nature between these two types of liquids, data and correlations developed for petroleum fractions must be applied to coal liquids with caution. Two independent studies were recently undertaken to form a data base on the surface tension of coal liquids - one by Hwang et al. (1982) at Exxon Research and Engineering Company and the other by Gray and Holder (1982) at Gulf R&D Company. A summary and comparison of their studies are discussed below.

### Experimental Program

Hwang et al. (1982) studied five Illinois (bituminous) and four Wyoming (subbituminous) coal liquids produced by the Exxon Donor Solvent (EDS) process. A drop weight surface tension apparatus capable of measuring data at high temperature and pressure was used for measuring the surface tension of the coal liquids. The apparatus was calibrated with pure samples of hydrocarbons over a wide range of temperature and pressure and the literature data were reproducible within  $\pm$  3%. A detailed description of the apparatus and the experimental procedure are described in Hwang et al. (1982).

The experimental data reported by Gray and Holder (1982) were taken by the Wilco Research Company. Surface tension data were collected on narrow boiling coal liquid fractions (Heart cut 4HC-B, 6HC, 7HC-A, 10HC-A, 15HC-A and 18HC-1) and also on vacuum tower overhead, heavy distillate product and recycle slurry obtained from the PDU-99 unit, at temperatures up to 672 K and pressures to 13.8 MPa. The reproducibility of their data was checked by measuring surface tension of two pure compounds (decaline and n-hexadecane) where the data could be reproduced with a maximum deviation of 4% or less. In general, the surface tension of coal liquids decreased with increasing temperature and pressure and increased with increasing boiling point of the liquids. The authors reported that an increase in pressure led to a decrease in surface tension of the coal liquid though the decrease was only marginal for coal liquids derived from the EDS process (Hwang et al., 1982). As expected, heavy distillate and vacuum tower overhead samples had almost the same surface tension because the boiling ranges of those two liquids are very similar. The recycle slurry stream showed surface tension values very different from other process streams probably because of large content of pyridine soluble material in that stream.

### Available Correlations

Hwang et al. (1982) from their study concluded that the correlations available for petroleum fractions and pure components are not accurate to represent the surface tension of coal liquids derived from the EDS process. The average deviation between the experimental data and the correlations which relate mixture surface tension to component parachor and other mixture properties was about 16%. Hwang et al. (1980) measured the surface tension of coal liquids having a wide boiling range obtained from the EDS process and correlated their data with the following expression:

$$\sigma_{r} = 0.0837 (1 - T_{r})^{0.868} (\frac{14.7}{P})^{MT}$$
(1)  

$$M = \text{constant} = 1.84 \times 10^{-4}$$

$$T = \text{temperature (}^{O}F\text{)}$$

The surface tension data of narrow boiling coal liquids were correlated by Gray and Holder (1982) with reduced temperature. The general form of this correlation can be written as

$$\sigma(T,P) = a_1 (1-T_r)^{a_2}$$

$$\sigma(T,P) = \text{surface tension of coal liquid (dyne/cm) at}$$

$$\text{temperature T(}^{o}F) \text{ and pressure (psia)}$$
(2)

where  $a_1$  and  $a_2$  are constants or  $a_1$  is a function of the Watson characterization factor. The data were also correlated in terms of reduced surface tension as:

$$\sigma_{r} = a_{3} \left(1 - T_{r}\right)^{a_{4}}$$
(3)

where

$$\sigma_{r} = \frac{\sigma (T, P)}{T_{c}^{1/3} P_{c}^{2/3}}$$
(4)

and  $a_3$  and  $a_4$  are constants. The applicability of these equations to actual experimental data and the resulting deviations are described in detail by Gray and Holder (1982).

Stephenson (1981) presented the following correlations to predict the surface tension of SRC-II distillate cuts at any temperature and pressure as:

$$\sigma_{\rm r} = 0.0676 \ (1 - T_{\rm r})^{0.350} \ (\frac{14.7}{\rm P})^{0.336} \tag{5}$$

At present, no correlation is available to calculate the surface tension of coal liquids in the presence of a solid. Until such data are available, the previous correlations are to be used for coal liquid slurries with great caution.

#### Conclusions

Surface tension is an important physical property of coal liquids and is essential for the rational design of a coal liquefaction reactor. Surprisingly, there is an extreme searcity of experimental data on this property. Only two sets of studies are reported, one by Hwang et al. (1982) and the other by Gray and Holder (1982). Hwang et al. tried to correlate their data from fundamental properties like the parachor while Gray and Holder used semi-empricial correlations. In any case, both sets of authors agree that the available correlations are inadequate to predict the surface tension of coal liquids and more experimental data are urgently needed.

## Nomencature

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<sup>a</sup> 1, a <sub>2</sub> , a <sub>3</sub> , a <sub>4</sub>	Constants 1/3
K <sub>w</sub>	Watson Characterization Factor ( $=\frac{Tb^{1/3}}{SG}$ )
P	Pressure (psia)
Pc	Critical Pressure (psia)
SG	Specific Gravity
Т	Temperature ( <sup>o</sup> F)
т <sub>ь</sub>	Boiling Point ( <sup>o</sup> F)
<sup>т</sup> с	Critical Temperature ( <sup>o</sup> F)
Tr	Reduced Temperature
σ	Surface Tension (dyne/cm)
σ <sub>r</sub>	Reduced Surface Tension, defined as in Equation

(4)

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#### PRANDTL NUMBERS AND HEAT TRANSFER

OF COAL LIQUIDS

#### Introduction

Direct coal liquefaction is a highly exothermic process invloving a complex network of series and parallel reactions. Efficient removal of the heat generated by reaction is very critical for proper thermal control and safe operation of coal liquefaction reactor. This cannot be accomplished by theoretical approach alone and an empirical approach utilizing the information available from a bench-scale reactor may be necessary to scale up the data for the design of a commercial reactor. One such approach is the use of "Dimensional Analysis" which is very popular among chemical engineers. The objective of this report can be stated as follows:

. To investigate the Prandtl numbers associated with coal liquids. The Prandtl number is an important dimensionless number used in heat transfer correlations.

• To investigate the applicability of available heat transfer correlations to coal liquids. These heat transfer correlations are usually expressed as functions of dimensionless numbers, e.g., Reynolds number, Prandtl number and Nusselt number. Actual pilot plant data are used in our analysis and final recommendations are made about their suitability to coal liquids.

## Prandt1 Number

Forced convection heat transfer is the most frequently employed mode of heat transfer in the coal liquefaction industry. Coal liquids from the dissolver unit are pumped through heat transfer equipment having widely different flow conditions and flow geometry. Flow is generally turbulent and the flow duct varies in complexity from circular tubes to baffled and extended surface heat exchangers. Heat transfer correlations involve Reynolds numbers  $(N_{Re})$  which is a function of the flow geometry and fluid properties and the Prandtl number  $(N_{Pr})$  which is entirely a thermal property of the liquid. These two dimensionless numbers are usually expressed as a function of the Nusselt number  $(N_{Nu})$ , which involves the convective heat transfer coefficient associated with a particular system. Correlations available in the literature and their application to coal liquids will be discussed in the next section of this report.

The Prandtl number, an important dimensionless number associated with heat transfer, is a fundamental property of the fluid and is a function of its physical properties. This is defined by equation (1)

$$N_{Pr} = \frac{C_{p}}{k}$$
(1)

where  $C_p$  is the heat capacity of the liquid (kJ/kg.k),  $\mu$  is viscosity of the liquid (mPa.s) and k thermal conductivity of the liquid (w/m.s). Experimental values of  $C_p$ ,  $\mu$  and k for different boiling fractions of coal liquids have been reported by Gray and Holder (1982). Frandtl numbers calculated from these data are shown in Figure III-30 and III-31. For any specific cut of coal liquid,  $C_p$  and k are very weak functions of temperature while  $\mu$  is not. Increase of temperature shows a significant decrease of  $\mu$  and consequently  $N_{Pr}$ . The effect of temperature was more pronounced for higher boiling cuts of liquids than lower ones. At higher temperature (> 400 K)  $N_{Pr}$  reaches an asymptotic value of 5.0 for cut 2 and 20.0 for cut 12. In general, it can be said that the  $N_{Pr}$  decreases with increasing temperature and increases with increasing boiling point of the coal liquid. Typical coal liquefaction reactions are carried out at approximately 800-900 °F and 28 MPa. However,

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experimental data on the physical properties are not available at such high temperature to calculate the Prandtl numbers. Extrapolation of low temperature data shows that depending upon boiling point of the coal liquids, the N<sub>Pr</sub> will vary from 5-30.0 at typical reaction conditions inside the preheater or the dissolver.

### Prandtl Number for Pure Compounds

Coal liquids are generally a mixture of different types of hydrocarbons, namely, aliphatic, alycyclic and mainly aromatic or heterocyclic hydrocarbons. The Prandtl number for some pure hydrocarbons were calculated and compared with those calculated for coal liquids. Physical property data for such liquids are readily available (Perry and Chilton, 1973, Reid, Prasunitz and Sherwood, 1977). Figure III-32 shows the data for pure aliphatic compounds; Figure III-33 shows the data for pure aromatic compounds and Figure III-34 shows the data for pure phenolic compounds. The same general trend of Prandtl number as a function of temperature as observed for coal liquids is found. Figure III-32 shows that Pr increases with increase in boiling point of the liquid (i.e., higher carbon number) and reaches an asymptotic value of 5-10 for temperatures greater than 600 K. Figures III-33 and III-34 show the Prandtl number of some selected aromatic compounds which constitute a major portion of the coal liquids. In general, it can be concluded that phenolic compounds (Figure III-34) have higher Prandtl numbers than aromatic compounds at lower temperature (< 400 K) but the reverse is true at higher temperature (> 400 K).

## Heat Transfer in Coal Liquids

The basic objective of this section is to examine the applicability of the heat transfer correlations to coal liquids. No comprehensive study on this particular aspect of coal liquids has been done so far. Gulf R&D

(Parimi, 1981) has conducted a detailed experimental investigation into the heat transfer characteristics of coal slurries in a sectionalized preheater and only one set of data were taken (baseline run) where the study was done with coal liquid only (in absence of any coal particles). These data were used by the present authors. The method of our analysis is summarized as follows:

(a) The preheater coil was divided in thirteen sections (for Run #R-1) and the inlet and outlet temperatures of the coal liquids and the skin temperature profile in each of these sections are given by Parimi (1981).

(b) Enysical property data (heat capacity, density, and viscosity) were also taken from the report (Parimi, 1981). Thermal conductivity data were also taken from the same report; however, they were significantly scattered over the temperature range of interest. Therefore, a least square fit was performed and the resulting equation, given as follows:

$$k = 0.1065 - 7.72 \times 10^{-5} T$$
 (2)  
 $T = {}^{0}F$ 

was used in our analysis.

(c) A simple energy balance around each section of the tube gives us the following equation

$$\ln \frac{T_{\rm L} - T_{\rm S}}{T_{\rm 0} - T_{\rm S}} + \frac{h_{\rm expt}}{\rho V C_{\rm p}} \left(\frac{4L}{D}\right) = 0$$
(3)

 $T_L$ ,  $T_S$ ,  $T_0$ , K and D data are taken from the report (Parimi, 1981). The film heat transfer coefficient ( $h_{expt}$ ) and Nusselt Number ( $Nu_{expt} = hL/D$ ) can be evaluated from equation 3 after substitution of the physical property data. (d) Depending on the Reynolds number and the physical properties of the fluid inside the tube, different correlations are available in the literature to predict the film heat transfer coefficient in a straight tube. Turbulent flow equations for predicting heat transfer coefficient are usually valid only at Reynolds number greater than 10,000. The transition region lies in the region of 2000  $< N_{Re} < 10,000$ . Under the conditions of the experiment,  $N_{Re}$  varies between 3000 - 30,000, that is, from the beginning of transition region to highly developed turbulent flow. No simple equation exists for predicting a smooth transition from laminar to turbulent flow. However, Hausen's equation (Perry and Chilton, 1973) is valid in the range of 2100 - 10,000 and was used by the present authors. This equation is:

$$N_{Nu} = 0.116 (N_{Re}^{2/3} - 125) N_{Pr}^{1/3} [1 + (D/L)^{2/3}] (\mu_b/\mu_w)^{0.14}$$
(4)

For  $N_{Re} > 10,000$ , 0.7  $< N_{Pr} < 700$ , L/D > 60, the Dittus - Boelter equation (Kern, 1965) is effective for predicting the heat transfer coefficent. This equation is given as

$$N_{Nu} = 0.023 N_{Re}^{0.8} N_{Pr}^{0.4}$$
(5)

A third equation investigated by the present authors is given by Petukhov (1970). This equation is valid for  $10^4 < \text{Re} < 5 \times 10^6$  and 0.5 < Pr < 2000 and is given as

$$N_{Nu} = \frac{(\zeta/8)^{N_{Re}} N_{Pr}}{K_{1}(\zeta) + K_{2} (N_{Pr}) (\zeta/8)^{1/2} (N_{Pr}^{2/3} - 1)}$$
(6)  
$$\zeta = (1.82 \log N_{Re} - 1.64)^{-2}$$
(7)
$$K_1(\zeta) = 1 + 3.4\zeta$$

$$K_2 (Pr) = 11.7 + 1.8 Pr^{-1/3}$$
 (9)

(8)

#### Results and Discussion

Plots of  $\boldsymbol{C}_{_{\!\boldsymbol{D}}},\;\boldsymbol{k},\;\boldsymbol{\rho}$  and  $\boldsymbol{\mu}$  against bulk fluid temperatures are shown in Figures III-35 and III-36. Variations of the Reynolds number and the Peclet number calculated from these physical property data for each section of the preheater are shown in Figure III-37. As expected, with increasing section number which also means increasing skin temperature of the preheater, the Reynolds number increases almost linearly. A log-log plot of heat transfer coefficient and Nussetlt number, both experimental (i.e., calculated from equation 3) and predicted by three different correlations namely Hausen (equation 4), Dittus-Boelter (equation 5) and Petukhov (equation 6) are shown in Figures III-38 and III-39. Our analysis shows that the Dittus-Boelter equation fits the data best (Average Absolute Deviation, AAD = 8.95%) for both the transition and the turbulent region. Petukhov's correlation is not as good (AAD = 12.26%) and has a tendency to underpredict and overpredict at lower and higher ranges respectively. Hausen's correlation gave the worst fit. (AAD = 16.68%) especially at lower values of the Reynolds number. The excellent fit of Dittus-Boelter equation for both the transition and turbulent region is surprising, since this equation is normally used for  $N_{Re} > 10,000$ . Petukhov's correlation is almost as good as the Dittus-Boelter correlation, however it is more complex in nature and difficult to use.

## Nomenclature

с <sub>р</sub>	Heat capacity
D	Diameter
h <sub>expt</sub>	Experimental Film Heat Transfer Coefficient
L	Length of tube
N <sub>Nu</sub>	Nusselt number
N <sub>Pr</sub>	Prandtl number
NRe	Reynolds number
k	Thermal Conductivity
к1	Defined by equation 8
<sup>K</sup> 2	Defined by equation 9
TL	Temperature of fluid at outlet
т <sub>о</sub>	Temperature of fluid at inlet
т <sub>s</sub>	Skin temperature
v	Velocity of the fluid

# Greek Symbols

μ	Viscosity of fluid
μ	Viscosity at bulk temperature
μ <sub>w</sub>	Viscosity of wall temperature
ρ	Density of fluid
ζ	Defined by equation 7

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Figure III-34 Heat Capacity and Thermal Conductivity Values Versus Bulk Fluid Temperature for SRC-II Liquid



Figure III-35 Viscosity and Density Values Versus Bulk Fluid Temperature for SRC-II Liquid

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Figure III-35 Reynolds Number and Peclet Number Versus Section Number for Slurry Preheater for SRC-II



Figure III- 37 Convective Heat Transfer Coefficient Versus Reynolds Number for Slurry Preheater for SRC-II



### Figure III-38 Nusselt Number Versus Reynolds Number for Slurry Preheater for SRC-II

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