High Temperature Simulated Distillation

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History of Simdis

- ASTM D2887
- Boiling range >100F to 1000F
- Cannot determine any residue >1000F
- (Normalizes results to 100%)

- High Temperature Simdis
- Boiling range >97F to 1382F
- Determines % residue above 1382F

Typical High Temp Simdis Result

AC Simdis version 04.09.001

Instrument 2 High temperature **ITS** **1**

Sample name	: 1600-1	Instrument	: 2
Method name	: C:\HPCHEM\2\METHODS\HT750C.M	Vial	: 1
Sample type	: SHELL	Injection	: 1
Sequence name	: 2041703C.S	Seq. line	: 5
Operator	:	Sample (g)	: 0.2118
Acquired on	: 4/21/03 1:47:14 PM	Solvent (g)	: 20.8045
Processed on	: 4/21/03 2:38:16 PM	ISTD (g)	: 0.0000
Data File	: 2041703C\001F0501.D\FID1A.CH	Start Elution	: 0.10
Blank used	: 2041703C\085F0401.D\FID1A.CH	End Elution	: 46.35S
BP Calibrant	: 2041703\090F0101.D\FID1A.CH	Found recovery	: 95.0%
Last Reference	: 2041703C\095F0201.D\FID1A.CH On spec.	Used recovery	: 95.0%
Cal. method	: External Standard Method	Response	: 2.6118e-008

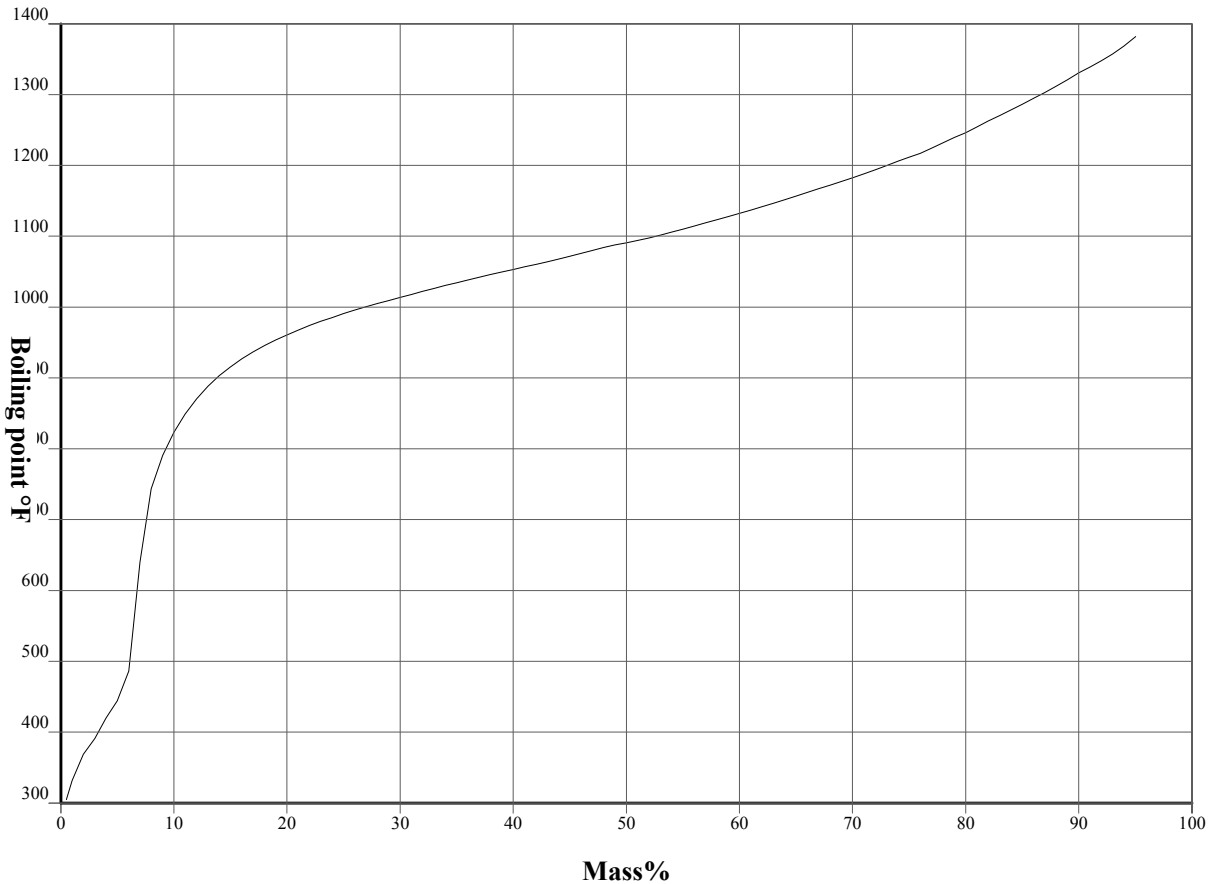
Boiling point distribution:

Mass%	BP(°F)	Mass%	BP(°F)	Mass%	BP(°F)	Mass%	BP(°F)	Mass%	BP(°F)
IBP	305	20	961	40	1053	60	1132	80	1246
1	331	21	968	41	1057	61	1137	81	1254
2	369	22	974	42	1060	62	1142	82	1262
3	391	23	980	43	1064	63	1146	83	1270
4	420	24	985	44	1067	64	1151	84	1278
5	444	25	991	45	1072	65	1157	85	1286
6	486	26	996	46	1076	66	1162	86	1295
7	640	27	1000	47	1080	67	1167	87	1303
8	744	28	1005	48	1084	68	1172	88	1312
9	791	29	1009	49	1088	69	1177	89	1321
10	823	30	1014	50	1091	70	1183	90	1330
11	849	31	1018	51	1094	71	1188	91	1339
12	870	32	1022	52	1098	72	1194	92	1348
13	888	33	1026	53	1102	73	1200	93	1357
14	903	34	1030	54	1106	74	1206	94	1368
15	916	35	1034	55	1110	75	1211	95	1381
16	927	36	1038	56	1114	76	1217	95.0	1382
17	937	37	1042	57	1119	77	1224		
18	945	38	1046	58	1123	78	1232		
19	953	39	1050	59	1128	79	1239		

Instrument 2 High temperature **ITS** **2**

Sample name	: 1600-1	Instrument	: 2
Method name	: C:\HPCHEM\2\METHODS\HT750C.M	Vial	: 1
Sample type	: SHELL	Injection	: 1
Sequence name	: 2041703C.S	Seq. line	: 5
Operator	:	Sample (g)	: 0.2118
Acquired on	: 4/21/03 1:47:14 PM	Solvent (g)	: 20.8045
Processed on	: 4/21/03 2:38:16 PM	ISTD (g)	: 0.0000
Data File	: 2041703C\001F0501.D\FID1A.CH		

Boiling point Distribution plot:



Instrument 2 High temperature **ITS** **3**

Sample name	: 1600-1	Instrument	: 2
Method name	: C:\HPCHEM\2\METHODS\HT750C.M	Vial	: 1
Sample type	: SHELL	Injection	: 1
Sequence name	: 2041703C.S	Seq. line	: 5
Operator	:	Sample (g)	: 0.2118
Acquired on	: 4/21/03 1:47:14 PM	Solvent (g)	: 20.8045
Processed on	: 4/21/03 2:38:16 PM	ISTD (g)	: 0.0000
Data File	: 2041703C\001F0501.D\FID1A.CH		

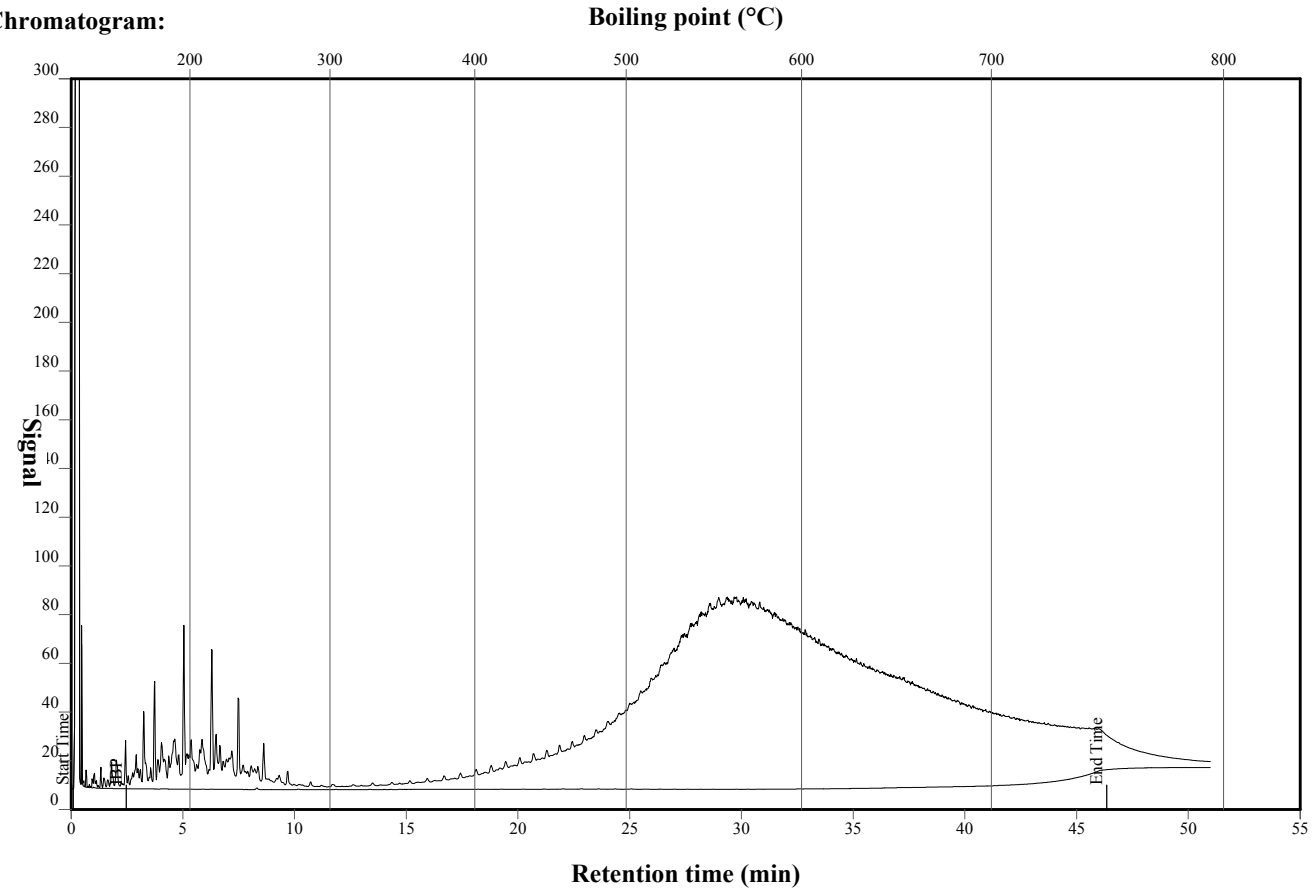
Cutpoints and fractions results:

BP(°F)	Cutpoint Mass%	Fraction Mass%	BP(°F)	Cutpoint Mass%	Fraction Mass%	BP(°F)	Cutpoint Mass%	Fraction Mass%
155	0.0	0.0	500	6.2	2.9	900	13.8	5.7
265	0.2	0.2	600	6.8	0.6	1000	26.9	13.1
350	1.5	1.3	650	7.1	0.2			
400	3.3	1.8	750	8.1	1.0			

Instrument 2 High temperature **ITS** **4**

Sample name	: 1600-1	Instrument	: 2
Method name	: C:\HPCHEM\2\METHODS\HT750C.M	Vial	: 1
Sample type	: SHELL	Injection	: 1
Sequence name	: 2041703C.S	Seq. line	: 5
Operator	:	Sample (g)	: 0.2118
Acquired on	: 4/21/03 1:47:14 PM	Solvent (g)	: 20.8045
Processed on	: 4/21/03 2:38:16 PM	ISTD (g)	: 0.0000
Data File	: 2041703C\001F0501.D\FID1A.CH		

Chromatogram:



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Instrument 2 High temperature **ITS** **1**

Sample name	: 1603-3	Instrument	: 2
Method name	: C:\HPCHEM\2\METHODS\HT750C.M	Vial	: 2
Sample type	: Sample Cryo	Injection	: 1
Sequence name	: 2041703C.S	Seq. line	: 7
Operator	:	Sample (g)	: 0.2186
Acquired on	: 4/21/03 4:08:59 PM	Solvent (g)	: 19.0087
Processed on	: 4/21/03 5:00:01 PM	ISTD (g)	: 0.0000
Data File	: 2041703C\002F0701.D\FID1A.CH	Start Elution	: 0.09
Blank used	: 2041703C\085F0601.D\FID1A.CH	End Elution	: 46.35S
BP Calibrant	: 2041703\090F0101.D\FID1A.CH	Found recovery	: 99.3%
Last Reference	: 2041703C\095F0201.D\FID1A.CH On spec.	Used recovery	: 99.3%
Cal. method	: External Standard Method	Response	: 2.6118e-008

Boiling point distribution:

Mass%	BP(°F)	Mass%	BP(°F)	Mass%	BP(°F)	Mass%	BP(°F)	Mass%	BP(°F)
IBP	<97	22	330	42	501	62	658	82	859
3	99	23	342	43	509	63	668	83	874
4	146	24	349	44	515	64	676	84	888
5	164	25	358	45	521	65	687	85	904
6	177	26	371	46	530	66	696	86	920
7	188	27	380	47	539	67	706	87	937
8	196	28	388	48	548	68	716	88	956
9	211	29	397	49	554	69	726	89	976
10	212	30	408	50	562	70	736	90	998
11	226	31	419	51	571	71	747	91	1022
12	236	32	425	52	576	72	756	92	1048
13	242	33	432	53	581	73	767	93	1076
14	259	34	442	54	590	74	777	94	1105
15	266	35	449	55	599	75	787	95	1140
16	275	36	456	56	604	76	796	96	1178
17	285	37	464	57	613	77	806	97	1222
18	290	38	472	58	623	78	815	98	1280
19	304	39	480	59	629	79	824	99	1348
20	314	40	488	60	640	80	835	99.3	1382
21	321	41	493	61	650	81	847		

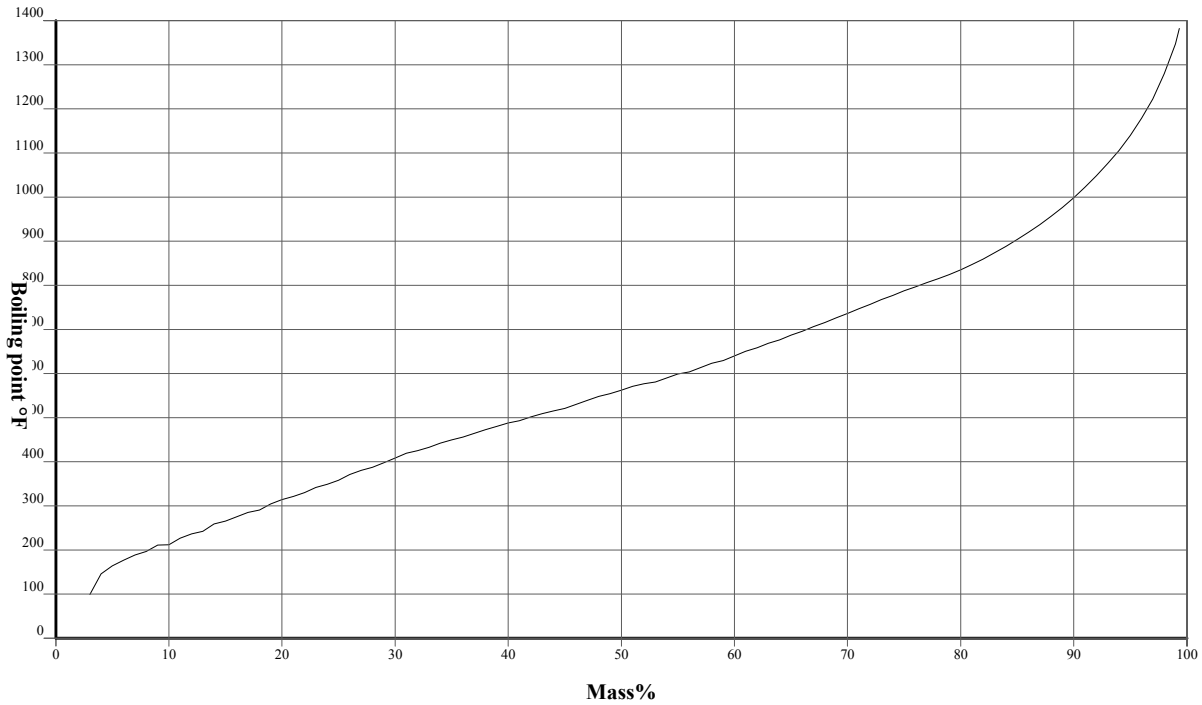
Crude Oil

AC Simdis version 04.09.001

Instrument 2 High temperature **ITS** **2**

Sample name	: 1603-3	Instrument	: 2
Method name	: C:\HPCHEM\2\METHODS\HT750C.M	Vial	: 2
Sample type	: Sample Cryo	Injection	: 1
Sequence name	: 2041703C.S	Seq. line	: 7
Operator	:	Sample (g)	: 0.2186
Acquired on	: 4/21/03 4:08:59 PM	Solvent (g)	: 19.0087
Processed on	: 4/21/03 5:00:01 PM	ISTD (g)	: 0.0000
Data File	: 2041703C\002F0701.D\FID1A.CH		

Boiling point Distribution plot:



Crude Oil

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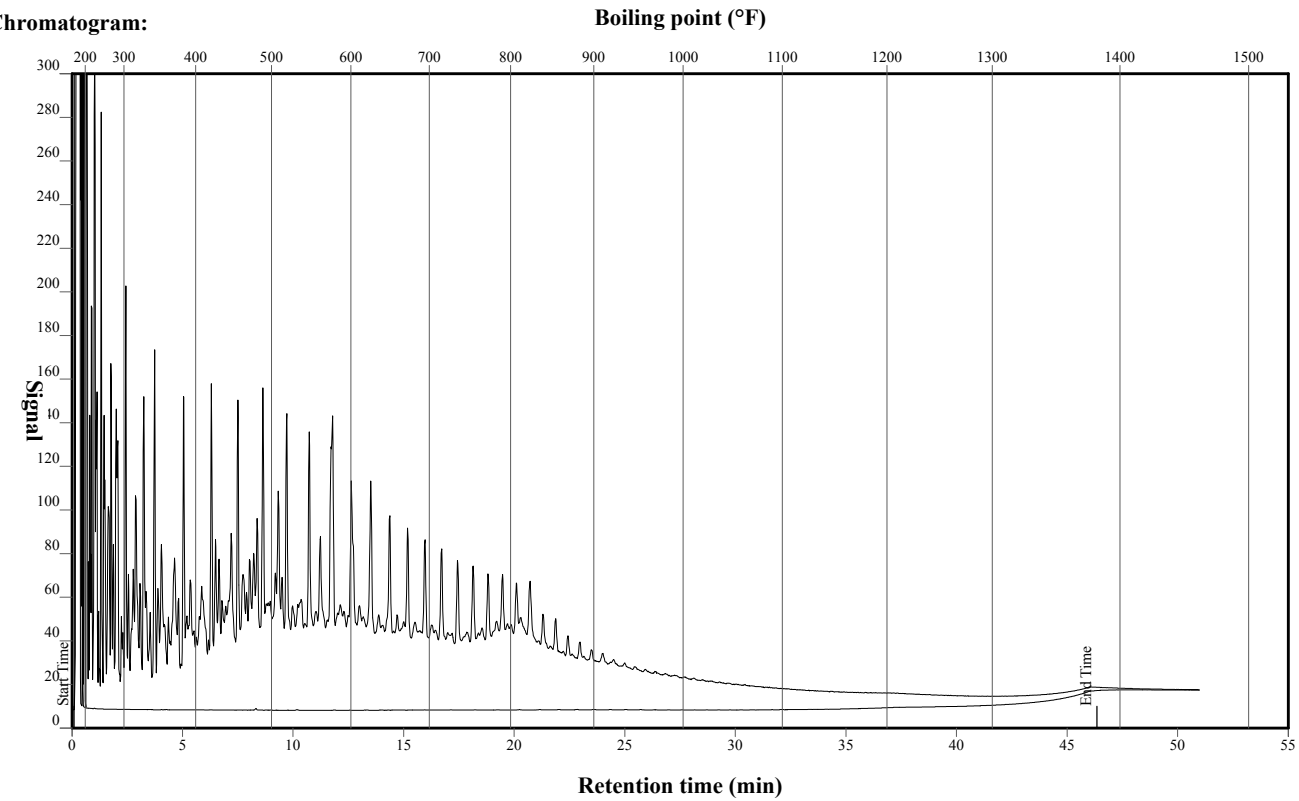
Instrument 2 High temperature **ITS** **4**

Sample name	: 1603-3	Instrument	: 2
Method name	: C:\HPCHEM\2\METHODS\HT750C.M	Vial	: 2
Sample type	: Sample Cryo	Injection	: 1
Sequence name	: 2041703C.S	Seq. line	: 7
Operator	:	Sample (g)	: 0.2186
Acquired on	: 4/21/03 4:08:59 PM	Solvent (g)	: 19.0087
Processed on	: 4/21/03 5:00:01 PM	ISTD (g)	: 0.0000
Data File	: 2041703C\002F0701.D\FID1A.CH		

Chromatogram:



A Picture worth a thousand words

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Instrument 2 High temperature **ITS** **4**

Sample name	: 1600-1	Instrument	: 2
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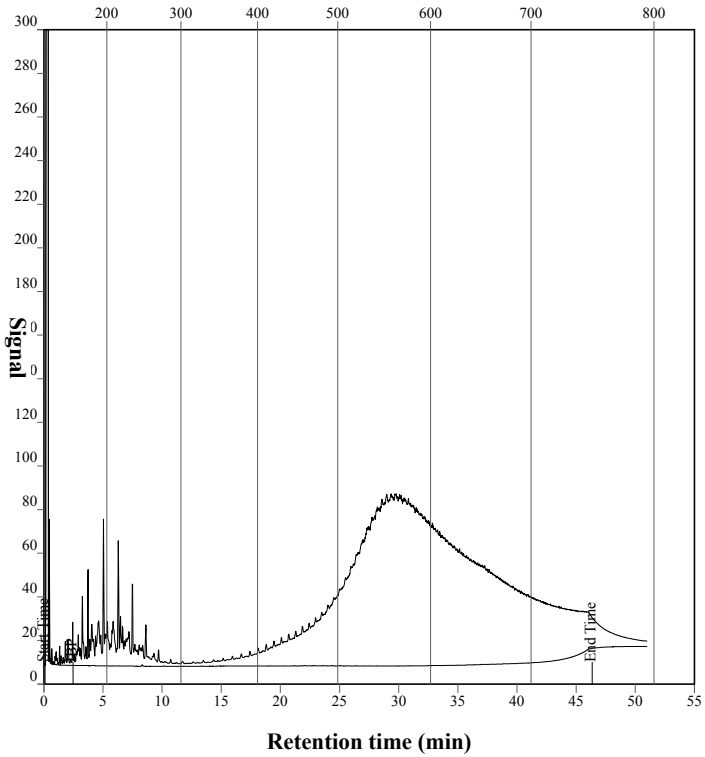
Data File : 2041703C\001F0501.D\FID1A.CH

Chromatogram: **Boiling point (°C)**



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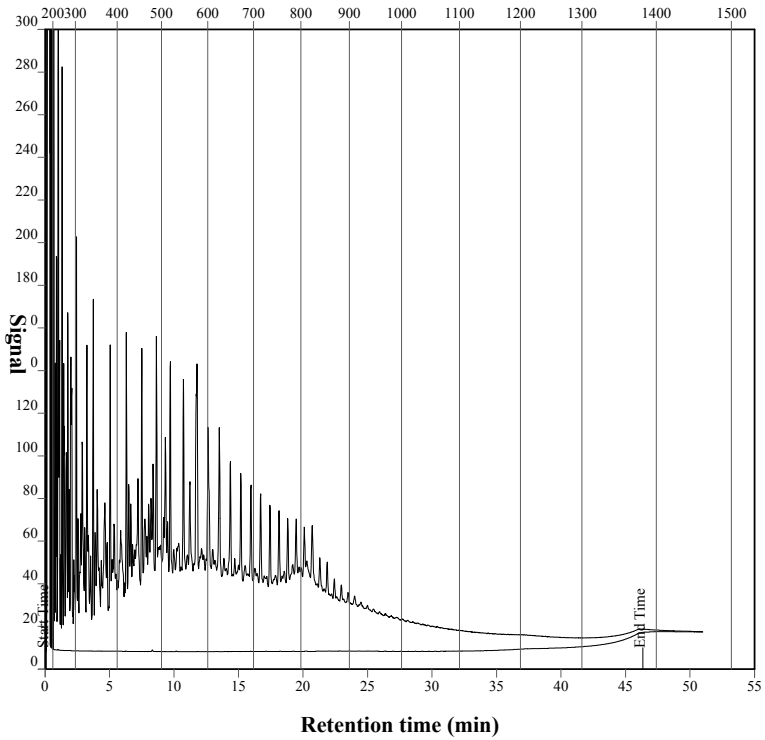
Instrument 2 High temperature **ITS** **4**

Sample name	: 1603-3	Instrument	: 2
Method name	: C:\HPCHEM\2\METHODS\HT750C.M	Vial	: 2
Sample type	: Sample Cryo	Injection	: 1
Sequence name	: 2041703C.S	Seq. line	: 7
Operator	:	Sample (g)	: 0.2186
Acquired on	: 4/21/03 4:08:59 PM	Solvent (g)	: 19.0087
Processed on	: 4/21/03 5:00:01 PM	ISTD (g)	: 0.0000

Data File : 2041703C\002F0701.D\FID1A.CH

Chromatogram: **Boiling point (°F)**



Advantages to Using HTSD

- MUCH faster than conventional TBP analysis (2 days or longer)
- Accuracy is adequate for use with most refinery models
- Lower cost than D2892/D5236
- More information on back end than D2887 or D5307

There ARE Disadvantages….

- No fractions are generated/cannot be characterized.
- Information on the front end (C1-C5) is fuzzy due to CS2 elution.
- VERY technique-dependent. Requires STRICT adherence to quality protocols.
- Still slight controversy on whether it accurately reflects distribution in high aromatic crudes.

ASTM Activity

- D6358- *Boiling Range Distribution for Petroleum Distillates in Boiling Range from 174 to 700C by Gas Chromatography*

- *Closer than previous methods, but not fully encompassing the range for crude oil.*

ASTM Activity

- Robustness for crude oils in progress
- Preliminary data not very precise
- Problems on the front end (quenching factor debates)
- Problems on the back end (recovery statistics)
- D5307 took 25 years to work out a compromise

Summary

- Good tool for characterizing and monitoring crude oil (with limitations)
- ASTM Standard? Gonna be a while…