

Caption list

Figure 1. nP-GC×GC group type separation of a diesel. For a better understanding elution zones of saturates, aromatics, diaromatics and triaromatics are plotted. Bands of C₁₃, C₁₄ and C₁₅ alkylbenzenes are represented with straight lines. Experimental conditions are reported in Table 1.

Figure 2. rP-GC×GC group type separation of a diesel. The pattern describes elution zones of saturates, aromatics, diaromatics and triaromatics in a reversed order compared to nP-GC×GC. Bands of C₁₃, C₁₄ and C₁₅ alkylbenzenes are represented with straight lines. Experimental conditions are reported in Table 1.

Figure 3. Separation between saturates (S) and aromatics (A) in nP-GC×GC and in rP-GC×GC. Chromatograms correspond to one modulation cycle of the raw chromatogram at the elution time of anthracene.

Figure 4. GC×GC detailed group type separation of a diesel: elution zones of saturates, aromatics, diaromatics and triaromatics are plotted according to the number of carbon atoms. The number inside each zone indicates the number of carbon atoms of the alkyl chain or alkyl groups.

Figure 5. Composition of the diesel: distribution of hydrocarbons per chemical class and per number of carbon atoms.

Figure 6. GC×GC simulated distillation of the diesel for each chemical group.

Figure 7. Comparison of simulated distillation obtained by GC×GC and by ASTM D2887.

Figure 1.

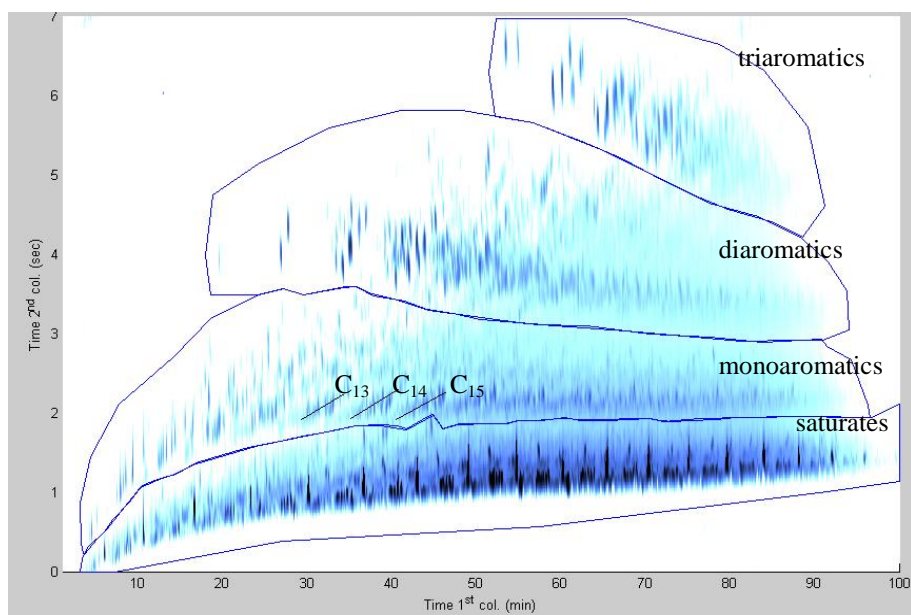


Figure 2.

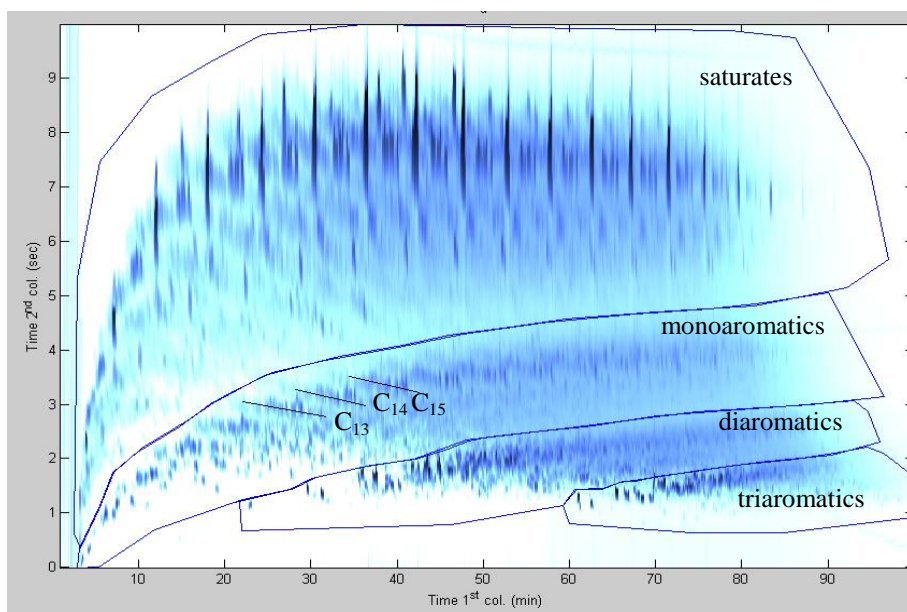


Figure 3

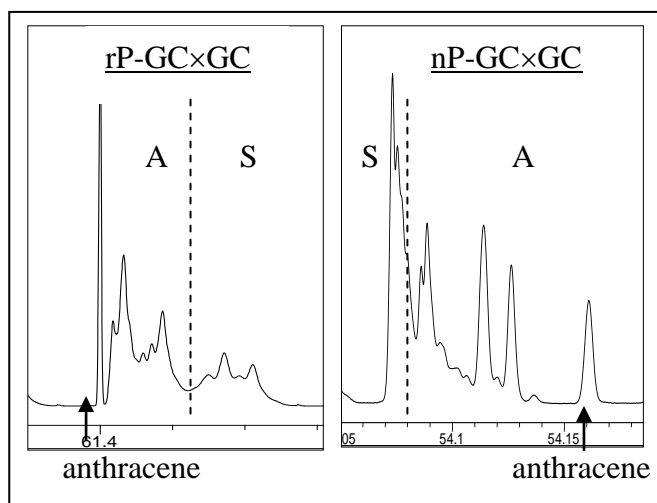


Figure 4

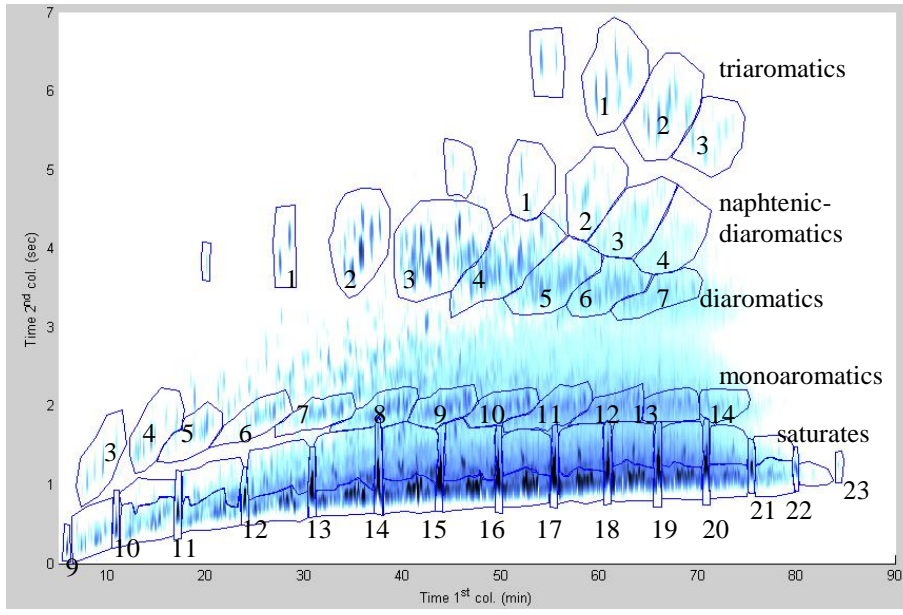


Figure 5

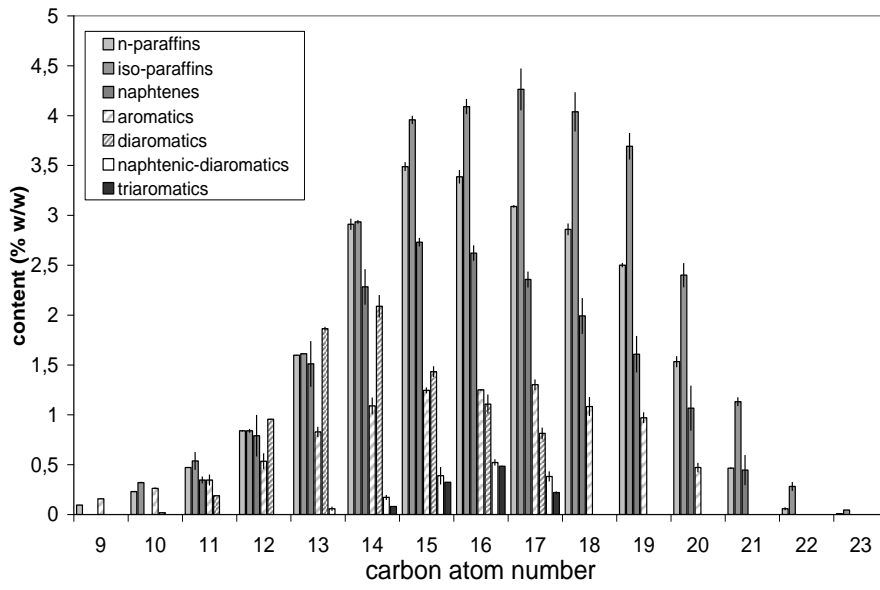


Figure 6

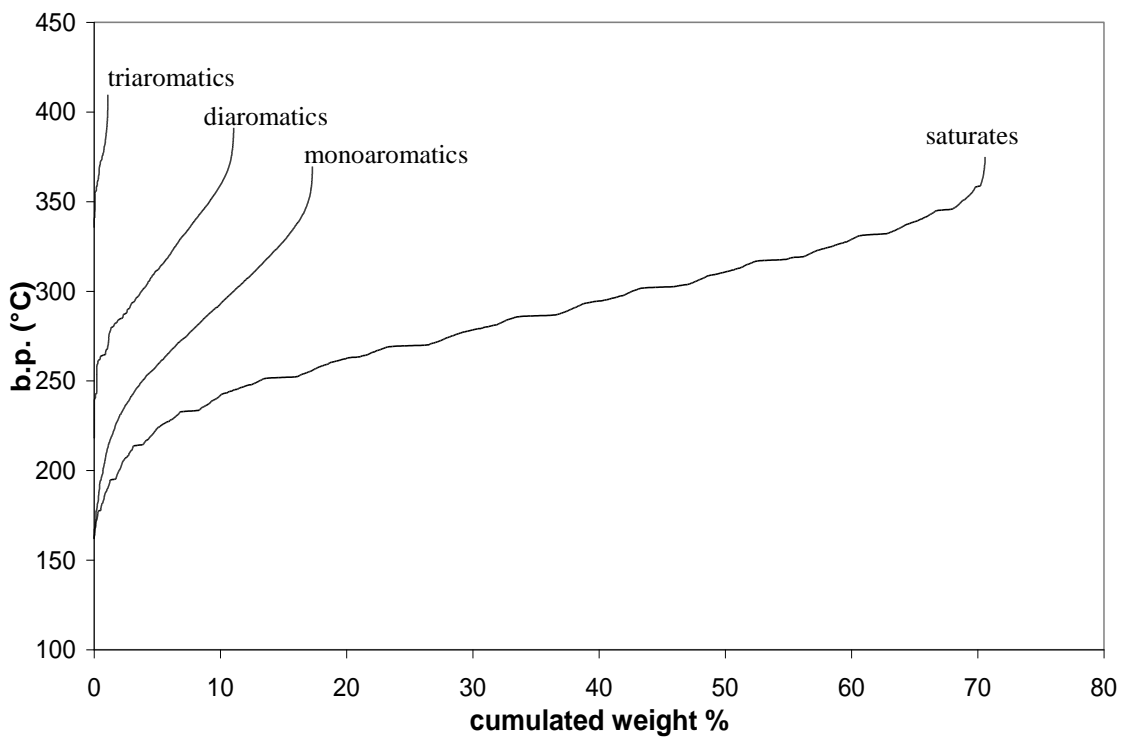


Figure 7

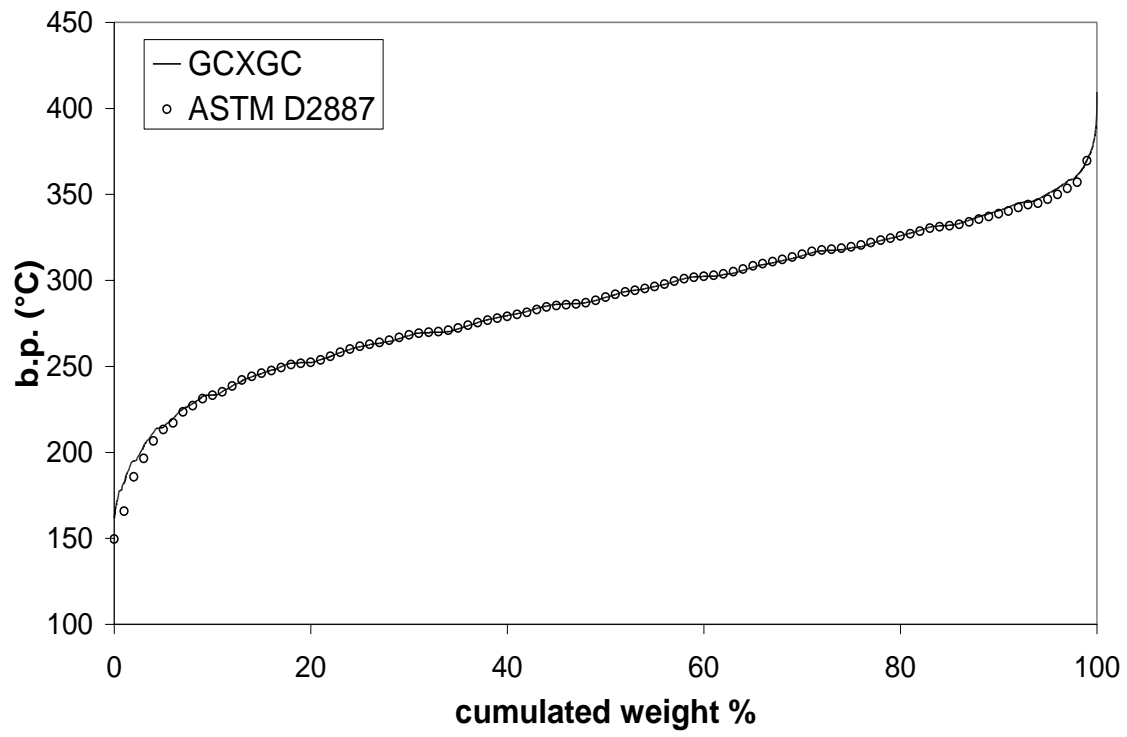


Table I. Operating conditions of GC×GC

	nP-GC×GC	rP-GC×GC
1 st column	PONA ^a , 10m×0.2mm i.d.; 0.5µm	BPX50 ^b , 10m×0.25mm i.d.; 0.25µm
2 nd column	BPX50 ^b , 0.8m×0.1mm i.d.; 0.1µm	DB1 ^c , 0.8m×0.1mm i.d.; 0.1µm
Column oven	50°C-280°C; 2°C/min	
Carrier gas	He; constant pressure, 200kPa	
Injection	0.2µl, split ratio 1:100; 280°C	
Detection	FID, 300°C	
Acquisition rate	100 Hz	
Modulation period	7 s	10 s

^{a, c} dimethylpolysiloxane, Agilent technologies (Massy, France)

^b (50%phenyl)polysilphenylene-siloxane, SGE (Courtaboeuf, France)

Table II. Composition of the synthetic hydrocarbon mixture

compound	b.p. (°C)	¹ t _r (min) ^a	² t _r (s)
n-decane	174	10.83	0.31
n-dodecane	216	23.84	0.67
n-tetradecane	254	37.26	0.75
n-hexadecane	287	49.51	0.86
n-octadecane	316	60.65	0.90
n-eicosane	344	70.74	0.97
n-propylbenzene	159	7.51	0.86
isobutylbenzene	167	10.31	1.02
indane	176	11.42	1.76
indene	182	11.71	2.22
tetraline	208	18.94	2.57
1-phenyloctane	264	40.06	1.79
1-phenyldecane	298	52.43	1.86
1-phenyldodecane	328	63.74	1.84
naphthalene	218	19.99	3.67
1-methylnaphthalene	245	28.33	3.98
1,3-dimethylnaphthalene	263	35.57	3.76
2,3,5- trimethylnaphthalene	-	44.49	3.76
fluorene	295	44.96	4.97
phenanthrene	336	55.46	6.16
anthracene	340	56.04	6.30
2-methylanthracene	-	62.46	5.73
9,10-dimethylanthracene	-	72.90	6.72

^a first dimension retention time is considered for the apex of most intense modulated peaks

Table III. Composition (% , w/w) of the diesel obtained by LC, MS, and GC×GC.

	LC (n=4)	MS (n=10)	nP-GC×GC (n=3) <i>raw data</i>	rP-GC×GC (n=3) <i>raw data</i>	nP-GC×GC (n=3) <i>corrected data</i>
saturates	70.4 ± 0.3	71.7 ± 0.9	68.3 ± 0.5	69.8 ± 0.5	70.6 ± 0.6
monoaromatics		18.8 ± 0.4	18.3 ± 0.2	17.1 ± 0.3	18.0 ± 0.3
diaromatics		8.7 ± 0.2	12.1 ± 0.3	11.7 ± 0.2	10.3 ± 0.3
triaromatics		0.8 ± 0.1	1.4 ± 0.1	1.4 ± 0.1	1.1 ± 0.1