USE OF MATHEMATICAL EXPRESSIONS FOR THE ESTIMATION OF SELECTED DIESEL FUEL PROPERTIES

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ABSTRACT
Mathematical expressions are presented, which predict some of the most important properties of diesel fuels. The experiments were performed using a fuel matrix of 128 gas oils, which covered the cetane index range 23-62. Although other parameters were also considered, the majority of the predictions were based on the distillation curve and the density of the fuels. Very good predictions were obtained for the aniline point, the kinematic viscosity at 40 °C, and for the fuels' aromatic content. The adjusted correlation coefficients in all cases is over 0.96.

LIST OF SYMBOLS

a,b,c,d,e,f,g,h,i	constants
ANIL	aniline point (°C)
AROM	aromatic content of the fuel (vol %.)
DENS	fuel density (g/mL at 15 °C)
D_{10}	distillation temperature for the 10% vol. of the fuel (°C)
D_{50}	distillation temperature for the 50% vol. of the fuel (°C)
D_{90}	distillation temperature for the 90% vol. of the fuel (°C)
FBP	final boiling point of the fuel (°C)
p	probability, the t-test to give a number equal or higher than t-ratio
R^2	correlation coefficient
R^2_{adj}	adjusted correlation coefficient
S	sulphur content of the fuel (wt %)
s	standard deviation

Greek Letters

ν_{40} kinematic viscosity (cSt at 40 °C)

INTRODUCTION
The properties of the gas oil streams in a modern refinery, vary widely, depending on the nature of the feedstock and the operating conditions. Straight atmospheric or cracking processes produce gasoils with properties that usually do not meet commercial specifications. Critical properties, such as the ignition quality, expressed with the cetane number increasingly become more severe, mainly for environmental reasons. Following production, the quality of the final gas oil products (diesel fuel) is adjusted by blending various gas oil streams in adequate quantities.
Modern blending processes need mathematical expressions that can predict accurately the amounts of each component to be blended, in order to meet the specifications of the market. The traditional use of tables and nomograms from the refineries for the estimation of the fuel blend properties, cannot satisfy the needs of the automated processes used in modern blending facilities[1-3]. Therefore, it would be desirable to find mathematical expressions for the most important specifications, using such parameters as the fuel distillation curve and density.
In the past, several investigators tried to identify the impact of the various fuel properties, either on the engine operating conditions or on emissions. The cetane number, as measured in a standard CFR engine, is the most significant property of diesel fuels, and for calculation purposes it can be approximated by the calculated cetane index [4-6]. The diesel fuel aromatic content, a property usually determined using chromatographic methods was found to correlate well with emissions from diesel engines [7-12]. The aniline point is related to the ignition quality of diesel

fuels through the diesel index [13, 14]. The kinematic viscosity is related to particulate emissions and performance of diesel engines, because of its impact on the droplet size distribution of the fuel at the injection system [15,16].

This work is an effort to present reliable mathematical expressions for the fuel's aromatic content, aniline point, and kinematic viscosity mainly using data from the distillation curve and the density.

EXPERIMENTAL SECTION

Sixteen gasoils with different properties were used as base fuels in this course of experiments, with their cetane index in the range of 23-62. They included straight run fuels from atmospheric distillation and cracking processes, i.e. light cycle oil from a fluid catalytic cracking unit and gasoils from visbreaker and hydrocracker. From these base fuels, 120 blends were prepared, covering a large spectrum of specifications that reflect both current and future trends. The properties of the total 126 fuels (base fuels and their mixtures), are listed in Table 1. All measurements were done according to the appropriate ASTM procedures.

STATISTICAL ANALYSIS

The data of the various fuel properties were analysed using standard statistical techniques. For each property, the parameters considered were the standard deviation s, the correlation coefficient R^2, and the adjusted correlation coefficient R^2_{adj}, which gives a more accurate behaviour of the model used. Each expression was tested through the t-test and probability number p, to ensure that only significant terms are used in the mathematical expressions [17]. All statistical parameters of the fuel properties considered in this paper, are listed in Table 2.

ESTIMATION OF THE KINEMATIC VISCOSITY

The kinematic viscosity of the fuel ν, was determined at 40 °C. The best results were obtained from the following equation:

$$\nu_{40} = a \cdot DENS + b \cdot DENS^2 + c \cdot D_{10}^2 + \frac{d}{D_{10}} + e \cdot D_{50}^2 + \frac{f}{D_{50}^2} + g \cdot D_{90}^2 + \frac{h}{D_{90}} + i \qquad (1)$$

Statistical parameters are given in Table 2. The results are depicted in Figure 1, where it can be seen that most of the points are close to the diagonal.

ESTIMATION OF THE ANILINE POINT

Aniline point is a simple procedure that gives an indication of the aromatic content of the fuel. The proposed equation for the aniline point is given below:

$$\begin{aligned} ANIL = {} & a \cdot DENS + b \cdot (e^{-3.5 \cdot (DENS-0.85)} - 1) + c \cdot (D_{10} - 215) + d \cdot (D_{10} - 215)^2 + e \cdot (D_{50} - 260) + \\ & + f \cdot (D_{90} - 310) + g \cdot (D_{90} - 310)^2 + h \cdot S^2 + i \end{aligned} \qquad (2)$$

In this case all variables have very high t-ratios and p-values equal to zero. The statistical parameters are given in Table 2. This means that all the predictor variables are significant. The results are given graphically in Figure 2.

ESTIMATION OF THE AROMATIC CONTENT

The aromatic content for diesel fuels is an important property since it affects both the density and the resulting emissions. The experimental determination of this specification requires special columns and it takes several hours to complete, ASTM D1319. Chromatographic techniques such as HPLC and SFC are also employed, but their instrumentation is very expensive. Modern techniques as FTIR give fast and good results. A mathematical expression for the calculation of aromatic content would be attractive. The following equation was found to give very good results:

$$AROM = a \cdot DENS^2 + b \cdot D_{10}^2 + \frac{c}{D_{10}} + \frac{d}{D_{50}} + e \cdot D_{90}^2 + \frac{f}{D_{90}} + g \cdot ANIL^2 + h \cdot S^2 + i \qquad (3)$$

In Table 2 are given the statistical parameters of the above equation. Graphical representation of the results shows that practically all the points are very well behaved, Figure 3.

CONCLUSIONS

Mathematical expressions which predict some important properties of diesel fuels have been experimentally determined, using a fuel matrix of 128 base fuels and blends. Very good predictions were obtained for the kinematic viscosity at 40 °C, the aniline point and the aromatic content. In all cases the adjusted correlation coefficients were just less than unity. These expressions can be used for a very accurate prediction of the actual values of these properties, when they cannot be measured directly.

ACKNOWLEDGEMENTS

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Table 1. Fuel Properties

Cetane Index	IBP (°C)	D_{10} (°C)	D_{50} (°C)	D_{90} (°C)	FBP (°C)	Density (g/ml, 15 °C)	v_{40} (cSt)	Aniline Point (°C)	Aromatic Content (% vol.)	Total Sulfur (% wt)
23.5	188	250	288	346	372	0.9550	3.85	20.9	73.0	1.82
24.3	154	242	276	341	369	0.9510	3.21	1.4	77.4	0.33
26.0	166	238	275	344	368	0.9420	3.16	7.0	74.3	0.30
27.0	185	235	274	340	366	0.9330	3.11	12.4	71.1	0.27
27.2	191	239	285	347	369	0.9330	3.62	19.8	69.4	0.28
27.3	190	249	290	355	372	0.9403	3.79	27.9	67.5	1.64
28.4	188	233	272	337	364	0.9240	3.06	17.5	67.9	0.24
28.6	188	252	288	347	373	0.9326	3.75	32.0	61.3	1.53
29.0	180	242	293	370	380	0.9346	3.85	20.4	65.8	0.34
30.2	193	233	270	334	360	0.9150	3.01	22.6	64.8	0.21
32.1	196	232	269	333	357	0.9060	2.96	27.6	61.6	0.18
32.4	194	247	296	354	369	0.9154	4.20	36.5	61.1	0.24
32.7	195	251	287	334	363	0.9100	3.64	43.0	51.9	1.22
34.0	205	252	290	356	382	0.9136	3.99	44.2	52.2	1.29
34.2	198	232	268	331	355	0.8970	2.92	32.1	58.5	0.15
35.8	185	228	254	332	361	0.8889	2.59	43.2	43.8	1.05
36.0	198	231	267	326	351	0.8880	2.87	36.8	55.4	0.12
36.8	189	247	287	328	361	0.8930	3.57	50.4	45.0	0.97
36.9	201	250	304	358	373	0.9012	4.78	46.8	54.2	0.19
37.5	185	225	257	337	369	0.8827	2.84	48.4	41.1	1.11
37.6	206	254	292	357	385	0.9012	4.07	50.6	46.3	1.12
38.3	200	230	267	323	348	0.8790	2.83	41.3	52.2	0.09
39.2	190	249	307	359	379	0.8941	4.91	55.1	52.2	0.18
40.2	185	223	262	353	369	0.8757	3.08	52.8	38.2	1.18
40.6	200	229	265	319	348	0.8700	2.78	45.9	49.0	0.05
40.8	206	255	294	357	383	0.8905	4.25	56.6	41.1	0.95
41.6	186	220	265	357	379	0.8706	3.16	55.0	35.1	1.25
42.9	198	227	265	313	344	0.8610	2.77	50.2	45.9	0.02
43.7	183	214	272	368	373	0.8642	3.42	58.5	32.2	1.32
43.8	185	218	272	363	376	0.8642	3.42	58.5	32.1	1.32
44.0	188	243	284	321	347	0.8691	3.48	60.3	33.8	0.64
44.1	206	256	295	359	386	0.8810	4.35	61.2	36.3	1.23
44.2	183	209	275	368	379	0.8618	3.50	60.8	30.7	1.35
44.5	185	215	275	368	379	0.8618	3.50	60.8	30.9	1.35
44.5	165	251	296	351	369	0.8771	4.01	59.1	38.1	0.12
44.7	196	229	268	323	353	0.8595	2.97	53.4	43.1	0.02
44.8	198	229	268	314	341	0.8578	2.85	53.8	42.3	0.05

Table 1. Fuel Properties (Continued)

Cetane Index	IBP (°C)	D_{10} (°C)	D_{50} (°C)	D_{90} (°C)	FBP (°C)	Density (g/ml, 15 °C)	v_{40} (cSt)	Aniline Point (°C)	Aromatic Content (% vol.)	Total Sulfur (% wt)
45.7	202	230	266	320	345	0.8561	2.80	55.1	41.2	0.03
45.8	182	210	284	365	375	0.8511	3.14	62.7	26.5	1.15
46.2	194	231	272	329	360	0.8580	3.11	56.4	40.0	0.02
46.5	185	215	284	372	385	0.8592	3.72	62.4	29.3	1.39
46.5	197	231	272	314	340	0.8550	2.93	56.9	39.1	0.07
46.7	219	257	316	362	381	0.8772	5.65	60.5	44.2	0.13
47.1	199	247	297	352	373	0.8691	4.11	63.8	32.8	0.18
47.5	208	257	297	340	386	0.8720	4.43	65.4	31.9	0.69
47.5	188	219	251	346	369	0.8439	2.8	63.2	23.5	0.91
47.5	206	231	265	321	347	0.8511	2.83	59.7	36.6	0.03
47.7	158	254	299	352	371	0.8701	4.13	65.4	33.9	0.10
47.8	225	268	327	371	384	0.8752	6.35	66.0	38.3	0.20
48.1	210	259	314	362	381	0.8742	5.29	61.9	42.1	0.12
48.1	194	235	278	338	363	0.8565	3.32	60.0	37.2	0.02
48.5	196	234	276	314	338	0.8518	3.02	60.6	35.5	0.10
48.5	188	225	261	355	388	0.8472	2.98	63.7	24.8	0.56
48.9	194	220	244	324	367	0.8355	2.45	64.5	20.5	0.66
48.9	182	210	284	365	375	0.8511	3.14	62.7	26.4	1.15
49.0	189	225	257	351	394	0.8435	2.80	64.1	23.4	0.92
49.0	214	261	302	360	386	0.8704	4.48	67.2	30.6	0.63
49.2	191	220	238	256	322	0.8247	2.06	65.6	16.2	0.28
49.4	195	220	240	270	354	0.8274	2.23	65.2	17.7	0.41
49.4	192	237	282	340	366	0.8550	3.56	63.0	34.2	0.02
49.4	203	232	264	323	347	0.8462	2.87	64.3	32.3	0.04
49.6	202	252	305	360	375	0.8638	4.67	68.7	29.2	0.27
49.6	191	225	252	346	391	0.8396	2.62	64.4	22.0	0.79
49.7	195	235	278	314	336	0.8500	3.08	62.7	33.1	0.11
49.8	195	226	246	333	395	0.8357	2.46	64.7	20.5	0.69
49.8	197	222	238	256	322	0.8239	2.06	65.6	16.2	0.28
50.2	191	224	246	359	381	0.8336	2.92	69.6	16.8	0.16
50.5	205	231	269	369	385	0.8462	2.58	73.8	18.9	0.17
50.5	170	257	300	354	373	0.8641	4.25	65.5	31.6	0.08
50.7	206	259	301	360	386	0.8650	4.55	69.8	28.1	0.56
50.9	190	239	287	342	368	0.8535	3.76	66.2	31.4	0.03
50.9	197	224	237	248	265	0.8200	1.94	66.4	14.7	0.15
50.9	209	258	299	361	388	0.8638	4.51	68.6	27.8	0.58
51.1	180	221	272	342	368	0.8430	3.16	68.6	28.0	0.28

Table 1. Fuel Properties (Continued)

Cetane Index	IBP (°C)	D_{10} (°C)	D_{50} (°C)	D_{90} (°C)	FBP (°C)	Density (g/ml, 15 °C)	v_{40} (cSt)	Aniline Point (°C)	Aromatic Content (% vol.)	Total Sulfur (% wt)
51.4	195	236	281	314	334	0.8475	3.15	65.3	30.5	0.13
51.6	205	227	241	257	301	0.8225	2.03	67.4	14.9	0.19
51.6	208	235	263	327	350	0.8412	2.90	68.9	27.6	0.05
51.6	198	222	240	270	354	0.8226	2.23	65.2	17.6	0.41
51.9	205	229	242	278	377	0.8282	2.18	67.8	15.2	0.18
52.0	165	214	279	349	372	0.8420	3.28	70.2	22.5	-
52.1	204	238	263	372	391	0.8404	3.23	72.4	16.7	0.26
52.1	228	274	333	375	388	0.8732	7.20	71.3	32.0	0.26
52.2	201	236	275	375	392	0.8452	3.77	73.8	17.2	0.3.0
52.4	214	237	254	368	390	0.8349	2.83	71.8	16.2	0.23
52.4	196	234	246	352	385	0.8302	2.49	68.2	15.7	0.22
52.4	187	219	268	333	359	0.8374	2.88	68.0	27.8	0.12
52.9	207	235	282	343	364	0.8460	3.57	70.1	24.1	0.28
53.0	203	239	273	337	358	0.8432	3.22	70.2	26.4	0.04
53.1	193	239	283	314	332	0.8451	3.23	67.9	27.7	0.16
53.2	188	247	292	348	370	0.8520	3.98	69.0	28.5	0.03
53.3	207	241	285	377	395	0.8475	4.07	75.2	17.4	0.32
53.8	193	230	267	290	302	0.8335	2.62	66.8	24.6	0.78
54.0	202	234	256	301	327	0.8303	2.57	69.0	18.5	0.18
54.1	210	259	299	365	390	0.8561	4.61	77.6	18.2	0.24
54.1	198	248	301	354	373	0.8530	4.52	72.2	23.2	0.15
54.2	195	243	282	345	361	0.8451	3.59	71.8	25.1	0.04
54.5	161	259	301	355	374	0.8554	4.41	71.0	26.0	0.05
54.7	191	244	284	314	331	0.8431	3.29	70.2	25.4	0.25
54.8	186	251	296	349	370	0.8505	4.26	71.6	25.6	0.03
54.8	210	244	334	370	385	0.8589	4.02	76.8	21.0	0.17
55.0	204	241	302	378	392	0.8492	4.43	75.4	17.7	0.32
55.1	186	238	270	311	330	0.8355	2.27	70.6	20.6	0.19
55.4	202	235	270	297	309	0.8330	2.71	70.3	19.2	0.62
55.6	186	248	293	351	367	0.8471	4.23	73.1	23.9	0.03
55.6	198	225	253	273	282	0.8213	2.24	66.5	20.3	0.68
55.9	195	238	279	309	328	0.8370	3.06	70.6	22.5	0.09
56.0	232	290	340	380	390	0.8712	8.16	76.7	25.7	0.33
56.0	212	254	303	353	380	0.8510	4.60	72.8	25.3	1.07
56.1	218	252	297	353	379	0.8483	4.16	74.3	20.5	0.89
56.3	225	270	320	364	385	0.8597	5.81	77.2	21.2	1.01
56.5	210	254	305	367	390	0.8505	4.57	73.8	23.1	0.15

Table 1. Fuel Properties (Continued)

Cetane Index	IBP (°C)	D_{10} (°C)	D_{50} (°C)	D_{90} (°C)	FBP (°C)	Density (g/ml, 15 °C)	v_{40} (cSt)	Aniline Point (°C)	Aromatic Content (% vol.)	Total Sulfur (% wt)
56.9	185	252	290	324	350	0.8431	3.60	72.8	23.0	0.15
57.1	184	255	293	335	356	0.8451	3.87	73.3	22.9	0.11
57.1	211	250	291	341	366	0.8432	3.69	71.2	22.1	1.00
57.2	180	260	300	353	369	0.8490	4.55	-	22.6	0.03
57.2	183	258	289	346	364	0.8470	4.19	73.9	22.7	0.07
57.6	188	249	285	313	329	0.8411	3.36	72.2	23.1	0.19
57.6	214	263	304	346	368	0.8500	4.51	72.8	22.6	1.23
57.8	194	260	305	360	386	0.8493	4.44	74.8	22.0	0.25
58.5	231	286	338	383	405	0.8642	7.85	77.2	23.4	0.20
58.8	221	281	324	363	385	0.8586	5.96	75.2	26.4	1.18
59.2	195	235	270	295	306	0.8252	2.81	74.6	17.5	0.03
59.9	216	285	335	380	397	0.8603	6.35	78.6	20.8	0.34
60.6	207	254	304	362	392	0.8410	4.53	81.0	18.6	0.08
61.5	239	312	351	382	390	0.8692	9.33	81.9	19.6	0.40
62.8	222	276	325	375	398	0.8489	6.12	83.4	19.2	0.09

Table 2. Statistical Parameters of Estimating Equations

Parameter	Equation (1)	Equation (2)	Equation (3)
a	124.080E+0	-12.248E+2	83.020E+0
b	-69.740E+0	-20.747E+1	24.970E-4
c	18.222E-5	38.215E-2	70.080E+2
d	38.601E+2	-24.400E-4	-11.009E+3
e	6.260E-5	12.106E-2	-32.528E-5
f	152.261E+3	55.730E-3	-19.659E+3
g	2.580E-5	87.490E-5	-71.388E-4
h	10.611E+2	34.537E-1	42.522E-1
i	-91.250E+0	10.945E+2	93.290E+0
s	2.472E-1	2.481E+0	1.654E+0
R^2	9.620E-1	9.780E-1	9.890E-1
R^2_{adj}	9.590E-1	9.770E-1	9.880E-1

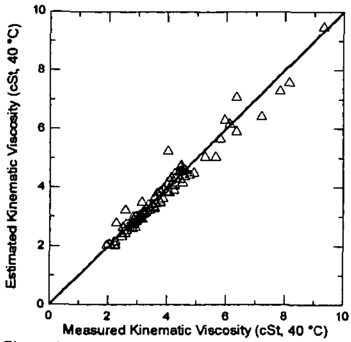

Figure 1. Estimated v's Measured Kinematic Viscosity

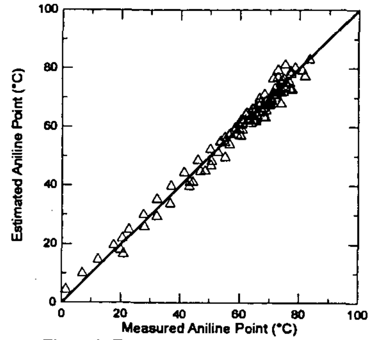

Figure 2. Estimated v's Measured Aniline Point

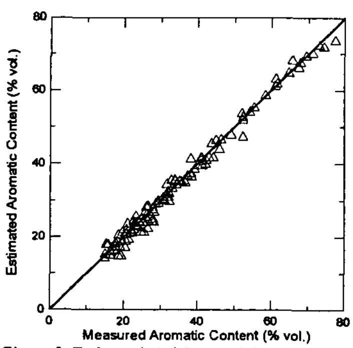

Figure 3. Estimated v's Measured Aromatic Content