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Research article

A multivariate statistical analysis to evaluate and predict ignition quality of marine diesel fuel distillates from their physical properties

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ABSTRACT

Ignition quality of diesel fuels used in compression ignition engines is mainly described by their respective Cetane Number (CN). The most widely accepted method for CN measurement is the ASTM D613, involving a variable compression ratio Cooperative Fuel Research (CFR) engine. However in the recent years other alternative methods based on a Constant Volume Combustion Chamber (CVCC) concept have gained significant popularity mainly due to lower cost of acquisition, maintenance and operation, still being able to provide accurate results. Other widely accepted parameters for the characterization of ignition quality of diesel fuels are cetane indices. These are empirical mathematical equations, based on simple physicochemical properties (such as density and distillation characteristics) and usually correlate well with CN. However, they are accurate enough within narrow limits and are very prone to produce misleading results when involving modern fuels, or biofuels and their blends. In this work, an effort was made to investigate the room for improvement for the prediction of CN, apart from the use of the most widely accepted method of Calculated Cetane Index (CCI), standardized by ASTM D4737, with regard to today's used marine diesel fuels. A total of 47 distillate marine diesel fuels (with high sulfur content compared to automotive diesel fuels) has been employed in order to create multivariate regression models to predict CN equivalents. Thus, useful conclusions were drown in an attempt to evaluate the importance of various physicochemical properties with regard to ignition quality, as well as a first step to the potentiality of revaluation of empirical mathematical models currently in use.

1. Introduction

Cetane Number (CN), one of the most substantial properties of a diesel fuel, is used to indicate its behavior right after the injection inside the cylinder of a compression ignition engine, therefore its ignition quality. It is usually estimated by the time delay period between the start of injection and the start of combustion, generally referred to as Ignition Delay (ID) [1,2].

ID depends on many factors related to the engine itself, such as compression ratio, injection pressure, injection nozzle, cylinder and piston geometry, but also the fuel. To be able to deliver high ignition quality, a diesel fuel usually has to perform short ID times. The shorter the ID, the less premixed fuel and air accumulate inside the cylinder before combustion [1–6]. Thus, when combustion finally takes place, the rate of burning remains within reasonable limits, avoiding too high pressure rise rates that increase noise, decrease efficiency and can damage the engine [1,3–7]. It is clear, then, that a high CN indicates short ID, for a given fuel [1]. Furthermore, fuels with low ignition quality characteristics exhibit poor exhaust emissions performance [1,2,8–10].

To measure the ignition quality of a given fuel typically a Cooperative Fuel Research (CFR) engine is used, as mandated by ASTM D613 method [11]. This procedure is however time consuming, requires skilled personnel and large amounts of expensive chemicals as standards as well as reference and sample fuels, let alone the high expense of acquiring and maintaining a CFR engine [12].

These factors have led to the development of alternative methods to estimate CN, some of them involving instrumentation built around a Constant Volume Combustion Chamber (CVCC) where the sample fuel is actually burned [6,13], and some of them employing empirical equations that use commonly measured physicochemical properties of the fuel to determine the ignition quality of the fuel [6,12,14–20].

The idea behind CVCC methods is to simulate the prevailing conditions inside a compression ignition engine, right before the fuel injection, then inject the sample fuel and measure the ID observed during the auto-ignition process. CVCC methods are not a new concept. The idea to use a CVCC to measure the ID of a diesel fuel goes back to 1930′s [6]. These methods have evolved through years of research and development to become nowadays the most popular experimental procedures for the evaluation of a fuel's ignition quality, due to more

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Table 1
Fuel properties.

Sample ID	Sulfur Content		Density, 15 °C	Viscosity, 40 °C	Distillation Properties					Aromatic Content			Ignition Quality Properties		
					IBP[a]	T10[b]	T50[b]	T90[b]	FBP[c]	Mono[d]	Di[d]	Tri+[d]	CCI	CCAI	DCN
	% m/m	mg/kg	kg/m^3	mm^2/s	°C	°C	°C	°C	°C	% m/m	% m/m	% m/m			
Test Method	ISO 8754	EN ISO 20846	EN ISO 12185	ASTM D7042	EN ISO 3405					EN 12916[e]			ISO 4264		ASTM D7170[f]
1	0.46		941.7	3.154	174	234	284	345	364	19.8	45.8	7.7	24.7	898.7	21.5
2	0.77		910.6	3.513	199	230	294	374	393	23.1	25.5	7.3	33.5	863.9	29.2
3	0.10		851.4	5.943	184	227	340	393	397	22.0	2.0	0.6	57.1	788.6	59.8
4		10	835.4	3.734	210	245	289	345	370	18.0	2.4	0.3	59.7	786.7	57.7
5		9	830.6	3.054	175	209	282	352	367	19.4	1.4	0.1	56.9	788.7	54.3
6	0.18		855.2	3.621	206	238	291	356	371	19.4	8.6	2.2	50.9	807.5	49.6
7	0.35		873.3	3.582	196	234	288	366	381	20.7	14.5	3.9	44.0	825.9	42.3
8	0.53		892.2	3.524	196	232	289	370	386	21.9	20.1	5.6	38.3	845.4	34.9
9	0.07		850.6	5.930	196	251	340	387	406	21.2	2.3	0.7	60.3	787.9	61.3
10	0.08		836.5	2.570	182	206	261	344	364	23.7	4.3	0.5	50.4	800.8	49.3
11	0.19		874.3	2.955	195	225	266	338	370	35.3	11.2	2.1	40.2	833.6	34.9
12	0.36		886.7	3.144	194	225	266	355	379	31.1	16.1	3.9	37.9	843.8	32.6
13	0.54		899.0	3.320	194	226	277	365	384	27.1	20.9	5.6	35.7	854.2	30.3
14		280	861.7	2.780	206	221	261	315	349	39.7	6.2	0.3	42.0	823.1	37.7
15	0.13		853.9	3.363	180	207	286	372	388	23.7	8.1	1.4	47.9	808.7	46.1
16		52	830.2	2.967	171	207	275	346	369	20.5	1.9	0.3	55.6	789.3	53.8
17	0.18		891.2	3.708	173	224	293	361	383	29.4	17.3	7.1	37.4	842.7	36.8
18	0.08		820.6	2.258	140	182	244	325	356	19.2	2.6	0.8	51.4	789.9	51.8
19	0.17		892.9	4.624	161	234	300	366	380	27.4	20.9	6.3	38.2	837.4	38.3
20	0.15		837.4	2.831	186	219	268	333	365	24.7	5.8	0.4	52.4	798.2	51.1
21	0.05		841.2	2.904	214	235	265	330	364	15.0	13.2	0.2	52.0	801.1	51.4
22	0.08		874.6	5.436	204	255	318	376	394	25.9	12.3	2.5	48.0	814.4	47.0
23	0.06		873.2	7.052	224	272	290	304	318	28.5	8.6	1.3	45.2	805.8	51.5
24	0.10		859.0	3.459	173	203	294	369	396	24.7	11.2	1.3	46.6	812.8	45.4
25	0.10		851.6	2.705	167	194	271	357	388	24.6	9.9	1.5	45.8	814.0	44.2
26	0.10		838.1	3.889	165	203	290	395	402	16.2	2.9	0.1	53.3	788.1	53.7
27	0.10		868.1	4.046	186	228	301	359	378	29.8	10.7	1.1	45.8	816.8	45.4
28	0.10		844.1	2.528	170	200	265	343	368	24.2	8.4	0.9	47.9	809.1	47.2
29	0.10		845.2	3.580	170	218	285	358	388	21.4	5.4	0.9	52.0	797.9	51.1
30	0.08		827.6	2.738	169	203	270	341	374	20.8	3.9	0.9	55.4	789.6	53.6
31	0.10		843.2	2.909	170	203	277	350	379	23.9	4.6	1.1	50.2	803.0	47.8
32	0.07		828.4	2.740	172	202	270	345	368	21.8	4.2	0.8	55.0	790.4	52.0
33	0.10		880.7	6.400	223	265	326	394	394	27.6	12.6	2.0	47.7	815.9	46.7
34	0.14		888.1	5.699	192	258	318	377	391	26.7	16.5	2.7	43.4	826.5	43.2
35	0.18		895.7	5.242	185	244	311	371	375	25.8	20.4	3.3	38.7	836.5	39.1
36	0.14		862.2	5.360	185	230	332	383	403	21.7	6.8	1.4	51.5	802.4	54.5
37	0.18		870.3	4.978	170	216	316	381	387	21.5	11.5	2.1	45.4	812.6	49.8
38	0.21		881.8	4.542	173	221	316	379	397	21.3	16.1	2.9	41.5	826.9	44.6
39	0.25		889.6	4.291	170	222	305	375	387	21.0	20.6	3.6	38.5	836.4	41.0
40	0.15		878.0	5.983	215	254	321	376	394	29.2	15.2	5.7	46.7	815.1	47.6
41	0.12		882.6	5.153	200	246	314	374	392	29.0	13.0	4.3	43.7	823.9	44.5
42	0.09		887.4	4.404	195	233	300	367	390	28.7	10.8	2.8	39.9	833.4	39.9
43		290	824.8	4.197	171	260	291	366	387	15.2	4.6	0.7	66.4	772.3	62.5
44	0.04		847.2	5.264	215	265	308	374	394	22.1	6.6	1.0	59.7	787.9	56.2
45	0.05		860.0	4.689	176	210	314	380	394	24.8	7.0	1.1	48.8	804.1	50.3
46	0.05		866.8	5.801	185	241	322	380	393	26.7	7.8	1.2	49.8	804.7	51.3
47	0.04		853.3	3.997	169	195	296	375	393	22.9	6.2	0.9	48.4	802.4	49.0

[a] IBP: Initial Boiling Point.
[b] T_{10}, T_{50}, T_{90}: Volume recovery temperatures of 10%, 50%, and 90%.
[c] FBP: Final Boiling Point.
[d] Content in monoaromatics, diaromatics and tri+ aromatics.
[e] EN 12916 precision limits for mono-aromatic content in the range from 6% m/m to 30%, m/m, di-aromatic content from 1% m/m to 10% m/m, tri + −aromatic content from 0% m/m to 2% m/m, polycyclic aromatic content from 1% m/m to 12% m/m, and total aromatic content from 7% m/m to 42% m/m.
[f] ASTM D7170 precision limits for DCN from 35.0 to 59.6.

affordable acquisition and maintenance of the apparatus itself, easy operation, less needed amount of sample fuel and chemical agents, fast and accurate results. It should be noted that since the CN determined by CVCC methods is not measured in the actual CFR engine, which is the defined source of CN, the values deriving from the CVCC approach are known as the Derived Cetane Number (DCN). CVCC methods have been standardized by ASTM and other standardization organizations specifically for each alternative CVCC device. Modern formalized methods include ASTM D6890 [21] (EN 15195, IP 498) for the Ignition Quality Tester (IQT), ASTM D7170 [22] (EN 16144, IP 567) for the Fuel Ignition Tester (FIT) and ASTM D7668 [23] (EN 16715, IP 615) for the Cetane Ignition Delay 510 (CID 510).

Empirical mathematical equations for the estimation of CN are no new concept either. They have been used routinely in refineries to help during common processes such as blending distillates from various streams. Such equations, also known as cetane indices, are however tailored to the specific use for which they are intended and may require frequent revision and readjustment. Furthermore, they produce satisfactory results within usually narrow limits in terms not only of actual ignition quality performance, but also of physical and chemical characteristics of the fuel [6,16].

The most popular empirical mathematical equation currently in use is without doubt the one formalized under ASTM D4737 method and also used in EN ISO 4264 [15,16,24]. The derived Calculated Cetane