Discrimination of BFO Quality on Multivariable Analysis of Combustion Process in Modified FIA Vessel

Hiroshi Tajima*1; Atsushi Takeda*2; Kousuke Okazaki*1; Dai Yamanishi*3; Satoshi Kawauchi*4

*1: Kyushu University, Kasuga, Japan 816-8580, tasima@ence.kyushu-u.ac.jp, +81-92-583-7592
*2: Nippon Yuka Kogyo CO., LTD., Yokohama, Japan 245-0053, bunseki@nipponyuka.com, +81-45-811-2731
*3: National Fisheries University, Shimonoseki, Japan 759-6595, yamanishi@fish-u.ac.jp, +81-83-286-5111
*4: National Maritime Research Institute, Mitaka, Japan 181-0004, kawauchi@nmri.go.jp, +81-422-41-3112

Statistical analyses of ROHR (rate of heat release) curves from a modified FIA (Fuel Ignitability Analyser) were introduced for the first time to distinguish trouble-inducing bunker fuel oils (TIO) from trouble-free fuel oils (TFO). The modified FIA employed longer injection duration, higher spray quality, and higher air temperature, which made its combustion conditions closer to those in an actual marine diesel engine. In this study, Linear Discriminant Analysis (LDA) and the Mahalanobis Taguchi System (MTS) were applied to extract effective variables from ROHR curves. Very promising results were obtained, and thus a reliable method for the distinction of bunker fuel oils was realized.

1. Introduction

The oil refining industry has been biased to supply more hydrogen-rich and much less sulphuric fuels for on-road facilities to pass their tight emission regulation. Conversely, bunker fuel oil (BFO) for large marine diesels wears more carbon-rich, cracked and aromatic feature in both its residual components and its cutter stocks. In extreme cases, so-called “gap fuels”, having almost no middle distillates between these two components, are reportedly being produced. As a result, combustion relating problems such as excessive piston ring wear, cylinder liner scuffing, exhaust valve stick, and so on, have been major issues on maritime transportation for the last decade. Some are certainly believed to be caused by trouble-inducible BFOs.

FIA has been regarded as the most practical and simulative test device for the ignitibility and combustibility of heavy fuel oils. Its latest version, FIA/FCA (Fuel Ignitability / Combustibility Analyser) is authorized in the British standard IP 541-06 for testing heavy fuel oils. Although the ECN (Estimated Cetane Number) acquired by the FIA/FCA measurement is generally recognized as a better index than FIA-CN, some of the authors stated [1] that the test conditions of the FIA/FCA are still improper in evaluating the fuel combustibility in an actual marine diesel engines since its injection duration is too short to cause diffusive combustion and neither its spray quality nor the in-cylinder temperature are compatible with the actual ones. And there is too much overlap between TIOs and TFOs in ECN or FIA-CN to discriminate each other because both indexes are determined only by the averaged ignition delay time.

All these above strongly lead to the necessity for new measurement procedures of FIA and for new evaluation method of total fuel quality other than ignition delay. The modified FIA system was proposed in the previous study [2] and statistical analyses on ROHR curves were newly proposed to discriminate TIOs from TFOs. Linear Discriminant Analysis (LDA) and Mahalanobis Taguchi System (MTS) were applied as two major multivariable analyses to extract effective variables from ROHR curves. LDA was applied to examine the statistical nature of the ROHRs, the MTS was extensively applied to more TFO and TIO samples to show the full potential of the statistical analysis. An additional MTS analysis was also tried with the basic properties of BFOs’ and it was proved to improve the reliability of the discrimination practically.

2. Experimental Apparatus and Conditions

2.1 Modified FIA-100/4
A modified FIA partially developed in Kyushu University is virtually the FIA-100/4 vessel with a revised injection system of electronically controlled unit. The combustion chamber is pure cylindrical shape with \( \phi 65 \) mm in diameter and 190 mm in height. This means the chamber volume is approx. 630 cm\(^3\). Since the measurement procedures with the modified FIA were explained in detail in the papers from the authors, major differences in experimental conditions from the conventional FIA/FCA system are summarized in Table 1. Higher injection pressure, smaller nozzle hole and constant fuel viscosity secured higher spray quality. Added to it, its higher initial air temperature makes the ignition delay much closer to the one in an actual diesel condition. Of course the residual components will not evaporate completely at this temperature level under pressurized condition, but it would be still better to get some contribution to the ignition process from the lighter residual components especially when the cutter stocks are highly difficult to ignite. Above all, its injection period of 20 ms with rectangle-shaped injection rate, which is surely longer than the ignition delay of a BFO of poorer ignitibility, enables quantitative evaluation of combustibility in the diffusive combustion mode and sensitive detection of after-burning phase. In the modified FIA, 85 mm\(^3\) of sample oil was injected from of single-hole nozzle of \( \phi 0.16 \) mm during 20 ms of injection with superb repeatability.

<table>
<thead>
<tr>
<th></th>
<th>FIA-100 FCA</th>
<th>Modified FIA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Injection pressure</td>
<td>20~25 MPa</td>
<td>55 MPa const.</td>
</tr>
<tr>
<td>Injection period</td>
<td>4~5 ms</td>
<td>20 ms</td>
</tr>
<tr>
<td>Hole diameter</td>
<td>( \phi 0.25)~0.35 mm</td>
<td>( \phi 0.16 ) mm</td>
</tr>
<tr>
<td>Fuel temperature</td>
<td>80~130 °C</td>
<td>40~150 °C</td>
</tr>
<tr>
<td>Fuel viscosity</td>
<td>No control</td>
<td>20 cSt const.</td>
</tr>
<tr>
<td>Air pressure</td>
<td>4.5 MPa</td>
<td>4.5 MPa</td>
</tr>
<tr>
<td>Air temperature</td>
<td>480 °C</td>
<td>550 °C</td>
</tr>
</tbody>
</table>

### 2.2 Tested BFOs

In general, collecting the real TIOs from the damaged marine vessels is feasible only for the limited numbers of inspecting institutions. That is always a problem in accomplishing the research on quality evaluation of BFOs. For this study, 19 kinds of TIOs and over 90 kinds of TFOs were gathered up with help from NIPPON YUSEN KABUSHIKI KAISHA (NYK LINE) and NIPPON YUKA KOGYO CO., LTD. Although the number of TIOs is still insufficient to apply statistical analysis, it was a maximum over full-year efforts of fuel sampling under the conditions of 380 cSt grade kept in all the TIOs and TFOs. This viscosity level is most popular worldwide, so that nonbiased distributions could be expected in all aspects. Every BFO sample was measured its elemental properties before the combustion analysis, and three combustion tests were conducted all in all. Firstly FIA-CN and ECN of the sample were calculated according to the ignition delays in FIA/100-4 and FIA-100 FCA respectively. Then the detailed ROHR analysis was applied in the modified FIA based on Statistics.

### 2.3 Multivariable Analysis

There seems to be no ultimate variable or ultimate combination of two or three variables from FIA/FCA analysis to discriminate TIOs from TFOs perfectly. For example, ignition delay and any other indexes such as main combustion duration or maximum ROHR timing have been traditionally used to draw correlation diagrams to distinguish TIOs from TFOs. As is generally known, the results seem not very useful or promising in evaluating fuel quality. The authors reached to the conclusion that dozen of variants should be integrated and so-called multivariable analysis should be applied. In multivariable analysis, each variable (explaining variable) represents just minor difference in ROHR curves between TFO and TIO, so that only the total score (objective variable) counts being contributed by all the explaining variables. In this study, two different multivariate analysis methods were introduced. One was Linear Discriminant Analysis (LDA) and the other was Mahalanobis
Taguchi System (MTS). Since both the analyses are described even in educational materials on Statistics, only the analysis concept, procedures, merits and demerits of the both methods are concerned below.

2.4 Linear Discriminant Analysis

LDA is qualitative evaluation of samples in a $n+1$ dimensional space of $n$ variables. Additional dimension: $z$ is for a linear discriminant function ($LDF$): $Z$. In that space, this function means an $n$ dimensional plane and every sample is expressed as a point on that plane, so that all the samples are divided into positive members or negative ones across a line of intersection between $z = 0$ plane and $Z$ plane. The goal of LDA is to find the best $LDF$ to distinguish both members most clearly. $LDF$ or discriminant score of a certain sample is expressed as follows.

$$Z_j = a_0 + \sum_{i=1}^{k} a_i \bar{x}_{ij}$$  \hspace{1cm} (1)

$\bar{x}_{ij}$ is a normalized value of a $i$th variable of a $j$th sample, $a_i$ is a discriminant coefficient for the $i$th variable in a total of $k$ variables, and $a_0$ is a constant term. As a first step, it should be requested to create from ROHR curves as many explaining variables as possible. Selection of the variables was done by the step-wise method during the $LDF$ determination process. Merits and demerits of LDA are itemized as follows.

○ Whether a sample belongs to TFOs (positive) or TIOs (negative) is uniquely decided by the sign of the discriminant score. Quality of the fuel can be quantified according to the discriminant score ($Z_j$).

○ The contribution of each explaining variable in fuel discrimination is evaluated by its coefficient in the $LDF$ including both its absolute value and its sign.

● As for the samples of near-zero discriminant score, validity of the distinction is considerably limited.

● Based on unlikely assumption that both TFOs and TIOs are expected to be equivalent populations in their variance and covariance, since TIO has small number of samples and large variations.

All in all, LDA is not supposed to be an ideal method in discriminating TIOs from BFO samples. The main reason to apply LDA technique is to duplicate the check for the availability of multivariable analysis and to examine the effectiveness of a certain variable from small number of samples.

2.5 Mahalanobis Taguchi System

The basic concept of MTS and the analysis procedure of the MTS adopted in this study are shown in Figure 1. MTS is relatively new analysis method introduced by Taguchi et al. utilizing a generalized Mahalanobis distance (GMD, hereafter) described below in order to discriminate a group of abnormal events (TIOs in this study) from a group of normal or reference events (TFOs). The GMD is calculated for TIOs and TFOs separately and a nominal distribution is supposed only in the GMDs of TFOs. A GMD: $D_j^2$ for a $j$th normal or abnormal member is described as follows.

$$D_j^2 = \frac{1}{k} Y_j^T R^{-1} Y_j$$  \hspace{1cm} (2)

$Y_j$ means an array of the variables for the $j$th nominal or abnormal member, and $R$ is a correlation matrix defined among the nominal groups and used in common. MTS has essential advantage to other data mining methods like LDA in terms of needing no equivalent population for abnormal members. There are variations of MTS algorithm especially for the selection of the effective variables. In this study, the calculation scheme of Nakatsugawa and Ohuchi [3] was adopted. In their scheme, a gamma distribution is assumed to the GMD of the nominal samples, and the threshold level and its confidence interval are
Theoretically derived, which should be set in the GMD scattering space to define the boundary between the nominal group and the abnormal group, and also to secure its significance level. For both a threshold level and a confidence interval, one can set a cumulative probability and level of significance respectively by assuming a gamma distribution \( (a, b) \) of GMD: \( D^2_{n,j} \) only for the nominal groups (expressed by suffix n) as below.

\[
P(D^2_{n,j} \leq s) = \int_0^s \frac{b^a}{\Gamma(a)} x^{a-1} e^{-b x} \, dx
\]

where \( s \) is the GMD threshold level, which gives the theoretical probability \( P \) getting the nominal samples under that level. \( \Gamma \) is a gamma function. Then, the goodness of fit of the gamma distribution is examined by Kolmogorov and Smirnov test.

\[
F(d) - \lambda_x \leq S_n(d) \leq F(d) + \lambda_x
\]

\( d \) means sorted samples by GMD order and \( S_n \) gives the normalized sampling distribution from 0 to 1. \( F(d) \) is also the cumulative probability of the same gamma distribution for \( d \), and \( \pm \lambda_x \) results in the confidence interval of these analysis. The details of the elicitation process have to be spared because of space limitations. Creating as many variables as possible is regarded to be better in MTS. So the selection of variables is essential for getting effective analysis and the standard method for that purpose is to evaluate larger-the-better SN ratio, by which one can determine the significance of a certain variable in increasing the GMD of TIOs. The influence of the variable is eventually evaluated by its presence or absence in an orthogonal array of factorial of 2. The effective variables are determined so as to maximize the GMDs of TIO group and there is a theoretical chance to identify an extremely positive member as a negative.

- Nominal distribution is not expected from negative ones (TIO) but from positive members (TFO), which drastically reduces TIO sampling efforts and realizes more robust and practical analysis.

- Larger GMD variation is secured in the TIO group, whereas the deviation in the TFO group is much smaller, so that the dynamic range of the discrimination gets wider and visibly clearer.

- The effective variables are determined so as to maximize the GMDs of TIO group and there is a theoretical chance to identify an extremely positive member as a negative.

- Sufficient number of positive members with statistically nominal nature is necessary in the analysis.

![Diagram of Discriminating concept and analysis procedures of MTS](image)

\( P(D^2_{n,j} \leq s) = \int_0^s \frac{b^a}{\Gamma(a)} x^{a-1} e^{-b x} \, dx \)
3. Experimental Results and Discussion

3.1 ROHR Measurement in Modified FIA

The examples of ROHR curves observed in the modified FIA are exemplified in Figure 2. At least ten measurements for each sample were secured in this research. Sample numbers are added after each “TFO” or “TIO” reading in the figures. (a) TFO#3 represented a typical TFO sample of good ignitability and combustibility, and (b) TIO#7 was its counterexample from the TIO samples of poor ignitability and combustibility. The ignition delay of a typical TFO group was around 3 ~ 3.5 ms and that of a typical TIO group lengthened to 5 ~ 7 ms, and the distinction of the ROHR curves between these groups was very easy even by “visual judgment”. One can say concretely that such a judgment is based on the factors numbered in the Figure 3. TFO case: “1” shorter ignition delay, “2” steeper rise of ROHR by main combustion, “3” rather lower ROHR peak by premixed combustion, “4” stable and “5” near constant ROHR during diffusive combustion period, which was brought by the balance between fuel supply from the constant injection rate of modified FIA and fuel consumption to the diffusive combustion. “6” clearer bending of ROHR at the end of injection since the after-burning decays more quickly from the above mentioned constant value. TIO case: “7” longer ignition delay, “8” moderate rise of ROHR by main combustion, “9” trend of higher ROHR peak by premixed combustion. “10” vibrating combustion process in “11” totally chevron shape of ROHR derived from the larger spray body at the ignition timing. “12” rather smoother transition to after-burning phase from main combustion, therefore “13” only subtle bending of ROHR observed at the injection end.

In Figure 2 (c), (d), TFO#21 of relatively long ignition delay among the TFO group is compared with TIO#12 of relatively short ignition delay, which is actually shorter than that of TFO#21. At first glance, one must say TFO#21 wears more...
characteristics expected in the typical TIOs and TIO#12 can be said to be a more TFO-looking sample. With these kinds of samples, it is prohibitively difficult to discriminate TIOs from TFOs, and this could always happen around the boundary between TFO and TIO in recent years, so that the effective discrimination has never reached with using two or three conventional variables (ignition delay and combustion period and combustion end time, etc.).

3.2 LDA Results on ROHR Curves

Figure 3 shows the discrimination result of LDA. Considering the precursive position of LDA in this study, the number of TFO samples was limited to 27 without any selection to save analysing time. Additional samples equivalent to the "gap fuel" mentioned in the introduction were prepared as GFO#1, GFO#2 and GFO#3 for a small blind test. They are the mixtures of 70 % of LCO and 30 % of straight asphalt (SA), 40 % of LCO and 60 % of SA, and 40 % of gas oil and 60 % of SA respectively. GFO#1 can be regarded as TIO with confidence, GFO#3 as TFO, and GFO#2 in between. In ideal LDA, TFOs (positive members) and TIOs (negative members) scatter separately across the line of zero discriminant score, that is Z=0 axis. If considerable samples locate around the vicinity of zero discriminant score, the discriminant probability of LDA greatly decreases and the applicability multivariable analysis should be limited in the fuel quality evaluation. According to the results shown in the figure, one can safely say that multivariable analysis is definitely useful in discriminating TIOs from most of TFOs. In fact, only one TFO mistakenly tested negative as a type I error in the test, but blindly tested GFO#1 and GFO#2 showed positive score as large as typical TFOs' unexpectedly. This implies that the number of TFO samples was not enough at this LDA calculation and some selection was necessary before statistical analysis.

3.3 MTS Analysis Results with Quasi-Blind Test

Figure 3 shows the discrimination results of MTS analysis. In this case, the number of TFO samples was increased to 62 for the statistically better results, whereas two TIO samples were excluded because the failure of the engine burning them were thought to be derived from other reason like commingling of sea water. As referred above, total 31 initial variables were prepared and 17 variables left after the selection. The mean value of the generalized Mahalanobis distances over TFO samples should be unity, so that normal group concentrates around log₁₀(GMD)=1 line and shows much smaller fluctuation compared with that of TIO samples. So, the dynamic range of the discrimination is much wider than that of LDA and only the TIO group is enhanced in the figure. The threshold level of 1.60 was calculated through equation (3) by setting the cumulative probability 0.95. In the method of Nakatsugawa and Ohuchi, the threshold level was set so as to equalize number of type I error with number of Type II error. From the 62 of positive samples, 2 or 3 of type I error (and also 2 of type II error) could be expected as shown in the figure. The confidence interval of ±0.17 was also derived through equation (4) with the significance level of gamma distribution approximation assured within 5 % of rejection probability. Since additional 4 positive samples were
included within the confidence interval around the threshold level, the net discrimination probability went down to 0.886. In the figure, semi-blindly tested 31 TFOs were also plotted. Unfortunately 12 of 31 samples tested negative or “gray”, which means 62 TFO samples are not enough and more nominal TFO population is required. The net discrimination probability went down again to 0.809. All in all, fairly better discrimination of TIOs would be possible on MTS analysis especially when compared with the results on FIA/FCA.

3.4 MTS Analysis Results with Fuel Properties

Before the FIA/FCA tests, physical properties of a bunkered BFO on its inspection chart was acquiring major concern in estimating its combustion quality. Some of the properties such as concentrations of Al+Si or Sulphur in the fuel could be still effective in discrimination of TIOs, although they do not seem to have direct correlation with ignitability or combustibility of the fuel. Another advantage in adopting fuel properties exists in utilization of the combined indexes proposed by other researchers. That is, CCAI (Calculated Carbon Aromaticity Index) [4], the combustibility / ignitability indexes by Nomura et al. [5], simplified ring analysis by Ogawa, and so on, could be adopted as the new candidates of discriminant variables. The results are exemplified in Figure 4 with 8 variables from the FIA tests and 7 variables from fuel properties after the aforementioned selection procedures. The GMDs are plotted normally here instead of logarithmically, since they are relatively distributed in narrower range than in Figure 3. As shown in the figure, all the TIOs stay above the threshold level, and the number of blind test samples above the lower edge of the confidence interval was clearly reduced. The property related variables surviving through the selection are Al+Si, Na, kinematic viscosity, CCAI, Nomura’s two indexes, number of Naphthene ring by Ogawa. This strongly indicates the effectiveness of the combined indexes extracting the useful information from a couple of the basic properties.

4. Conclusions

Statistical analyses on LDA (Linear Discriminant Analysis) and MTS (Mahalanobis Taguchi system) were introduced to ROHR (rate of heat release) curves from a modified FIA (Fuel Ignitability Analyser) and physical properties of BFO (Bunker Fuel Oil) for the first time to discriminate trouble-inducible bunker fuel oils (TIO) from normal trouble-free fuel oils (TFO). Following results were reached.

○ Over 20 variables were studied out from ROHR curves measured in the modified FIA and their effectiveness was successfully confirmed by both LDA and MTS technique.

○ The net discrimination probability finally reached to just over 80% because of insufficient number of nominal TFOs. All in all, fairly much better discrimination of TIOs would be possible on MTS analysis than simple ECN measurements in FIA/FCA.

○ Physical properties were tentatively added to discriminant variables on MTS analysis, and Al+Si, kinematic viscosity were recognized as effective as well as the combined indexes proposed by other researchers.

References

Figure 4 MTS discriminant results utilizing physical properties of BFO