L.E. CURCIO, Refinery Automation Institute LLC, Morristown, New Jersey

IMO 2020 and the importance of nonlinear blending properties calculation

With 2020 here, fuel blenders, shipowners, and fuel oil producers and users are concerned about what will happen this year, with the sulfur content in bunker fuel reduced from 3.5 wt% to 0.5 wt%, as per International Maritime Organization 2020 (IMO 2020) rules.

This concern is justified, since there will be a proliferation of very-low-sulfur fuel oil (VLSFO) blends in an attempt to cut costs. Many of the 0.5 wt%-sulfur bunker properties are nonlinear and directly affect cost.

IMO 2020 and fuel properties. Literature describes how to blend low-sulfur components and how to estimate prices, but no articles address the practical issues of wide varieties in specifications—e.g. VLSFO peddled with 20 cSt–30 cSt, 80 cSt–120 cSt, and those closer to 300 cSt–380 cSt.[1] Mixing these fuels guarantees compatibility and stability problems, which creates the possibility of engine-damaging sludge.

Bunker fuel asphaltenes are the cause of compatibility problems. These problems come from the precipitation of asphaltenes in the form of sludge, clogging filters, decreasing effectiveness of purifiers, and discarded asphaltene sludge energy. Stability is basically a time-dependent compatibility issue, whereby the asphaltenes precipitate during the ship voyage. Surprisingly, the asphaltene content of bunker residual fuel is not included in ISO8217-2017 specs.[2]

Stability and compatibility[3] are not the only blend properties that blenders and shipowners must worry about. In bunker blending, more than 23 properties must be monitored simultaneously to ensure that specifications are met. If even one of those properties is off-spec, the final-product bunker fuel cannot be sold.

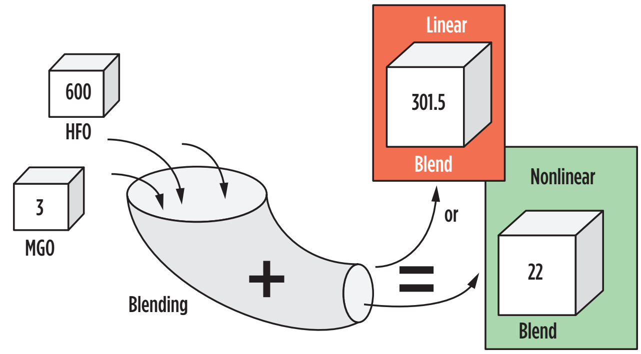

FIG. 1. Linear vs. nonlinear viscosity analysis.

For example, if a fuel producer wants to make a compatible and stable bunker fuel but its pour point value exceeds the one set in the ISO8217 specs, then the bunker cannot be sold because it is off-spec.

This article focuses on the nonlinearity of bunker component properties and how to deal with them. This might seem like an easy concept, but the majority of blenders and shipowners calculate bunker blend component properties *linearly*. This is a large mistake, one that overestimates or underestimates valuable or safety-related properties (i.e., viscosity, flashpoint, pour point, etc.) and can result in significant financial losses.

TABLE 1. Behavior of main bunker properties

Property	Linearity
Density	Linear
Sulfur	Linear
Ash	Linear
Conradson carbon	Linear
Water and sediment	Linear
Total sediment potential	Linear/nonlinear
Vanadium	Linear
Aluminum and silicon	Linear
ULO zinc	Linear
ULO phosphorous	Linear
ULO calcium	Linear
Specific energy	Linear
Acid number	Linear
Sodium	Linear
H_2S	Linear
Asphaltenes	Linear
Flashpoint	**Nonlinear**
Pour point	**Nonlinear**
Viscosity	**Nonlinear**
CCAI (calculated carbon aromaticity index)	**Nonlinear**
BMCI (Bureau of Mines co-relation index)	**Nonlinear**
Toluene equivalent	**Nonlinear**
Xylene equivalent	**Nonlinear**
Compatibility	**Nonlinear**

Linear vs. nonlinear measurement of fuel properties. What is the difference between linear and nonlinear? Why is considering blend nonlinearity so important? The answer is not a complex one. Since the bunker fuel oil and hydrocarbon-based components do not "attract" each other, chemical interactions modify the behavior of the solution or blend when the components are mixed together.

As an example, **FIG. 1** shows the blending of two components (of equal quantities of 1 t): heavy fuel oil (HFO) with a viscosity at 50°C of 600 cSt, and marine gas oil (MGO) with a viscosity at 50°C of 3 cSt. The linear calculation is (600 + 3) ÷ 2 = 301.5 cSt. However, a blend sample analyzed by a lab gives the result of 22 cSt. The reason for this difference is that the strong interactions between molecules in the blend make the phenomena highly nonlinear. The molecules differ in structure, size and/or thermal stability (differing blend behavior). The nonlinear molecular interactions show a difference in class:

- Nonlinear blends at paraffins, olefins, naphthenes and aromatics (PONA)
- Paraffins and naphthenes
- Paraffins and olefins.

Despite this behavior, the linear blends are of the same molecular class (e.g., paraffins and paraffins, or olefins and olefins, etc.).

Bunker fuel oil has more than 23 specs,[4] most of which are nonlinear. Focusing on the most important spec from a financial point of view, **TABLE 1** shows which bunker properties are linear and which one are nonlinear.

Bunker blend properties equations. As discussed in the previous section, bunker has more than 23 specifications to be met simultaneously. Some are linear, and some are nonlinear. The most important bunker properties are density, viscosity, sulfur, pour point, flashpoint and compatibility. As shown in **TABLE 1,** sulfur and density are calculated linearly, with "simple" linear wt% equations.

As an example, if the goal is to make a new, compliant 2020 bunker fuel (i.e., VLSFO), using the ISO8217-2017 specs, the resulting specs are shown in **TABLE 2.** Six blend components with their recipes in mass fraction are shown, along with the recipe specs and the blend results. These recipes are calculated linearly and nonlinearly to meet the ISO8217-2017 specs. The ultimate goal is to make a finished bunker product that meets all specifications.

If the blend results are compared, using linear equations vs. nonlinear equations, a number of differences emerge, as shown in **TABLE 3.** A large discrepancy can be seen, particularly on the nonlinear properties, when those properties are calculated linearly. For example, if calculated linearly, the viscosity has a value of 2,800 cSt; when calculated nonlinearly, its value is 300 cSt. This discrepancy is quite significant because the viscosity has a logarithmic trend.

The same thing happens with pour point and flashpoint, toluene equivalent and stability. If the pour point is calculated linearly, the value is 22°C, but it is 30°C when calculated nonlinearly. If the flashpoint is calculated linearly, the value is

TABLE 2. Bunker recipe for making VLSFO

			Blend results	
Blend components	**Blend recipe, wt%**	**Specifications**	**Linear**	**Nonlinear**
LSFO	32.78	Density, kg/m³	991	991
HSFO	7.72	Sulfur, wt%	0.48	0.48
LCO	46.54	Viscosity, cSt	**2,800**	**300**
LSFO 2	0	Pour point, °C	**22**	**30**
LSFO 3	12.96	Flashpoint, °C	**134.25**	**111.4**
No. 6	0	Ash, wt%	0.08	0.08
TOTAL	**100**	Conradson carbon, wt%	7.49	7.49
		Water and sediment, vol%	0.05	0.05
		Total sediment potential, wt%	0	0
		Vanadium, ppm	20.84	20.84
		Aluminum and silicon, ppm	47.6	47.6
		ULO zinc, ppm	0	0
		ULO phosphorous, ppm	0	0
		ULO calcium, ppm	0	0
		Specific energy, MJ/kg	40.45	40.45
		Acid number, mg KOH/g	0	0
		Sodium, mg/kg	0.74	0.74
		Toluene equivalent	**13.88**	**29.67**
		Asphaltenes, wt%	2.31	2.31
		CCAI	**854**	**854**
		BMCI	**79.6**	**79.6**
		Stability	**65.7**	**49.9**

134.25°C, and 1,11.4°C when calculated nonlinearly. For toluene equivalent and stability, if linear equations are used, the values are 13.88 and 65.7, respectively. If nonlinear equations are used, the values are 29.67 and 49.9, respectively.

These values not only create problems in term of meeting specifications for a compliant and compatible bunker fuel, but they can also have a significant economic impact. Translated into financial terms, dollars are being left on the table with each batch (**TABLE 4**).

Some important observations can be made from **TABLE 4.** If the linearly calculated final bunker blend is considered, a profit of $57/t can be secured. On the other hand, if the nonlinearly calculated final bunker blend is considered, the profit is $94/t. The change between the nonlinear profit model and the linear profit model is $37/t. This means that if a blender or a terminal operator is selling 100,000 t/mos of bunker fuel, if the linear equations are used, the blender or operator is leaving $3.7 MM/mos or $44 MM/yr on the table.

Adopting linear equations not only has a negative impact on the economics, but it also forces the blenders or terminal operators to produce a non-sellable product because the final blend values are off-spec.

In the abovementioned example, $3.7 MM/mos or $44 MM/yr is lost because of the linear/nonlinear issue. This article examines only one batch per month, but large refineries, terminals and blenders produce more than one batch per month and certainly more than 100,000 t. This shows how financially important it is to consider the nonlinearity of bunker blends in blending calculations.

Properties calculation methods.[4] The main differences between linear and nonlinear blending are summarized below.

The first approach usually taken is the linear approximation method, because it is very easy. This equation clusters classes of molecules into "lumps" and uses a %mass/volumetric equation to describe their behavior (Eq. 1):

$$Q_b = Q_{11} \times M_1 + Q_2 \times M_2 + \dots\ Q_i M_i \qquad (1)$$

where:

Q_b = Property of blend
Q_i = Property of component i
M_i = Mass (or volume) fraction of component i in blend

Due to the money involved, the molecular interaction (which the linear approach ignores) must be taken into consideration. The nonlinear blending properties can be calculated using several methods:

- Linear approximation with bonuses (good results if bonuses are updated constantly)
- Blending values (or dynamic bonuses) method
- Developing regressed equations using lab blend data
- Blending index (transformation) method.

The main blend properties are calculated using blending index:

TABLE 3. Bunker final blend properties, using linear and nonlinear equations

	Blend results	
Specifications	**Linear**	**Nonlinear**
Density, kg/m³	991	991
Sulfur, wt%	0.48	0.48
Viscosity, cSt	**2,800**	**300**
Pour point, °C	**22**	**30**
Flashpoint, °C	**134.25**	**111.4**
Ash, wt%	0.08	0.08
Conradson carbon, wt%	7.49	7.49
Water and sediment, vol%	0.05	0.05
Total sediment potential, wt%	0	0
Vanadium, ppm	20.84	20.84
Aluminum and silicon, ppm	47.6	47.6
ULO zinc, ppm	0	0
ULO phosphorous, ppm	0	0
ULO calcium, ppm	0	0
Specific energy, MJ/kg	40.45	40.45
Acid number, mg KOH/g	0	0
Sodium, mg/kg	0.74	0.74
Toluene equivalent	**13.88**	**29.67**
Asphaltenes, wt%	2.31	2.31
CCAI	**854**	**854**
BMCI	**79.6**	**79.6**
Stability	**65.7**	**49.9**

- Direct properties
  - o Flashpoint uses the index method (ethyl)
  - o Pour point uses the index method (ethyl)
  - o Viscosity uses the index method (ethyl, Refutas, etc.)
  - o Toluene equivalent uses a titration measurement only (no algorithm)
- Calculated variables
  - o CCAI uses the index method from ISO8217
  - o BMCI uses the Bureau of Mines co-relation index method
  - o Stability uses the ExxonMobil method for calculating compatibility.

It is important to consider the nonlinear calculations for properties like flashpoint, pour point and compatibility. The flashpoint of a fuel is the temperature at which vapor will ignite when an external flame is applied under standardized conditions. A flashpoint is defined to minimize fire risk during normal storage and handling. The minimum flashpoint for fuel in the machinery space of a merchant ship is governed by international legislation; the value is 60°C. Underestimating this calculation will create the possibility of explosions onboard.

The pour point is the lowest temperature at which a marine fuel can be handled without excessive amounts of wax crystals forming from a solution. If a fuel is below the pour point, then wax will begin to separate out and clog filters. An off-spec pour point from a linear correlation can cause the bunker fuel to crystallize, thereby inhibiting the flow.

TABLE 4. Economics comparing VSLFO finished price (using nonlinear equations) and VLSFO finished price (using linear equations) and relative giveaway per batch*

Nonlinear		Linear	
Blend cost, $/t	460	Blend cost, $/t	497
Sale price, $/t	554	Sale price, $/t	554
Profit, $/t	94	Profit, $/t	57

*Using 100,000 t as a reference volume

TABLE 5. Comparing linear, nonlinear and lab results

	Linear	Nonlinear	Laboratory
Viscosity, cSt	2,800	300	323
Flashpoint, °C	134.25	111.4	114.5
Pour point, °C	22	30	28.5

Stability is calculated by considering the toluene equivalent and the asphaltenes content. Although it is not recognized in the ISO8217-2017 specs, several patents exist, including the Exxon patent that shows the relationships between toluene, asphaltenes and stability.

Disputes over specifications. In the case of a dispute, a certificate of analysis from the lab can resolve doubts regarding the accuracy of a method. The nonlinear calculation results presented in **TABLE 3** have good agreement with the lab results, as shown in **TABLE 5.** The lab data are very close to the nonlinear correlation, within the reproducibility of the test method, which supports the use of nonlinear equations.

Takeaway. The IMO 2020 sulfur bunker regulations make it economically vital to consider the difference between linear and nonlinear property calculation results, and their potential impact on profit or loss. A terminal or refinery that produces 100,000 tpd of bunker fuel shows a difference of $44 MM/yr in profit just by considering the nonlinearity of the blend property calculation.

The economic benefit is not the only advantage of using the nonlinear correlation. As previously mentioned, using the wrong calculations for properties like flashpoint, pour point and compatibility can significantly impact the quality of the final bunker product, as well as the safety of operations. Blenders and terminal operators should sell compliant VLSFO that meets all specifications and is both stable and compatible. HP

LITERATURE CITED

[1] Barsamian, A., "Everything you want to know about IMO 2020 but are afraid to ask," *Hydrocarbon Processing*, July 2019.

Complete literature cited available online at HydrocarbonProcessing.com.

ELISEO CURCIO is the Vice President and CFO at Refinery Automation Institute LLC. He has more than 8 yr of experience in gasoline, diesel, bunker blending, ethanol nonlinear property correlations, octane boost, and naphtha and butane blending. He also teaches the gasoline, diesel and bunker blending optimization section of Refinery Automation Institute's public course in blending. As Manager, he is responsible for growing the business, acquiring new customers, and managing the company cashflow. Mr. Curcio holds BS and MS degrees in chemical engineering with high honors from the University of Calabria in Italy and an MS degree in advanced modeling and optimization from the Catholic University of Louvain in Belgium.

ONLINE ONLY

LITERATURE CITED

[1] Barsamian, A., "Everything you want to know about IMO 2020 but are afraid to ask," *Hydrocarbon Processing*, July 2019.

[2] Einemo, U., "ISO 8217:2017—what's new and why," International Bunker Industry Association, March 24, 2017, online: https://ibia.net/iso-82172017-whats-new-and-why

[3] Curcio, L. *et al.*, "IMO 2020 stability and compatibility headaches," *Hydrocarbon Processing*, December 2019.

[4] Curcio, L., "What is blending?" *Hydrocarbon Processing*, December 2017.