Kinematic Viscosity Prediction Guide: Reviewing and Evaluating Empirical Models for Diesel Fractions, and Biodiesel-Diesel Blends according to the Temperature and Feedstock

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Kinematic Viscosity Prediction Guide: Reviewing and Evaluating Empirical Models for Diesel Fractions, and Biodiesel-Diesel Blends according to the Temperature and Feedstock

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ABSTRACT

Experimental analysis of viscosity can be a straightforward and inexpensive analysis for few samples. However, in industrial processes that have high demands of properties measurements, the determination of viscosity and other properties involves time-consuming with sampling, analysis and availability of results. Also in refineries, the sampling routines for experimental determination of the viscosity of streams are not enough to represent variations that occur in the process, such as the shift of an oil tank in distillation units. In addition, besides requiring cost of operating personnel and laboratory analyst, all of these steps can take up to one shift until the result is available. Therefore, as an alternative, the use of predictive methods of kinematic viscosity are essential. Empirical methods have been used in simulations and design calculations of streams and mixture at industries regarding kinematic viscosity (KV) of petroleum fractions and fuels at different temperatures. However, there are uncertainties about the most accurate method to use at specific condition (temperature, feedstock, volume fraction) which might affect the KV prediction of fuels with unknown composition. Therefore, we assembled and evaluated several methods to predict KV of different diesel systems. In addition, new methods for predicting KV of diesel fractions at several temperatures were also developed for improving the estimation accuracy. As a result, we developed a guide with suggestions of the most accurate models to be applied for diesel fraction from assays, diesel fractions S500 from blend system at several temperatures, and biodiesel-diesel blends at different temperatures, volume fractions and feedstock.

Keywords: Empirical Equations; Prediction Method; Biodiesel; Diesel Fraction; Kinematic Viscosity

1. Introduction

Production of petroleum fractions and transportation fuels requires monitoring and control of some properties, such as viscosity. Besides essential for flow and hydraulic calculations, this property is also required during the blending process of petroleum fractions to increase profits through giveaway decreasing, adding less noble fractions, without deviating from fuel specification [1,2].

The examination of kinematic viscosity (KV) at 40° C is an important property, especially for fossil diesel, for the well-functioning of a given engine, influencing factors such as droplet size formation at the fuel atomization process for combustion quality [3]. Some concerns related to inadequate viscosity are leakage, in case of low KV, and poor atomization, incomplete combustion, deposit formation, and malfunctioning during cold weather [4]. As such, depending on the type of diesel engines, the kinematic viscosity target of fuels varies from 1.3 mm²/s to 4.1 mm²/s at 40°C for diesel fuel with light middle distillate, with specific sulfur concentration, according to ASTM D975-20a and ASTM 7467-20a [5,6].

Kinematic viscosity is also a crucial property for biodiesel, a biofuel derived from vegetable and animal oils applicable for Diesel engines. The biodiesel is a renewable source that can be an alternative of fossil diesel (non-renewable) in case of petroleum depletion and it is often blended with fossil diesel [7]. The application of biodiesel provides some benefits such as lower carbon dioxide emission and the increase of lubricity of the fuel in the engine, due to its higher KV [3,8]. However, the high KV of biodiesel, which varies according to feedstock, and volume fraction of biodiesel in a blended fuel, diminishes the quality of fuel atomization, and increases the formation of deposits in engines [9–11]. Thus, biodiesel KV must meet the specification, which ranges from 1.9 mm²/s to 6.0 mm²/s at 40°C [12], according to methods ASTM D445 and ASTM D7945 [5]. Those experimental tests depend on temperature and present satisfactory measurement for fluids with Newtonian flow behavior.

Experimental analysis of viscosity can be a straightforward and inexpensive analysis for few samples. However, in industrial processes, the determination of experimental viscosity or any other property involves sampling, analysis and availability of results. Therefore, besides requiring cost of operating personnel and laboratory analyst, all of these steps can take up to one shift until the result is available. Also in refineries, the sampling routines for experimental determination of the viscosity of streams are not enough to represent the variations that occur in the process, such

as the shift of an oil tank in the distillation unit. In addition, for minimizing giveaway in fuel blending systems, online optimization is necessary, with instantaneous values that is only possible through calculation methods. These methods are applicable for viscosity prediction of streams before and after blending (mixing calculations).

Viscosity prediction of fuels with high accuracy might not be a straightforward calculation, since it depends on its composition, chemical properties of each compound in the mixture [13], their interaction [14], temperature, and type of predictive model. For that, the prediction of kinematic viscosity can be carried out by two different approaches: rigorous calculations and empirical methods.

Rigorous calculations for viscosity prediction are based on theoretical concepts, such as statistical mechanics [15–21]. There are also semi-theoretical models with theoretical basis but also has some adjusted parameters. Rigorous methods might require complex data at molecular level, such as repulsion diameter, intermolecular potential attractive energy, structure theory, molar mass, and so on [22].

Some theories for viscosity prediction were developed based on Brownian motion, and equations of state in function of density and complex parameters such as rigid sphere diameter of the molecules, and coefficients of shear [16]. There is also a theory relating the flow with activation energy so that the calculation includes several parameters such as the molar free energy of activation of flow, molar volume for Newtonian behavior [23, 24]. For non-polar and polar pure liquid viscosity, the corresponding-states method has been applied for equilibrium and transport properties of pure materials [17] and requires critical properties, and size or shape parameter [25].

For hydrocarbon mixtures, rigorous methods also can be used. There are some studies for KV prediction of mixtures requiring composition content, pressure, temperature, thermal conductivity, some fitted parameters in function of n-alkane and aromatics, molar mass, and critical properties [26–28].

In front of the complexity of theoretical models application, empirical methods are often used in simulations with interactive calculations and project optimization to predict KV based on a correlation between viscosities and other properties.

KV can also be obtained through conversion model instead of a predictive one applying the standard ASTM D341, which requires only KV at two different temperatures to obtain KV at specific temperature [29].

For feasibility, predictive empirical methods have been developed requiring as input only properties easily measured and frequently available, such as density and boiling temperature. These methods are highly useful when the composition and other difficult properties are unknown [1,2,30–33]. However, as a drawback, empirical methods are developed for a specific system so that the range of validity is narrow and might not be applicable without restrictions [34].

Some individual studies have been conducted for kinematic viscosity prediction for fossil compounds, such as the development of new correlations for petroleum fraction [35, 36], and crude oil blends [14, 37]. There are also studies with assessment and development of models to predict kinematic viscosity of biodiesel-diesel blends [38–43] and specially a recent evaluation models at 40°C [44].

Therefore, due to the abundance of empirical models and numerous individual assessments of KV prediction, we evaluated existing methods at several conditions (temperature, feedstock, volume fraction) to verify the applicability and accuracy of KV predictive models for various systems, such as diesel fractions, and several biodiesel-diesel blends at different temperatures and volume fraction. We also developed new methods to predict KV of diesel fractions with higher accuracy than presented existing models. After that, we also developed a guide with indication of the most suitable methods to be used, according to the obtained accuracy represented by the minor % AAD from each evaluation.

2. Predictive Models of Kinematic Viscosity

Viscosity can be predicted by different types of models, such as semi-theoretical, theoretical, and empirical. Semi-theoretical models are based on the principle of corresponding states, applying reduced properties and theoretical models, which are based on models of statistical mechanics [1].

2.1. Prediction of kinematic viscosity of hydrocarbons

To predict the kinematic viscosity of hydrocarbons, there are several models that can be applied (Table 1). However, the calculation and the accuracy will mainly depend on the application range of each model and the required input parameters.

Abbot [2] has developed two methods to predict KV (cSt) at 37.8 °C and 98.9 °C, applying only API characterization factor (K_{API}) and API gravity (°API), shown in Equations (1) and (2). Results from those models presented a deviation of around 10-15%, for petroleum fractions, with KV from 0.5 cSt to 200 cSt at 100 °F, 0.3 cSt to 40 cSt at 210 °F, and with °API from 0 to 25, and K_{API} from 10 to 12.5 [2].

For undefined petroleum fraction, Aboul-Seoud and Moharam [30] have developed a method to predict KV (mm²/s) at any temperature (K), requiring only mid-boiling point (K), T_b , and specific gravity (sg) at 15.6 °C (Eq.(3)) [30].

With only mid-boiling point (K), T_b , it is also possible to predict KV (mm²/s) of petroleum fractions and hydrocarbons at any temperature T (K) by applying Mehrotra et al. [1] model (Eq.(4)).

Another model that requires only one input property is the one developed by Puttagunta et al. [45]. Their method (Eq.(5)) requires KV (mm²/s) at 37.8°C and is applicable for fractions with API gravities in excess of 30 degrees and API at low pressure. It is also recommended by the API-TDB – American Petroleum Industry – Technical Data Book on Petroleum Refining [45].

With more and different input parameters, the KV of petroleum fraction can be predicted by Beg et al. [46] method (Eq.(6)), applying parameters A and B, which are obtained from temperature at 50% volume distilled (T_{50}) and API gravity. This model can be applied only for data with boiling point from 200 °F to 850 °F [46]. Beg and Amin [31] also developed two more models to predict KV, Eq.(7) for heavy petroleum fraction and Eq.(8) for petroleum fraction with boiling point from 95 °C to 455 °C.

There is also another model to predict the KV of petroleum fractions at any temperature T (K) that requires three input properties, such as molecular weight, density at temperature T (ρ_T), and temperature at 50% volume distilled (T_{50}) (K) (Eq.(9)). In case of lack of molecular weight, density and temperature T, authors Fang and Lei [32] have suggested equations to obtain them, using density at 15.6°C ($\rho_{15,6}$), and T_{50} .

Also, there is a procedure to obtain KV from petroleum fractions by following the ASTM D341 [29] model. For that, one must apply two kinematic viscosities at two different temperatures (Eq.(10)).

There are also two models of KV prediction at 98.8°C, which are applicable for heavy oil with density from 929 kg/L to 1094 kg/L, and pour point of heavy oil from -33 °C to 15 °C (Equations (11) and (12)). Eq.(11) requires kinematic viscosity at 60°C and density at 20 °C, with AAD = 1.54 mm²/s. Eq.(12) only requires kinematic viscosity at 60°C, with AAD = 3.72 mm²/s [33].

Table 1 – Models to predict kinematic viscosity, ν , of pure hydrocarbon systems

Model	Equation	# Eq.
Abbot 1	$\log(\nu_{37.8}) = (4.39371 - 1.94733 K_{API} + 0.12769 K_{API}^2 + 3.2629$ $* 10^{-4} * API^2 - 1.18246 * 10^{-2} * K_{API} * ^\circ API$ $0.171617 K_{API}^2 + 10.9943 * API +$ $+) \frac{9.50663 * 10^{-2} * ^\circ API^2 - 0.860218 * K_{API} * ^\circ API}{^\circ API + 50.3642 - 4.78231 K_{API}}$	(1)
Abbot 2	$\log \nu_{98.9^\circ C} = \frac{8.0325 * 10^{-2} K_{API} + 1.24899 * ^\circ API + 0.19768 * ^\circ API^2}{^\circ API + 26.786 - 2.6296 K_{API}}$ $+ (-0.463634 - 0.166532 * ^\circ API + 5.13447 * 10^{-4}$ $* ^\circ API^2 - 8.48995 * 10^{-3} * K_{API} * ^\circ API$	(2)
Aboul-Seoud and Moharam	$\ln(\ln(\nu + 0.8)) = a_1 + a_2 * \ln(T)$ $a_1 = 4.3414 * (T_b * sg)^{0.2} + 6.6913$ $a_2 = -3.7$	(3)
Mehrotra et al.	$\log \log(\nu_T + 0.8) = a_1 + a_2 * \log(T)$ $a_1 = 5.489 + 0.148 * (T_b)^{0.5}$ $a_2 = -3.7$	(4)
Puttagunta et al.	$\log(\nu_T) = B * \left(\frac{559.67}{T + 459.67} \right)^S - 0.86960$ $B = \log(\nu_{37.8}) + 0.86960$ $S = 0.28008 * [\log(\nu_{37.8})] + 1.8616$	(5)
Beg et al.	$\nu = A * \exp\left(\frac{B}{T}\right)$ $B = \exp(5.471 + 0.00342 * T_{50})$ $A = -0.0339 * API^{0.188} + 0.241 * T_{50} / b$	(6)
Beg and Amin 1	$\nu = A * \exp\left(\frac{B}{T}\right)$ $B = -15.8342 * 10^{-4} + 374.357 * T_{50} - 0.2123 * T_{50}^2$ $A = 62.542 * 10^{-7} + 0.4274 * \exp(-15.06 * 10^{-4} * B)$	(7)

Beg and Amin 2	$v = A * \exp\left(\frac{B}{T}\right)$ $A = -1.954 * 10^{-3} + 0.0906 * \exp(-7.773 * 10^{-3} * M)$ $B = 67.45 + \exp(5.329 + 0.00329 * T_{50}) + 44.263 * (M/API)$	(8)
Fang Lei	$\ln(v_T/T) = 59.06 * T_{50\%}^{0.1546} * M^{0.4791} * \rho_T/T - (18.103 + \ln M)$ $\rho_T = [(\rho_{15.6}^2 - 1.1 * 10^{-3} * (T - 15.6))]^{0.5}$ $M = 219.05 * \exp(0.003924 * (T_{50\%} + 273.15)) * \exp(-3.07 * S) * (T_{50\%} + 273.15)^{0.118} * S^{1.88}$ $S = \rho_{15.6}/0.999024$	(9)
ASTM D341	$\log(\log(Z)) = A - B \log(T)$ $Z = v + 0.7 + \exp(-1.47 - 1.84 * v - 0.1 * v^2)$ $v = Z - 0.7 - \exp(-0.7487 - 3295 * (Z - 0.7) + 0.6119 * (Z - 0.7)^2 - 0.3193 * (Z - 0.7)^3)$	(10)
Santos and Fregolente 1	$v_{98.8^\circ\text{C}} = (0.657 * v_{60^\circ\text{C}})^{(1.4263 - 0.00069699 * d_{20^\circ\text{C}})}$	(11)
Santos and Fregolente 2	$v_{98.8^\circ\text{C}} = 0.6392 * v_{60^\circ\text{C}}^{0.7561}$	(12)

2.2. Prediction of kinematic viscosity of blends

Kinematic viscosity of blends (v_m) can be predicted by two types of methods, such as mixture-viscosity equations and parameter mixing rules [1]. Their application depends on component similarity.

2.2.1. Mixture-viscosity equations

One of the simplest approach to calculate some properties of mixtures is applying linear blending model and expressed by the weighted average of each blend component's property. The average can be based on volumetric, mole or mass fraction [45]. However, some properties, such as kinematic viscosity, cannot be expressed by linear blending but by other type of models [45]. Some empirical models for KV of mixtures (v_m) were developed for mixtures consisting of non-polar compounds and with similar structure [47] such as Chirinos [48] apud [37], Cragoe [49] apud [50], Arrhenius [51] apud [52], Bingham [53] apud [54], Linear [55], Kendal and Monroe [55], Refutas [56] apud [37], and Chevron [57] models (Table 2).

Based on mass fraction and KV of each component, the KV of a binary mixture can be predicted by Chirinos model (Eq.(13) [48] apud [37] and Cragoe method (Eq.(15) [49] apud [50]. However, for Cragoe model, two more parameters are required, L_i (Cragoe parameter of each compound i) and L (Cragoe parameter), which are calculated through the KV of each compound i (v_i) and mass fraction (w_i) [58] apud [49, 50].

Through volume fraction (V_i), the KV of a binary mixture of hydrocarbons can be predicted by applying Arrhenius model [51] apud [52], Bingham model [53] apud [54], or Linear model [55], Eq. (14), Eq.(16), and Eq. (18) respectively.

For KV prediction of a binary mixture based on mole fraction, x_i , Kendal and Monroe model [55] (Eq. 17) can be applied. This model is recommended by API-TDB [45] and it is widely used due to its satisfactory results [1]. Arrhenius model and Kendal and Monroe model (Equations (14) and (17), respectively) produce accurate results if the chemical structure of the two compounds is similar, such as non-polar and non-associated liquid, and if one of the compound is predominant [47].

Finally, there are Refutas model [56] apud [37] and Chevron model [57] (Equations (19) and (20), respectively), which are different from the previous methods, since they are based on index mixture. Also, similarly to Bingham [53] apud [54], Arrhenius [51] apud [52], and Linear [55] models, they are calculated on volumetric fraction.

Table 2 – Models of Mixing of pure component viscosities

Model	Equation	# Eq.
Chirinos	$\log(\log(v_m + 0.7)) = ((w_a * \log_{10}(\log_{10}(v_a + 0.7))) + (w_b * \log_{10}(\log_{10}(v_b + 0.7))))$	(13)
Arrhenius	$v_m = 10^{(\sum V_i * \log(v_i))}$	(14)
Cragoe	$v_m = 5 * 10^{-4} * \exp(1000 * \ln(\frac{20}{L}))$ $L = \sum w_i * L_i$ $L_i = 1000 * \ln 20 / (\ln v_i - \ln(5 * 10^{-4}))$	(15)
Bingham	$v_m = 1 / \sum (V_i * v_i)$	(16)
Kendal and Monroe	$v_m = (\sum (x_i * v_i)^{1/3})^3$	(17)
Linear	$v_m = \sum V_i * v_i$	(18)
Refutas	$VBI_i = 10.975 + 14.534 * \ln(\ln(v_i + 0.8))$	(19)
Chevron	$VBI_i = \frac{\log(v_i)}{\log(v_i * 1000)}$	(20)

2.2.2. Empirical models with additional parameters

Equations (13) to (20) can predict the KV of blends (v_m) composed by components with similar properties. Then, when this similarity decreases, the prediction deviation increases. Therefore, equations with additional parameters (Table 3) are more suitable for complex mixtures to obtain higher accuracy [59, 13].

Walther [37] model (Eq.(21)) requires a parameter C, which is obtained from regression analysis. This parameter is related to type of mixture, such as C = 0.8 for petroleum mixtures [37].

Lederer [60] (Eq.(22)) is an Arrhenius model modification that estimates KV through parameter alpha and the effective mole fraction, x'_A . Alpha parameter is called degree of association and is calculated through experimental KV of the mixture [60]. According to the literature, Lederer [60] and Cragoe [49] apud [50] models provide a similar and satisfactory prediction for blend of petroleum fractions with low viscosity ratios [52]. In addition, Shu [61] developed a correlation to obtain alpha for heavy oil and petroleum fractions (Eq.(23)) [61].

Power model, a modification of Kendal and Monroe [23] model (Eq.(24)), and Miadonye et al. [36] model (Eq.(25) use mass fraction to predict KV. Miadonye et al. model has two parameters, related to viscosity interaction (a) and viscosity reduction (n). This model was developed to predict KF of bitumen(v_B) and diluent blend (v_D) [36].

As a recommendation of API-TDB, there is Twu Bulls [45] model to predict the KV of a binary mixture, requiring KV at two different temperatures (T, in degrees Rankine) to estimate m and b parameters (Eq.(26).

Table 3 – Mixture models with additional parameters

Model	Equation	# Eq.
Walther	$\log(\log(v_m + C))$ $= x_a * \log_{10}(\log_{10}(\text{visc}_a + C) + x_b$ $* \log_{10}(\log_{10}(\text{visc}_b + C))$ $\ln(\mu_m) = x'_A \ln \mu_A + x'_B \ln \mu_B$	(21)
Lederer	$x'_A = \frac{\alpha x_A}{\alpha x_A + x_B}$ $x'_B = 1 - x'_A$	(22)

Model	Equation	# Eq.
Shu (alpha for Lederer model)	$\alpha = \frac{17.04 * (\rho_A - \rho_B)^{0.5237} * \rho_A^{3.2745} * \rho_B^{1.6316}}{\ln(\mu_A/\mu_B)}$	(23)
Power	$v_m = \left(\sum (w_i * \text{visc}_i)^n \right)^{1/n}$ $v_m = \exp(\exp(a * (1 - w_D^n)) + \ln v_D - 1)$	(24)
Miadonye et al.	$a = \ln(\ln v_B - v_D + 1)$ $n = v_D / (0.9029 * v_D + 0.1351)$	(25)
Twu and Bulls	$\ln(\ln(v_m + 0.7)) = m * (\ln T) + b$	(26)

3. Methodology

After reviewing predictive methods of KV (Table 1, Table 2, and Table 3), we calculated it applying, as input, some experimental properties provided by Brazilian oil industries and from the literature. Posteriorly, once R^2 might be inappropriate to validate the performance of nonlinear models, we evaluated their performance by the average of absolute difference between the calculated property and the value of experimental property. We calculated average absolute deviation percentage, %AAD (Eq. (27)), and average absolute deviation, AAD (Eq.(28)). As a result, comparing the %AAD of each predictive method, the most appropriate and accurate one is the equation that provided predicted KV with the minor %AAD.

$$\%AAD = \frac{100 * 1}{N} \sum_{i=1}^N \left| \frac{v_{calculated,i} - v_{experimental,i}}{v_{experimental,i}} \right| \quad (27)$$

$$AAD = \frac{1}{N} \sum_{i=1}^N |v_{calculated,i} - v_{experimental,i}| \quad (28)$$

3.1. Approach for KV prediction of Diesel fraction from petroleum assays

To predict KV of diesel fraction, we applied data (56 samples) from petroleum assays. The characterization of the petroleum can be represented by the specific range of values for some properties, such as specific gravity at 15°C from 0.82 to 0.91, °API from 24.15 to 41.83, KV at 20°C from 3.82 mm²/s to 15.23 mm²/s, KV at 40°C from 2.59 mm²/s to 7.83 mm²/s, KV at 50°C

from 2.20 mm²/s to 5.97 mm²/s, KV at 100°C from 1.18 mm²/s to 2.26 mm²/s, and KV at 150°C from 0.76 mm²/s to 1.24 mm²/s (Table 4) [62].

Table 4 – Properties of experimental data of diesel fraction from petroleum assays

Properties	Minimum value	Maximum value	Average value
Specific gravity at 15°C	0.82	0.91	0.86
°API	24.15	41.83	32.87
Kinematic viscosity @ 20 °C (mm ² /s)	3.82	15.23	7.29
Kinematic viscosity @ 40 °C (mm ² /s)	2.59	7.83	4.22
Kinematic viscosity @ 50 °C (mm ² /s)	2.20	5.97	3.37
Kinematic viscosity @ 100 °C (mm ² /s)	1.18	2.26	1.50
Kinematic viscosity @ 150 °C (mm ² /s)	0.76	1.24	0.89

We also calculated KV at several temperatures for diesel fraction, applying methods developed to obtain KV through KV data at different temperatures (Eq.5 and Eq.10) (Table 5). As mentioned previously, methods requiring KV at specific temperature to obtain KV in a different temperature are not considered predictive but a conversion one.

Table 5 – Input Properties applied to calculate KV at T temperature

Model	Target Calculation: KV at T	Properties as Input
Eq.(5)	KV at 40°C	KV data at 20 °C, 50°C, 100 °C and 150 °C Three different systems:
Eq.(10)	KV at 100 °C	KV at 40 °C and 20°C, 40 °C and 50°C, and 50 °C and 100°C Three different systems
Eq.(10)	KV at 20 °C	KV at 40 °C and 50°C, 100 °C and 150°C, and 40 °C and 150°C Three different systems
Eq.(10)	KV at 50°C	KV at 40 °C and 50 °C, 40 °C and 150 °C, and 100°C and 150 °C Three different systems
Eq.(10)	KV at 40°C	KV at 20 °C and 50 °C, 20 °C and 150 °C, and 100°C and 150 °C Three different systems
Eq.(10)	KV at 150°C	KV at 40 °C and 20 °C, 40 °C and 50 °C, and 100°C and 50 °C

To estimate KV by Eq.(8), it was necessary to calculate molecular weight, since this is a difficult property to acquire, through mean average boiling point of petroleum fraction (°R), T_b ,

and specific gravity at 60 °F/60 °F, s. The method for molar mass prediction (Eq.(29) is applicable for a boiling point from 90 °F to 1050 °F, API gravity from 14.4 to 93.1, and specific gravity from 0.63 to 0.97, and it is recommended by API-TDB [45].

$$M = 20.486 * \left(e^{1.165*10^{-4}*Tb-7,78712*d_{60F/60F}+1.1582*10^{-3}*Tb*d_{60F/60F}} \right) * Tb^{1,26007} * d_{60F/60F}^{4,98308} \quad (29)$$

3.2. Approach for KV prediction of Diesel fraction S500 from blending systems

To evaluate KV prediction methods, we applied 95 data of diesel S500 from blending system from Brazilian oil industries, which has specific properties (Table 6). All the models presented previously were evaluated, except Eq.(11) and Eq.(12), once they have been developed for heavy oil, as well as Eq.(7), designated for heavy petroleum fraction.

Table 6 – Properties of experimental data of diesel S500

Properties	Minimum value	Maximum value	Average value
Density at 20°C (kg/m³)	827.10	862.90	845.13
Kinematic viscosity @ 40 °C (mm²/s)	2.30	4.20	3.11
Temperature at 30% volume distilled (T_{30} (°C))	120.60	216.90	186.97
Flash Point (°C)	39	72	47.39

3.3. Approach for improving KV prediction of diesel fractions

To obtain higher accuracy, we applied diesel data from petroleum assays to develop new models at temperatures from 20 °C to 150 °C and also a new method to predict KV at any temperature. In addition, since 40°C is a crucial temperature to monitor kinematic viscosity for diesel specifications, we combined diesel fraction data from assays and diesel S500 from blending system to generate a model to amplify the restriction range for KV prediction at 40 °C.

Lastly, new methods were tested and validated with different data. Those new equations that predict KV at any temperature and KV at 40 °C were also evaluated through diesel S500 data to compare results from existing models.

3.4. Approach for KV prediction of diesel-biodiesel blends: effect of temperature, volume fraction, and biodiesel feedstock at KV prediction

To evaluate the accuracy of predictive methods (models with additional parameters and models for mixing pure component viscosities) of KV and their application for mixtures of fossil fuel and renewable fuel, such as biodiesel, diesel and biodiesel, 431 data from literature were applied. Those data comprehend density and KV at several temperatures, such as at 20 °C, 30 °C, 40 °C, 60°C, 80 °C, and 100 °C (Table 7). In addition, we applied data with varied volume fraction of diesel and data with several types of feedstock of biodiesel, such as soybean, yellow grass, castor, peanut, sunflower, canola, etc. (Table 8). For this study, all the methods were evaluated, except Shu (Eq.23), once it requires non available data such as density of each compound at specific temperature.

Table 7 – Average of KV at temperature T

Biodiesel type	Average KV (mm ² /s) at temperature T (°C)						Ref
	T=20.00 °C	T=30 °C	T=40.00 °C	T=60.00 °C	T=80.00°C	T=100.00°C	
Canola FAME	-	-	4.34	-	2.09	-	[40]; [4]
Castor FAME	-	-	14.77	-	-	-	[63]
Coconut FAME	-	6.15	-	-	1.41	-	[40]; [9]
Corn FAME	-	-	4.35	-	-	-	[4]; [64]; [42]
Cottonseed FAME	-	-	4.06	-	2.01	-	[40]; [4]
Diesel	3.94	-	3.5	1.82	1.37	1.09	[40]; [65]; [64]; [63]; [42]; [9] [66]
Jatropha FAME	-	6.44	4.48	-	-	-	[42]; [9]
Palm FAME	-	-	4.65	-	2.08	-	[40]; [63]
Peanut FAME	-	-	-	-	2.11	-	[40]
Pomace FAME	-	-	4.79	-	-	-	[42]
Rapeseed FAME	-	-	5.48	-	2.58	-	[40]; [64]
Sesame FAME	-	-	4.59	-	-	-	[42]
Soybean FAME	7.16	-	4.16	3.08	2.25	1.77	[40]; [65]; [4]; [42]; [66]
Soybean FAEE	-	-	5.83	-	-	-	[65]
Sunflower FAME	-	-	4.16	-	-	-	[4]; [42]
Waste FAME	-	6.76	4.75	-	-	-	[4]; [64]; [9]
Yellow Grease FAME	8.34	-	5.02	3.36	2.42	1.86	[42]; [66]

Table 8 – Diesel-biodiesel systems (several volume fractions and types of biodiesel) to evaluate KV prediction of mixtures

Blend system	% volume fraction of biodiesel	Ref
Diesel+ palm oil FAME	20; 40; 60; 80	[40], [63]
Diesel+ peanut oil FAME	5; 20	[40]
Diesel+ waste oil FAME	2; 5; 10; 20; 50; 75	[4], [64], [9]
Diesel+ sunflower oil FAME	2; 5; 10; 20; 50; 75	[4], [42]
Diesel+ canola oil FAME	2; 5; 10; 20; 50; 75	[40], [4]
Diesel+ yellow grease FAME	25; 20; 75	[66]
Diesel+ coconut oil FAME	5; 10; 20; 40; 50; 60; 75	[40], [9]
Diesel+ castor oil FAME	20; 40; 60; 80	[63]
Diesel+ jatropha oil FAME	2; 5; 10; 20; 50; 75	[42], [9]
Diesel+ corn oil FAME	2; 5; 10; 20; 50; 75	[4], [64], [42]
Diesel+ cottonseed oil FAME	10; 20	[4], [40]
Diesel+ rapeseed oil FAME	5; 20	[64]
Diesel+ sesame oil FAME	2; 5; 10; 20; 50; 75	[42]
Diesel+ pomace oil FAME	2; 5; 10; 20; 50; 75	[42]
Diesel+ soybean oil FAME	2; 5; 10; 15; 20; 25; 50; 75	[4], [66], [42]
Diesel+ soybean oil FAEE	5; 15; 20; 25; 50	[65]

4. Results and Discussion

4.1. Diesel fraction from petroleum assays

4.1.1. Evaluating empirical models of KV

For KV calculation of diesel fraction from petroleum assays, we observed that the best accuracy was from Eq.(10), with deviation around zero for KV at temperatures from 20 °C to 50 °C. Differently, the deviation from Eq.(10) was not zero for KV at 100°C (%AAD = 0.45) nor KV at 150°C (%AAD = 3.55). As a result from this evaluation, we observed that Eq.(10), independently of KV at a specific temperature, presented higher accuracy. However, we highlight that this is not a predictive model, since it requires two kinematic viscosities in different temperatures to obtain KV in another temperature, as well as Eq.(5). Therefore, if there are available KV in two different temperatures, we recommend applying Eq.(10) to obtain KV at the desired temperature. Otherwise, one must apply a predictive method.

For that, evaluating several methods shown at Table 1, we obtained different behavior and results for each model, according to specific temperature (Table 9). In another words, even though

all models can be applied for any temperature, we identified accuracy variation according to the temperature of kinematic viscosity.

Prediction of kinematic viscosity at 150 °C was more accurate if obtained through Eq.(6) with minor deviation (AAD = 0.04 mm²/s and % AAD = 4.70). For Kinematic viscosity at 100 °C, the most accurate model was obtained from Eq.(6) (AAD = 0.06 mm²/s and % AAD = 4.07). At 50 °C, kinematic viscosity prediction was more accurate applying Eq.(3) (AAD = 0.29 mm²/s and % AAD = 8.96). Eq.(3), Eq.(4), and Eq.(6) presented the highest deviation. At 40 °C, the most accurate model to predict KV was Eq.(3) (AAD = 0.41 mm²/s and % AAD = 10.21). Finally, at 20°C, the most accurate model to predict KV was Eq.(3) (AAD = 0.41 mm²/s and % AAD = 10.21).

Therefore, we assumed that KV prediction can be performed by specific equations depending on the temperature range. For example, at 150 °C and 100 °C, KV presents the same performance. Then, KV can be predicted by the same model, which is Eq.(6). For lower temperatures, such as 50°C, 40 °C, and 20 °C, Eq.(3) is the most appropriate model.

By this assessment of predictive methods, we realized that two input properties, such as mid boiling point and specific gravity or API gravity, are recommended to predict flow liquid behavior at temperatures from 20 to 150°C. Perhaps, because of that, Eq.(4) presented higher deviation, since it requires only mid-boiling point.

Table 9 – Results from KV (mm²/s) through predictive models for diesel fraction at specific temperature T (°C) by applying T30 and specific gravity

KV @ T	Model	AAD	%AAD	KV @ T	Model	AAD	%AAD	KV @ T	Model	AAD	%AAD
150°C	Eq.(6)	0.04	4.70	100°C	Eq.(6)	0.06	4.07				
	Eq.(3)	0.05	5.26		Eq.(9)	0.08	5.23				
	Eq.(5)	0.05	5.59		Eq.(3)	0.09	6.25				
	Eq.(9)	0.05	5.98		Eq.(8)	0.14	9.65				
	Eq.(8)	0.10	11.34		Eq.(5)	0.13	9.85				
	Eq.(4)	1.08	123.07		Eq.(4)	1.18	80.68				
50°C	Eq.(3)	0.29	8.96	40°C	Eq.(3)	0.41	10.21	20°C	Eq.(3)	0.84	13.14
	Eq.(6)	0.39	11.51		Eq.(4)	0.51	13.33		Eq.(5)	0.78	14.73
	Eq.(9)	0.42	12.90		Eq.(6)	0.66	15.68		Eq.(4)	1.10	16.40
	Eq.(8)	0.54	16.64		Eq.(9)	0.69	16.78		Eq.(6)	1.69	25.69
	Eq.(5)	0.48	17.64		Eq.(8)	0.83	20.48		Eq.(9)	1.70	26.19
	Eq.(4)	0.71	23.30						Eq.(8)	1.98	30.47

Assembling the results of KV predicted at several temperatures (20°C to 150 °C), except results from Eq.(5), which did not predict KV at T= 37.8 °C once it is an input of the equation, we obtained that Eq.(6) was the most accurate method to predict KV at any temperature, since it presented minor deviation (AAD= 0.328 mm²/s and %AAD = 8.22) (Table 10).

Table 10 – Results from KV prediction at any temperature T

Model	AAD (mm²/s)	%AAD
Eq.(6)	0.33	8.22
Eq.(3)	0.36	10.01
Eq.(5)	0.42	10.29
Eq.(9)	0.62	14.73
Eq.(8)	0.62	16.36
Eq.(4)	1.16	55.6

Once diesel fractions data have presented K_{API} from 12.56 to 13.86, Eq. (1) and Eq. (2) were not applicable in this study. In addition, we did not evaluate Eq.(11) and Eq. (12), since they have been developed for heavy oils. The Eq.(7) also was not evaluated because it is designated for heavy petroleum fraction.

4.2. Diesel fractions S500 from blending systems

4.2.1. Evaluating empirical models

Applying existing models to predict KV of diesel fraction S500 from blending systems at 40 °C, we observed that Eq.(3) presented a satisfactory accuracy (% AAD = 6.69) (Table 11). Comparing this result with KV prediction at 40 °C from diesel fraction from petroleum assays, we observed that Eq.(3) is the most appropriate existing model to predict diesel fraction KV at 40 °C.

Eq. (7), Eq. (11), and Eq. (12) were not evaluated, since they are not applicable for KV data of diesel S500, but for heavier fractions. Also, Eq.(5) was not evaluated once it requires KV at 37.8 °C.

Eq.(1) is originally developed to predict KV at 37.8°C, not 40 °C. However, it presented the second minor deviation (%AAD = 7.52). Therefore, Eq.(1) can also be applied to predict KV at 40 °C with accuracy similar to Eq.(3).

Table 11 – Results from existing models evaluation for KV at 40°C

Model	AAD (mm ² /s)	%AAD
Eq.(3)	0.21	6.69
Eq.(1)	0.23	7.52
Eq.(9)	0.34	10.93
Eq.(6)	0.35	11.12
Eq.(8)	0.44	14.07
Eq.(4)	0.88	28.12

4.3. Improving KV prediction of diesel fractions: Developing new models

Several equations for KV prediction from the literature presented low deviation, mainly at 150 °C and 100 °C. However, to achieve higher accuracy, we developed new equations for several temperatures, such as 20 °C, 40 °C, 50 °C, 100 °C, and 150 °C, and also for any temperature T (Table 12 and Fig. 1 to Fig. 12) for diesel fractions.

We analyzed the linear and nonlinear correlation among kinematic viscosity and properties, such as T10, T30, T50 (temperature at 10, 30 and 50 vol% distilled, respectively) and specific gravity to choose efficient parameters to predict KV. After calculations, T30 and specific gravity presented the most satisfactory performance through a nonlinear regression.

A new equation can predict KV at any temperature for diesel fraction (Eq.(35)) and it also presented lower deviation than the one from the existing models. In addition, we developed empirical methods to predict KV at specific temperature to improve accuracy (Eq. (30) to Eq. (34)). Those equations presented a deviation lower than 6% (Eq. (30) to Eq. (35)).

For KV at 40°C, we developed a new method including diesel fraction data from petroleum assays and diesel fraction S500 data from blending system. Therefore, Eq.(31) can be applied for a larger range of diesel fraction data, such as KV from 0.81mm²/s to 7.98 mm²/s, T_{30%} from 214.00°C to 280.91 °C, and specific gravity from 0.83 to 0.90.

We also tested those new equations with different data (testing data), which presented similar performance compared to training data, original data applied for developing new methods with adjusted coefficients (Table 12 and Fig. 1 to Fig. 12).

For KV prediction at any temperature, comparing results from the most accurate existing method (Eq.(6) with $\%AAD = 8.22$ (Table 10)), we observed that the developed method (Eq.(35)) presented higher accuracy, since its deviation was lower, $\%AAD = 5.50$ (Table 12).

For KV prediction at 40°C, applying diesel S500 data from blending system, we also observed a satisfactory prediction. As a result, Eq.(35) presented deviation $AAD = 0.11 \text{ mm}^2/\text{s}$ and $\%AAD = 4.00$, showing higher accuracy than the existing models.

The same occurred when we applied diesel S500 data to evaluate Eq.(31), which presented $AAD = 0.10 \text{ mm}^2/\text{s}$ and $\%AAD = 3.66$. Therefore, with similar performance (Fig. 13 and Fig. 14), to achieve higher accuracy from data similar to diesel S500, Eq.(35), and, mainly, Eq.(31), might be more efficient models to predict KV at 40 °C.

We also observed that the test achieved minor deviation compared to the original data. This performance can be explained due to obedience to restriction ranges of these new models.

Table 12 – New predictive KV models through T30 and specific gravity

T (°C)	Range	Method	Figure	AAD Regression (mm ² /s)	%AAD Regression	AAD Test (mm ² /s)	%AAD Test	Eq.#
20	<p>*For Regression (42 data) KV from 5.01 mm²/s to 10.11 mm²/s; T30 from 266.08°C to 280.83 °C; Specific gravity from 0.83 to 0.89</p> <p>*For Test (10 data) KV from 5.94 mm²/s to 9.62 mm²/s; from 272.45°C to 280.91 °C; °Specific gravity from 0.84 to 0.90</p>	v_{20} $= \frac{0.6832 * d_{15} * 1.1358 * T_{30\%}}{(0.2599 * T)^{0.8905 * d_{15}}}$ $- 5.0719 * T^{0.2000 / (0.0006 * T_{30})}$	Fig. 1	0.39	5.58	0.37	4.76	(30)
40	<p>*For Regression (42 data) KV from 2.40 mm²/s to 5.37 mm²/s; T30 from 214.00°C to 280.91 °C; Specific gravity from 0.83 to 0.90</p> <p>*For Test (10 data) KV from 2.50 mm²/s to 4.90 mm²/s; from 212.00°C to 280.77 °C; °Specific gravity from 0.83 to 0.88</p>	v_{40} $= \frac{1.1161 * d_{15} * 1.4200 * T_{30\%}}{(1.0014 * T)^{0.8688 * d_{15}}}$ $- 6.2297 * T^{0.0100 / (0.0030 * T_{30})}$	Fig. 3	0.20	5.00	0.16	4.39	(31)
50	<p>*For Regression (42 data) KV from 2.65 mm²/s to 4.16 mm²/s; T30 from 266.08°C to 280.83 °C; Specific gravity from 0.83 to 0.89</p> <p>*For Test (10 data) KV from 1.42 mm²/s to 1.73 mm²/s; from 272.45°C to 279.69 °C; °Specific gravity from 0.85 to 0.88</p>	v_{50} $= \frac{1.0171 * d_{15} * 1.2466 * T_{30\%}}{(0.7935 * T)^{0.9918 * d_{15}}}$ $- (6.0771 * T)^{0.0022 / (0.0016 * T_{30})}$	Fig. 5	0.15	4.57	0.08	2.37	(32)
100	<p>*For Regression (42 data) KV from 1.42 mm²/s to 1.73 mm²/s; T30 from 266.08°C to 280.83 °C; Specific gravity from 0.83 to 0.89</p> <p>*For Test (10 data) KV from 1.42 mm²/s to 1.73 mm²/s; from 275.36°C to 280.91 °C; °Specific gravity from 0.84 to 0.90</p>	v_{100} $= \frac{1.6576 * d_{15} * 1.2778 * T_{30\%}}{(1.5473 * T)^{0.8246 * d_{15}}}$ $- (6.0771 * T)^{0.0010 / (0.0034 * T_{30})}$	Fig. 7	0.04	2.78	0.05	3.15	(33)

T (°C)	Range	Method	Figure	AAD Regression (mm ² /s)	%AAD Regression	AAD Test (mm ² /s)	%AAD Test	Eq.#
150	*For Regression (42 data) KV from 0.81mm ² /s to 1.00 mm ² /s; T30 from 266.08°C to 280.91 °C; Specific gravity from 0.83 to 0.90 *For Test (10 data) KV from 0.85 mm ² /s to 1.73 mm ² /s; T30 from 272.45°C to 280.91; °Specific gravity from 0.85 to 0.90	$v_{150} = \frac{2.0081 * d_{15} * 0.8882 * T_{30\%}}{(2.0401 * T)^{0.6350 * d_{15}}}$ $- (6.077 * T)^{0.7820 * 10^{-5} / (0.0056 * T30)}$	Fig. 9	0.02	2.59	0.02	2.07	(34)
T	*For Regression (273 data) KV from 0.81mm ² /s to 7.98 mm ² /s; T30 from 214.00°C to 280.91; °Specific gravity from 0.83 to 0.90 *For Test (61 data) KV from 0.85 mm ² /s to 7.88 mm ² /s; T30 from 212.00°C to 280.91; °Specific gravity from 0.83 to 0.90	$v_T = \frac{1.8744 * d_{15} * 1.2115 * T_{30\%}}{(1.6853 * T)^{0.8103 * d_{15}}}$ $- (6.0668 * T)^{0.0092 / (0.0035 * T30)}$	Fig. 11	0.20	5.50	0.17	4.77	(35)

Fig. 1 - KV prediction with training data through Eq.(30) **Fig. 2** - KV prediction with test data through Eq.(30)

Fig. 3 - KV prediction with training data through Eq.(31) **Fig. 4** - KV prediction with test data through Eq.(31)

Fig. 5 - KV prediction with training data through Eq.(32) **Fig. 6** - KV prediction with test data through Eq.(32)

Fig. 7 - KV prediction with training data through Eq.(33) **Fig. 8** - KV prediction with test data through Eq.(34)

Fig. 9 - KV prediction with training data through Eq.(34)

Fig. 10 - KV prediction with test data through Eq.(34)

Fig. 11 - KV prediction with training data through Eq.(35)

Fig. 12 - KV prediction with test data through Eq.(35)

Fig. 13 - Test of Eq.21 through Diesel S500 data

Fig. 14 - Test of Eq.17 through Diesel S500 data

4.4. Diesel Blends

To evaluate the most applicable empirical methods to predict KV of diesel-biodiesel blend, we considered four categories of cases, such as (1°) KV prediction with no criteria of variables (temperature, volume fraction, and feedstock); (2°) KV prediction regarding volume fraction of biodiesel; (3°) KV prediction regarding temperature; and (4°) KV prediction regarding the biodiesel feedstock.

4.4.1. (1°) KV prediction with no criteria of variables (temperature, volume fraction, and feedstock)

For the first case of study, for models of mixing pure component viscosities, a satisfactory prediction was presented by the model with the minor deviation, which was Arrhenius [51] apud [52], with AAD = 0.06 mm²/s and %AAD = 1.62 (Fig. 15 and Table 1 at Supplementary material). For this case, no criteria was established, considering all biodiesel types (canola, castor, corn, cottonseed, coconut, jatropha, palm, peanut, pomace, rapeseed, sesame, soybean FAME, soybean FAEE, sunflower, waste oil, yellow grease), all temperatures (20 °C; 30 °C; 40 °C; 60 °C; 80 °C; 100 °C), all biodiesel volume fractions (2 %; 5 %; 7 %; 10 %; 15 %; 20 %; 25 %; 30 %; 40 %; 50 %; 60 %; 70 %; 75 %; 80 %; 90 %), with data from the literature [40], [65], [4], [63], [64], [42], [9], [66].

Fig. 15 – Suitable model of mixing pure component viscosities for diesel-biodiesel blend at any T

About models with additional parameters, we observed that higher accuracy can be obtained applying them (Table 13). For this case, the most appropriate model was Lederer [60] (Eq.22) with minor deviation $\%AAD = 0.73$ applying the parameter $\alpha = 0.89$. This model was also indicated as the most accurate by Hernández et al. [44] but for a different system, such as biodiesel-diesel blends at 40°C ($\alpha = 0.92$) [44].

Table 13 - Performance of each method with additional parameter - $\%AAD$ – at any temperature

Model	Any T	Parameter
Walther (Eq. 21)	2.37	C=2.48
Lederer (Eq. 22)	0.73	$\alpha=0.89$
Power (Eq. 24)	0.77	n=-0.01
Miadonye et al. (Eq. 25)	4.21	n is calculated according to Eq.

Fig. 16 - Suitable model of additional parameter for diesel-biodiesel blend at any T (20 °C to 100°C)

4.4.2. (2°) KV prediction regarding volume fraction of biodiesel

To understand the effect of volume fraction for KV prediction, as a second case, we evaluated the predicted KV at any temperature in three categories, such as biodiesel with volume fraction below 50%; with 50%; and with volume fraction more than 50 %. In this case, mixture-viscosity equations presented higher accuracy with minor %AAD compared to models with additional parameter. We also observed that the lowest accuracy (highest %AAD) was performed with 50% of volume fraction of biodiesel and, in general for all methods, the second lowest accuracy was performed with volume fraction of biodiesel more than 50%.

Arrhenius [51] apud [52] model (Eq. (14)) was the most appropriate model for less than 50% (%AAD=1.49) and greater than 50% (%AAD=1.53) of volume fraction of biodiesel. For volume fraction of biodiesel equal to 50%, the accuracy decreased, and the most appropriate model was Kendal, with %AAD = 2.37. Thus, Eq. (14) might be applicable for generalized volume fraction of biodiesel. However, we highlight that the accuracy of Eq. (17), Kendal and Monroe [55] model, can present higher accuracy if one component is dominant in quantity [47]. Also, Eq. (14) presented similar performance for volume fraction of biodiesel equal to 50%, with %AAD = 2.59 (Fig. 17 and Table 2.1 at supplementary material).

For models with additional parameters, which presented minor deviation considering the specific volume fraction, we observed that the most appropriate model for volume fraction equal to 50% of biodiesel was performed by Power model [36] (Eq. 24) ($\%AAD = 2.76$). For volume fraction greater than 50% of biodiesel, Lederer [60] (Eq. 22) and Power [36] methods were the most suitable, with $\%AAD = 2.30$ and $\%AAD = 2.32$, respectively. Also for volume fraction of biodiesel with less than 50%, Lederer [60] and Power [36] methods were the most suitable with $\%AAD = 2.27$ for both (Table 2.2 at supplementary material with appropriate parameters).

Further studies with specific data relating volume fraction with temperature is need to better evaluate the influence of both conditions. However, with this evaluation, we observed that kinematic viscosity prediction is influenced by composition, then we suggest to be aware of possibility of greater deviation when biodiesel concentration increases.

Fig. 17 – Performance of model with the minor deviation, according to volume fraction of biodiesel at any T(°C)

4.4.3. (3°) KV prediction regarding temperature

Analyzing the performance according to the temperature, as the third case, we observed that the most appropriate method and its accuracy varies according to the temperature (Table 1 and Table 15).

KV prediction presented the highest deviation at 20 °C (almost the double of average deviation, considering all temperatures with %AAD = 1.62). Since the difference between KV diesel and KV biodiesel is almost always the double, regardless of the temperature, we observed that it is not the value of KV at 20°C that affects the prediction result, but it might be the type of model. Hence, KV prediction at 20°C may not be appropriate to apply index mixture models, or KV at 20°C might not follow an additive property performance. Nevertheless, more studies need to be carried out with the same biodiesel source and with the same volume fraction to verify the influence of those parameters. In this study, we could not follow this procedure due to scarcity of data.

Table 14 – Evaluation of predicting methods of KV regarding temperature T

Biodiesel	Model	T (°C)	%Volume of Biodiesel	AAD (mm ² /s)	%AAD
canola, castor, corn, cottonseed, jatropha, palm, soybean, pomace, rapeseed, sesame, sunflower, waste oil, yellow grease	Cragoe (Eq. 15)	40	2; 5; 7; 10; 15; 20; 25; 30; 40; 50; 60; 70; 75; 80; 90	0.07	1.69
coconut, jatropha, waste oil	Kendal (Eq. 17)	30	5; 10; 20; 40; 50; 60; 75	0.04	0.92
soybean, yellow grease	Linear (Eq. 18)	20	25; 50; 75	0.16	2.83
soybean, yellow grease	Linear	60	25; 50; 75	0.05	1.87
canola, cottonseed, coconut, palm, peanut, rapeseed, soybean, yellow grease	Linear	80	20; 25; 50; 75	0.03	1.98
soybean, yellow grease	Linear	100	25; 50; 75	0.02	1.34

After evaluating methods with additional parameter and comparing results (Table 14 and Table 15), we concluded that methods with additional parameters performed higher accuracy than pure mixing methods. In addition, we observed that Lederer [60] method performed satisfactory results for almost all temperatures but for each temperature its parameter has a different value. Depending on the temperature, others also can be applied. We observed that methods with additional parameter performed with minor AAD among specific temperatures such as 30 ° C to 60 ° C. Therefore, to obtained the most satisfactory performance, we suggest applying determined methods for a specific temperature (Table 16). We just highlight that due to lack of data, for each temperature, a different type of data (different biodiesel feedstock) were applied. High variety of biodiesel feedstock were used at 40°C.

Table 15 - Performance of each method with additional parameter - %AAD – according to the temperature

Model	%AAD at specific Temperature (°C) and parameter					
	20	30	40	60	80	100
Walther (Eq.21)	2.83 (C=6710888.4)	0.46 (C=11.57)	2.21 (C=1.2)	1.87 (C=3399032.36)	2.28 (C=-6699883.19)	1.34 (C=-2488122.3)
Lederer (Eq.22)	2.24 ($\alpha = 1.74$)	0.47 ($\alpha = 1.19$)	0.73 ($\alpha = 0.89$)	1.41 ($\alpha = 1.54$)	1.58 ($\alpha = 1.54$)	1.07 ($\alpha = 1.37$)
Power (Eq.24)	2.79 (n=1.07)	0.46 (n=0.61)	2.21 (n=-0.1)	1.78 (n=1.37)	2.14 (n=2.20)	1.19 (n=1.35)
Miadonye (Eq.25)	13.3	7.38	3.43	8.74	26.9	24.17

Table 16 – The most appropriate method to predict KV of biodiesel-diesel blends considering the temperature

Biodiesel	Model	T (°C)	% Volume of Biodiesel	AAD (mm ² /s)	%AAD
soybean, yellow grease	Eq.22 ($\alpha = 1.74$)	20	25; 50; 75	0.13	2.24
coconut, jatropha, waste oil	Eq. 24 (n=0.61) or Eq.21 (C= 11.57) or Eq.22 ($\alpha = 1.19$)	30	5; 10; 20; 40; 50; 60;75	0.03	0.47

Biodiesel	Model	T (°C)	%Volume of Biodiesel	AAD (mm²/s)	%AAD
canola, castor, corn, cottonseed, jatropha, palm, soybean, pomace, rapeseed, sesame, sunflower, waste oil, yellow grease	Eq.22 ($\alpha = 0.89$)	40	2; 5; 7; 10; 15; 20; 25; 30; 40; 50; 60; 70; 75; 80; 90	0.03	0.73
soybean, yellow grease	Eq.22 ($\alpha = 1.54$)	60	25; 50; 75	0.04	1.41
canola, cottonseed, coconut, palm, peanut, rapeseed, soybean, yellow grease	Eq.22 ($\alpha = 1.54$)	80	20; 25; 50; 75	0.03	1.58
soybean, yellow grease	Eq.22 ($\alpha = 1.37$)	100	25; 50; 75	0.02	1.07

4.4.4. (4°) KV prediction regarding the biodiesel feedstock

For the fourth case of applying empirical methods of KV prediction regarding biodiesel feedstock, we observed that there was not only one the most suitable model to be applicable as well. Actually, the most appropriate model varied according to the biodiesel type, as well as temperature (Tables 3.1 and 3.2 at Supplementary Material). However, in general, Lederer [60] method was the method with the minor deviation and for each type of feedstock there is a specific optimum parameter to be applied (Table 17).

On the other hand, the system with the lowest accuracy was that of soybean FAEE biodiesel-diesel blend, with AAD = 1.04mm²/s and %AAD = 22.17, applying Linear [56] model at 40 °C (Table 5 at supplementary material). This might imply that the type of alcohol used during transesterification reaction affects the flow property, presenting higher KV, and consequently the accuracy of specific predictive method of KV. More studies might be necessary to verify the prediction of FAEE biodiesel.

Table 17 - Appropriate method based on feedstock biodiesel and temperature

Feedstock biodiesel	Temperature (°C)	AAD	%AAD	Parameter	Method
Canola	40	0.03	0.74	1.72	Walther
Castor	40	0.11	1.74	0.88	Lederer
Coconut	30	0.02	0.45	1.14	Lederer
Corn	40	0.03	0.84	-	Refutas
Cottonseed	40	0.02	0.73	-	Chevron and Cragoe
Jatropha	40	0.04	0.97	0.94	Lederer
Jatropha	30	0.01	0.29	11.57	Walther
Jatropha	40-30	0.97	0.05	1.25	Lederer
Palm	40	0.01	0.18	0.79	Lederer
Pomace	40	0.02	0.57	0.96	Lederer
Rapeseed	40	0.18	4.43	27.12	Walther
Sesame	40	0.03	0.71	0.96	Lederer
Soybean	20	0.13	2.22	1.80	Lederer
Soybean	40	0.06	1.63	-	Cragoe, Chevron, Refutas, Chirino, and Arrhenius
Soybean	60	0.04	1.48	1.55	Lederer
Soybean	100	0.02	1.03	1.37	Lederer
Soybean	80	0.03	1.65	1.54	Lederer
Soybean	20-100	0.07	2.07	-	Linear
Soybean FAEE	40	0.67	14.00	0.72	Lederer
Sunflower	40	0.03	0.72		Chevron and Cragoe
Yellow grease	20	0.07	1.37	1.47	Lederer
Yellow grease	40	0.04	1.24	1.40	Lederer
Yellow grease	60	0.02	0.80	1.18	Power

Feedstock biodiesel	Temperature (°C)	AAD	%AAD	Parameter	Method
Yellow grease	80	0.02	1.09	1.82	Power
Yellow grease	100	0.02	1.08	1.35	Power
Yellow grease	20-100	1.07	0.04	1.26	Power

One of the most feedstock used for biodiesel production is soybean and we observed different models for each temperature to better predict KV. For any temperature, the most appropriate method was Linear [56] method with minor deviation, %AAD=2.07 (Fig. 18 and Table 17 and Table 3.1 at supplementary material). Also Lederer [60] method performed satisfactory results with the second minor deviation (%AAD =2.40 with alpha=0.89).

Fig. 18 – KV prediction of biodiesel composed by soybean FAME at any temperature

On the other hand, the system with the lowest accuracy was that of soybean FAEE biodiesel-diesel blend, with AAD = 1.04mm²/s and %AAD = 22.17, applying Linear [56] model at 40 °C (Table 5 at supplementary material). This might imply that the type of alcohol used during

transesterification reaction affects the flow property, presenting higher KV, and consequently the accuracy of specific predictive method of KV. More studies might be necessary to verify the prediction of FAEE biodiesel.

At 40°C, we observed that the prediction of KV of soybean FAME blend presented a similar behavior to Cragoe [49] apud [50], Chevron [57], Refutas [56] apud [37], Chirino [48] apud [37], and Arrhenius [51] apud [52] models with the lowest deviation, AAD = 0.06 mm²/s and %AAD = 1.6 (Table 18).

Table 18 – Performance of KV prediction at 40 °C of biodiesel blends with soybean FAME

Model	AAD	%AAD
Cragoe	0.06	1.62
Chevron	0.06	1.62
Refutas	0.06	1.62
Chirino	0.06	1.63
Arrhenius	0.06	1.63
Kendal	0.06	1.67
Linear	0.07	1.91
Bingham	0.07	1.95

Finally, we highlight that Refutas [56] apud [37], Chirinos [48] apud [37] and Kendal and Monroe [55] models are not based on volumetric fraction to predict KV for blends. However, precise and similar results were obtained compared to models based on volumetric fraction.

In general, Miadonye et al. [36] and Power [36] models presented the highest deviation, with %AAD = 9.55 and %AAD = 8.45, respectively. However, Miadonye et al. model might have lower accuracy, since it was developed for bitumen. We also highlight that due to lack of density of compounds and/or of mixtures at specific temperatures, Shu [61] method was not evaluated and Walther [37] and Lederer [60] methods were evaluated through volume fraction instead of mass fraction.

4.5. Results overview: a KV prediction guide

As an overview of the results obtained in this assessment, we developed a guide with suggestions of the most appropriate models, regarding minor deviation, to predict kinematic viscosities according to diesel system, its properties, and temperature (Fig. 19).

For diesel fraction at 40°C, temperature to attend specifications, the most appropriate model was the new Eq.(31) presenting %AAD = 5.00, or the existing model Eq.(3), with %AAD = 10.21. For any other temperature, we suggest applying the new Eq.(35), with %AAD = 5.50, or the existing model Eq.(6), with %AAD = 8.22, or verifying a specific temperature and system at Table 12.

For diesel fraction blend system at 40 °C (temperature to meet specifications), the most appropriate model was Eq.(31), presenting %AAD = 5.00, and the existing model Eq.(3), with %AAD = 6.69.

For soybean biodiesel blend system at any temperature, the most appropriate model was Eq.(18), presenting %AAD = 2.07. For KV prediction at 40°C, we suggest applying some models of pure hydrocarbon mixtures, such as Eq. (13), Eq. (14), Eq. (15), Eq. (19), and Eq. (20), with %AAD = 1.63.

To achieve higher accuracy of KV prediction of diesel-biodiesel blend with a different biodiesel, and also at another temperature different from 40 °C, others models are more suitable (Table 16 and Table 17). In addition, in case of lack of biodiesel KV to be applied on calculations, we suggest consulting a list (Table 7) with average KV of several biodiesel types at 40 °C, obtained according to the literature.

In this guide, no model was suggested regarding volume fraction, since more studies are needed considering at specific temperature and feedstock biodiesel. However, we highlight that increasing biodiesel volume fraction might decrease the accuracy of these prediction models.

Fig. 19 – Guide for KV prediction with suggested models to apply according to diesel system and temperature

5. Conclusion

In this study, several models of KV prediction were analyzed to different conditions of diesel fraction and diesel blends.

For KV prediction of diesel fraction from petroleum assays, we obtained different behavior and results for each model, according to specific temperature. In another words, even though all models can be applied for any temperature, we identified accuracy variation according to the temperature of kinematic viscosity.

For KV prediction of diesel fraction S500 from blending systems at 40 °C, we observed that Eq. (3) presented a satisfactory accuracy (% AAD = 6.69)

To achieve higher accuracy, we developed new equations for KV at several temperatures, such as 20 °C, 40 °C, 50 °C, 100 °C, and 150 °C, and also for any temperature T (Table 12 and Fig. 1 to Fig. 12) for diesel fractions. As input for new methods, we studied T10, T30, T50 and specific gravity. We verified that the most satisfactory performance through a nonlinear regression to predict KV are applying T30 and specific gravity. Therefore, only methods with T30 as input were presented in this study. Those methods were tested with different data and provided satisfactory results.

For KV prediction of diesel blends, we considered four categories of cases, such as (1°) KV prediction with no criteria of variables (temperature, volume fraction, and feedstock); (2°) KV prediction regarding volume fraction of biodiesel; (3°) KV prediction regarding temperature; and (4°) KV prediction regarding the biodiesel feedstock.

As result for the first case, Eq. 14 was the most suitable method for KV prediction, with the minor deviation, AAD = 0.06 mm²/s and %AAD = 1.62.

For considering the study of the impact of volume fraction on KV prediction as the second case, we evaluated the KV prediction of blend with 50% of the biodiesel, greater than 50% of biodiesel and less than 50% of biodiesel. As results, Eq. 14 was the most accurate method for diesel blend with less and greater than 50% of biodiesel. For volume fraction of biodiesel equal to 50% the accuracy is poorer than the other two fractions and presented Eq.17 as the most accurate

method. For models with additional parameters the higher accuracy was obtained through Eq.22 and Eq. 24.

For the third and fourth case, we observed that the most appropriate method and its accuracy varies according to the temperature and biodiesel feedstock. Therefore, to achieve higher accuracy a specific method must be applied for a specific temperature and feedstock.

We concluded in general that, to obtain the highest accuracy for KV prediction, it is adequate to apply an appropriate model for specific condition and fuel properties. Except in case of soybean biodiesel-diesel blend, any type of KV prediction model (if mixture-viscosity equations or model with additional parameter) can provide similar performance. Also, some models might have their accuracy decreased when the volume fraction of biodiesel increases but more studies must be carried out to verify the influence of the volume fraction on the predictive methods.

Overall, interested researchers can follow the developed guide to choose the most appropriate model for achieving higher accuracy to predict KV of diesel fraction and its derivatives, according to the object of study, KV range, and temperature.

Nomenclature

KV	kinematic viscosity
K_{API}	API factor
ν_T	Kinematic viscosity at T temperature
d_{15}	Density at 15°C
API	API gravity
T_b	Boiling point
A, B	Parameters for liquid related to viscosity
Z	Parameter for viscosity temperature equation
w	Mass fraction
V	Volume fraction
x	Mole fraction
M	Molar mass

VBI	Viscosity blend index
ν_m	Mixture kinematic viscosity
AAD	Average absolute deviation
% AAD	Percentage average absolute deviation
ν_D	Diluent viscosity for Miadonye et al. model
ν_B	Bitumen viscosity for Miadonye et al. model
ρ_A, ρ_B	Density for fluid A and B for Shu model
$d_{60F/60F^-}$	Specific gravity at 60°F/60°F
T10, T30, T50	Temperature at 10, 30 and 50 vol% distilled
T	Temperature
FAME	Fatty acid methyl esters
FAEE	Fatty acid ethyl esters
C	Walther parameter
α	Alpha, a parameter from Lederer model
a, n	Constants from Miadonye additional parameter model

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