

An atomic contribution model for the prediction of speed of sound



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ARTICLE INFO

Article history:

Received 6 April 2013

Received in revised form 12 July 2013

Accepted 18 August 2013

Available online 26 August 2013

Keywords:

Speed of sound

Wada's constant

Atomic model

Predictive model

ABSTRACT

Speed of sound is an important property in many applications and it is being increasingly used in different technological areas. In this work a database of speed of sound and density at atmospheric pressure for n-alkanes, branched alkanes, n-alkenes, aromatics, alcohols, ethers and esters were collected from the open literature. Using these data a Wada group contribution model recently proposed by us was used as the basis for the development of a new atomic contribution model to predict speed of sound for all the families of compounds investigated in this work. It is shown that the proposed model is able to predict the speed of sound for compounds of these families with deviations close to the experimental reproducibility. This work also discusses the effect of branching on the Wada's constant, pointing out the importance of new measurements for this type of compounds.

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1. Introduction

As an important property in physical and chemical studies, speed of sound can be used in many areas, like in medicine [1], fuel level indicators in many modern aircrafts [2], or concentration monitoring in liquids [3]. When it is used in conjunction with other properties it allows the derivation of a wide range of thermophysical properties including isentropic and isothermal compressibility [4].

With the advent of renewable biofuels there has been a move into the blending of conventional hydrocarbon based fuels with renewable non-conventional fuels, like biodiesel, pyrolysis bio-oil, and alcohols or ethers. This fact is leading to a change in the chemical nature of fuels. The fluid properties of speed of sound and isentropic bulk modulus have important impacts on the injection process. The isentropic bulk modulus is a measure of a fluid's compressibility under pressure – it affects the amount of pressure rise that will occur from the fuel pump pulse. The speed of sound in the fuel affects the time required for the pressure rise to proceed through the fuel line and reach the injector. As an example, compared to petroleum fuel, biodiesel is less compressible and has a higher speed of sound. Both factors contribute to an advance in fuel injection timing. Injection timing advance can lead to earlier

start of combustion, which raises peak in-cylinder temperature, thereby increasing thermal NO_x formation [5]. The bulk modulus and speed of sound values are thus indispensable parameters for system modeling and for experimental injection rate determination [6].

Being important to predict thermophysical properties to solve engineering problems, many studies have been performed in order to develop accurate models that can represent speed of sound. Lafitte et al. [7] developed a modified version of SAFT model (Statistical Theory associating Fluid), the SAFT-VR MIE, predicting the speed of sound of some n-alkanes and comparing their deviation with SAFT SW-VR, obtaining average absolute deviations (AAD) of 2.52 and 12.17%, respectively for each model, modeling speed of sound at different temperatures and pressures. The following year, the same authors [8] analyzed their proposed modified SAFT for 1-alcohols and branched alcohols, and the model was used to calculate speed of sound in mixtures of alcohol+n-alkane, obtaining a AAD of 2.72% for pure alcohols. Paredes et al. [9–11] used the Prigogine–Flory–Patterson model to correlate density and speed of sound in n-hexadecane, n-dodecane, n-decane, and tetralin, obtaining AAD of 0.43, 0.36, 0.28 and 0.53%, respectively. Recently, Villiers et al. [12], evaluated three models: PC-SAFT, SAFT and CPA (cubic-plus-association) equations of state, for predicting the speed of sound of n-alkanes, obtaining overall AAD of 6.61, 24.8 and 8.83%, and of 1-alkanols, observing AAD of 7.65, 15.48 and 13.35%, for each model, respectively. Queimada et al. [13] used a model based on corresponding-states principle to predict speed of sound of several n-alkanes, including long-chains, with AAD of

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Table 1
Standard reproducibility uncertainty.

Property	Value
Density (kg/m ³)	0.46
Speed of sound (m/s)	2.4
10 ³ Wada's constant (SI)	0.002

1.6% using linear perturbation and 1.8% for 2nd-order perturbation. Freitas et al. [14] performed measurements of 3 FAMEs (fatty acid methyl ester) and 10 biodiesel fuels, and proposed a modified Auerbach model and compared the predicted speed of sound to the original Auerbach model, reporting overall AAD of 1.64% for the modified model and 9.13% for the original model.

The model to predict the speed of sound proposed in this work uses the Wada's constant that is described by Eqs. (1) and (2), where ρ is the density, M is the molar mass, u is the speed of sound and k_s is the isentropic compressibility.

$$\text{Wada} = \frac{k_s^{-1/7}}{\rho} M \quad (1)$$

$$k_s = \frac{1}{u^2 \rho} \quad (2)$$

This parameter is interesting as it is little influenced by temperature with a decreasing rate of less than 1% for a change of temperature of 100 K. Moreover, in a previous work [15] it was shown that it presented a linear behavior with respect to molecular weight for compounds belonging to same family (e.g. alkanes). Furthermore we have recently shown that the group contribution concept can be straightforwardly applied to this property and we determined contributions of groups occurring in hydrocarbons and fatty acid methyl esters and biodiesels [16]. In this work, we extend the study to include branched alkanes, esters, including acetates, FAME (fatty acid methyl esters) and FAEE (fatty acid ethyl esters), ethers, alcohols and aromatics, allowing an extension and revision of the proposed model by further enhancing the group decomposition into atoms through extensive analysis of this new atomic contribution method.

In this sense, the new model will be able to predict speed of sound of any compound pertaining to the studied classes, what allows the extrapolation of this work to substances with no experimental data available yet, as expected from any group/atom contribution group. This extension is particularly important to simulate properties of fuels, since several hundreds of substances may be identified even in a light fuel as gasoline, and for many of these substances there is no experimental speed of sound available. Also, the increasing need for renewable fuels will demand the knowledge of speed of sound of several oxygenates, and this work aims to contribute to these calculations.

2. Data of density and speed of sound

A literature review of data [10,14,16–30,15,31–126] for density and speed of sound of a variety of compounds of interest was undertaken. A list of the systems studied is presented in the supplementary data (Table S.1), comprising a total of 94 compounds including n-alkanes (18), branched alkanes (17), n-alkenes (11), aromatics (9), aliphatic alcohols (17), aliphatic ethers (3) and aliphatic esters (19).

Table 1 reports the experimental global reproducibility uncertainty, calculated according to [9], for all the compounds studied in this work, analyzing density, speed of sound and calculated Wada's constant from literature data, using Eq. (1). Besides their experimental uncertainty, it is also important to know the largest differences between the data reported by different authors for each

Table 2
The largest difference observed between different authors for the speed of sound.

Class	Density (kg/m ³)	Speed of sound (m/s)	10 ³ Wada's constant (SI)
n-Alkanes	0.8	4.5	0.006
Branched alkanes	3.8	25.0	0.020
n-Alkenes	3.4	4.0	0.015
Aromatics	3.1	9.6	0.008
Alcohols	2.2	21.0	0.006
Esters	2.1	17.0	0.010
Ethers	1.3	3.4	0.004

family as these provide another hint on the quality of the experimental data. These values are reported in Table 2.

As can be seen from comparison of Table 2 with Table 1, for many classes it is possible to find discrepancies between available data from different authors that are many times the reproducibility uncertainty in the database. Hence, literature needs more experimental data to allow for a critical analysis of the data and to eliminate inadequate data. Furthermore, these values are important to evaluate the model here proposed.

3. Results and discussions

The experimental Wada's constant values at 298.15 K were calculated from experimental density and speed of sound data using Eq. (1). This property is plotted in Fig. 1 as a function of chain length for hydrocarbon compounds and in Fig. 2 for the oxygenated families studied in this work. For n-alkenes, we found few density and

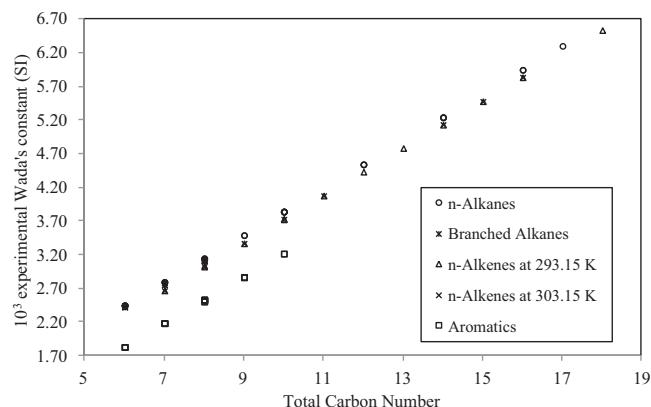


Fig. 1. 10³ Experimental Wada's constant for hydrocarbon compounds against the total number of carbons, at 298.15 K except when otherwise indicated.

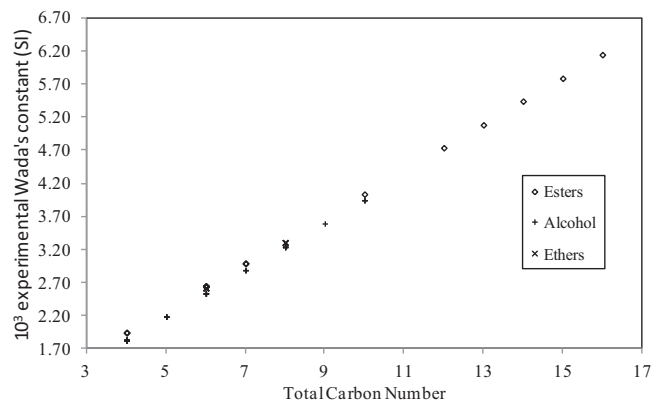


Fig. 2. 10³ Experimental Wada's constant for oxygenated compounds against the total number of carbons, at 298.15 K.

Table 3
Mean-square deviations for Wada's constant (SI) for the linear fittings.

Family	Mean-square deviation $\times 10^3$
Alkanes	0.013
n-Alkanes	0.009
Branched alkanes	0.018
n-Alkenes	0.005
Aromatics	0.007
Alcohols	0.004
Esters	0.004
Ethers	0.005

speed of sound experimental data at 298.15 K, so we represented in Fig. 1 data at 293.15 K and 303.15 K for this hydrocarbon family.

For all families in Figs. 1 and 2, we observe a linear behavior between Wada's constant and chain length. Furthermore, it is observed that these lines present approximately the same slope, i.e., they are essentially parallel. In the studied temperature range (293.15–303.15 K), no influence of temperature on alkenes Wada's constants was observed.

For each family presented in these two figures, a linear model relating the Wada's constant and total number of carbons in the compound was adjusted by the least squares method. The mean-square deviations between the Wada's constant calculated values and experimental data observed for each series are presented in Table 3.

Comparing results in Table 3 with Wada's constant standard reproducibility uncertainty presented in Table 1, one can see that, except for branched alkanes, all mean-square deviations are up to 3.5 times the standard reproducibility, which is a rather low deviation, especially when the highest discrepancies presented in Table 2 are taken into account. This result confirms the expectation of linear behavior between Wada's constant and carbon number.

However, for branched alkanes the behavior is not the same. In order to clarify the performance of the assumed linear behavior for alkanes Wada's constant, the difference between calculated values and experimental data, both at 298.15 K, are plotted in Fig. 3. The dashed lines represent the confidence interval for this difference that is calculated with a 95% confidence level from standard reproducibility uncertainty presented in Table 1.

As can be seen in Fig. 3, the hypothesis of linear dependency of Wada's experimental constant data is confirmed for the majority of the studied n-alkanes with 95% confidence level. On the other hand, deviations for branched alkanes present values that deviate considerably from the confidence region, suggesting that the linear model is limited to describe the influence of some types of branching on the Wada's constant.

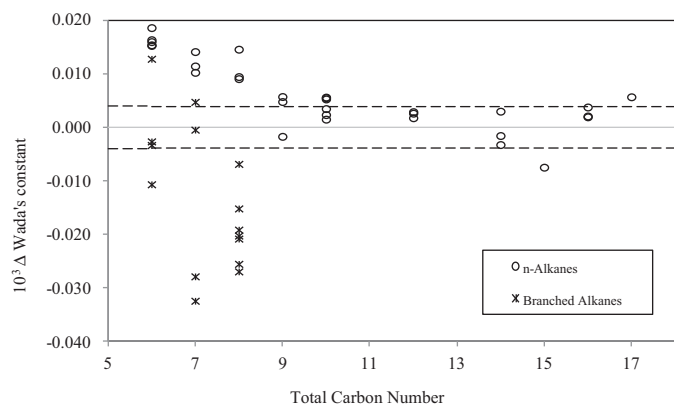


Fig. 3. Difference between experimental Wada's constant and calculated values for alkanes with the same number of carbons, at 298.15 K. Dashed lines are the confidence interval that cannot be distinguished from zero.

Table 4
Some values of experimental and predicted Wada's constants (SI) for non-linear alkanes.

Substance	10 ³ Experimental Wada's constant	10 ³ Predicted Wada's constant	Difference
2,2-Dimethylpentane	2.778	2.778	0.000
3,3-Dimethylpentane	2.746		0.032
2,4-Dimethylpentane	2.783		0.005
2,3-Dimethylpentane	2.751		0.027
3-Methylpentane	2.423	2.427	0.004
2-Methylpentane	2.440		0.013
2,2-Dimethylbutane	2.424		0.003
2,3-Dimethylbutane	2.416		0.011

Table 4 shows the values of Wada's constant for four isomers of dimethylpentane, two isomers of methylpentane, and two isomers of dimethylbutane. These values are compared with those predicted by the linear model fitted from the data set of Wada's constant to alkanes shown in Fig. 1. It is observed that for 2,2-dimethylbutane, 2,4-dimethylpentane, 3-methylpentane and 2,2-dimethylpentane at 298.15 K, linear model predictions represent Wada's constant within the confidence region, however the same is not true for 3,3-dimethylpentane, 2,3-dimethylbutane, 2-methylpentane and 2,3-dimethylpentane. Analyzing data from experimental Wada in Table 4, one can see that this property holds significant deviations between the position isomers. It is well known that first order group contribution methods are unable to predict this behavior and, therefore, second order group contribution methods have been proposed. However, there is still a considerable lack of experimental data of speed of sound for branched compounds limiting the analysis for this type of systems. Furthermore, the limited available data in the literature at the same experimental conditions present deviations of up to 0.020×10^{-3} to Wada's constant (SI), that are one order of magnitude above the standard reproducibility uncertainty found for other compounds studied in this work (Table 1).

As the analysis of branched compounds requires more experimental work to justify a more sophisticated proposal and since most of the results presented here indicate that there is a linear dependence between the Wada's constant and the number of carbons for the different families studied, this work proposes a new atomic contribution method for Wada's constant, which is simpler and demands less information than a group contribution method. For instance in an atomic based model the CH₃, CH₂, CH and C group contributions may be replaced by C (paraffinic) and H contributions.

For the development of a new atomic contribution method, it is essential to confirm the parallel dependency among Wada's constant data of the different families observed in Figs. 1 and 2. In order to verify this, the experimental Wada data for n-alkenes, aromatics, alcohol, ethers and esters were subtracted of those adjusted by the alkanes linear model with the same number of carbons. The results are shown in Fig. 4 for n-alkenes and aromatics, Fig. 5 for alcohols and ethers and Fig. 6 for esters. Bars represent the confidence interval for Wada's constant that is calculated with a 95% confidence level from the standard reproducibility uncertainty presented in Table 1.

Analyzing Figs. 4–6 it is possible to say that, with a 95% confidence, Wada experimental values of the different families of compounds studied in Figs. 1 and 2 deviate from those observed for alkanes by a constant independent of chain length. Therefore, the hypothesis of parallelism among Wada's constant data of the different families observed in Figs. 1 and 2 are corroborated for these series considering one or times the confidence interval in some cases. However, this analysis should be done with caution considering Table 2, since the literature data present high discrepancies in density and speed of sound when comparing different authors.

Table 5
Atomic contribution values for speed of sound estimation.

	C_{Par}	C_{Olef}	C_{Arom}	H	O_{Sp3}	O_{Alc}	O_{Sp2}
10^3 Wada's constant (SI)	0.0113	0.1234	0.1348	0.1694	0.1738	0.0940	0.2568
$10^3 \chi$ (K^{-1})	0.0191	0.0191	0.0191	0.0191	0.0191	-1.3064	0.3488

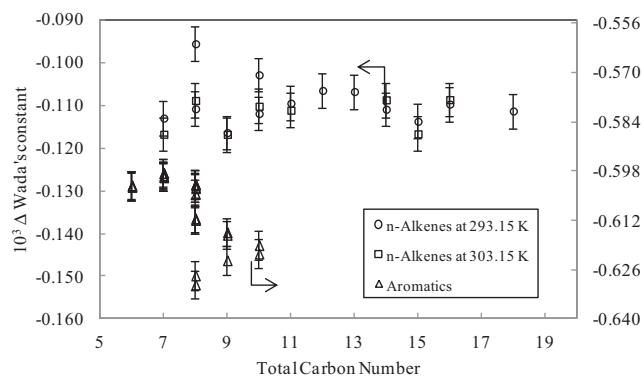


Fig. 4. Difference between experimental Wada's constant for n-alkenes or aromatics and calculated values for alkanes for the same number of carbons at 298.15 K except when otherwise indicated.

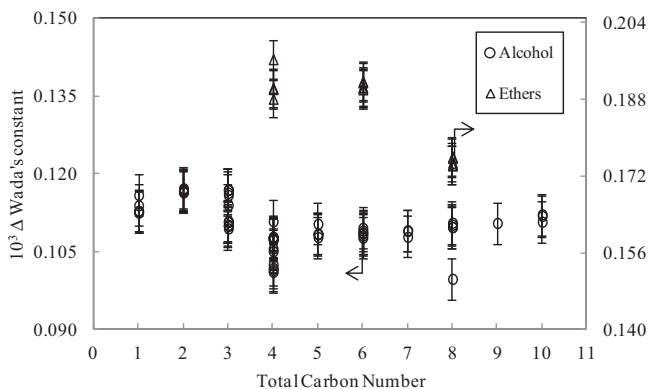


Fig. 5. Difference between experimental Wada's constant for alcohols or ethers and calculated values for alkanes for the same number of carbons, at 298.15 K.

The results above suggest that an atomic contribution method may be able to provide reliable estimative of Wada's constant within an acceptable error, with the possible exception of some branched alkanes. The increase of one carbon and two hydrogens in a series leads to the same increment to the Wada's constant regardless of the analyzed series. This increase could be obtained by the slope of the straight lines identified in Figs. 1 and 2. It is worth noting that the presence of branched esters did not lead to a different

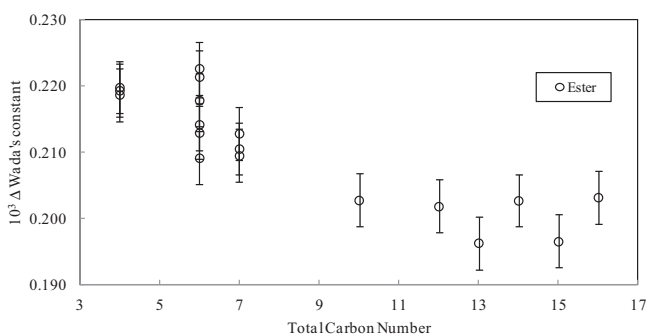


Fig. 6. Difference between experimental Wada's constant for esters and calculated values for alkanes with the same number of carbons, at 298.15 K.

behavior from that obtained with linear esters, which reinforces the concept of atomic additivity instead of group contribution of first order.

We propose thus a new model, based on atomic additivity, for calculating the Wada's constant. This new method includes seven contributions that are able to predict this property for all studied families of compounds, namely: C_{Par} (for paraffinic carbon), C_{Olef} (for olefinic carbon), C_{Arom} (for aromatic carbon), H (for hydrogen), O_{Sp3} (for ether oxygen), O_{Sp2} (for ester group, being the COO decomposed into one C_{Olef} , one O_{Sp2} and one O_{Sp3}), and O_{Alc} (for alcohol oxygen). This work uses the parameter χ , proposed in our previous work [16], to incorporate the effect of temperature on Wada's constant.

The new atomic contribution method for calculating the Wada's constant is based on the following equation

$$\text{Wada} = \sum_a v_a \text{Wada}_a (1 - \chi_a (T - 298.15)) \quad (3)$$

where v_a is the atom occurrence, Wada_a is the atom Wada's constant contribution at 298.15 K, χ_a is the atom linear temperature correction parameter and a runs over all atoms, however the only different values for χ_a are for O_{Alc} and O_{Sp2} , for others atomic contributions it has the same value.

Using the proposed method (Eq. (3)) along with Eqs. (1) and (2), after rearrangement the working equation for speed of sound is presented in Eq. (4).

$$u = \left[\frac{\rho^{6/7}}{M} \sum_a v_a \text{Wada}_a (1 - \chi_a (T - 298.15)) \right]^{7/2} \quad (4)$$

The atom Wada's constant contributions were obtained by least squares method to correlate speed of sound of n-alkanes, n-alkenes, aromatics, alcohols, saturated esters and ethers. It is worthwhile to mention that for the isomer *o*-xylene the experimental Wada's constant is very discrepant from those of the other isomers *p*- and *m*-xylene, and therefore this isomer was not used in the calculations. Also, this work limited the range of temperature for 288.15–343.15 K, since very few data were found at higher temperatures, at which the behavior of Wada's constant with temperature is quite dissimilar for the few data found. Adjusted Wada's constant contributions are presented in Table 5 while speed of sound mean-square deviations and AAD for each compound family is presented in Table 6.

In order to test the predictive performance of the new contribution method, speed of sound for FAEE and unsaturated FAMES and

Table 6
Results of mean-square deviations for calculated speed of sound using Wada's atomic contribution model.

Class	Mean-square deviations (m/s)	AAD (%)
n-Alkanes	3.4	0.22
n-Alkenes	7.2	0.48
Aromatics	8.4	0.54
Alcohol	9.0	0.61
Ethers	7.0	0.68
Saturated FAME and acetates	6.5	0.45
Global	6.8	0.42
FAEE	4.8	0.32
FAME and FAEE unsaturated	2.8	0.17

one FAEE were calculated with parameters presented in Table 5. Speeds of sound mean-square deviations and AAD for these families are also presented in Table 6.

The global deviation in the parameter estimation is only three times the experimental uncertainty in speed of sound, which is a quite reasonable result for this predictive approach. The extrapolation to saturated FAEE and unsaturated FAME and FAEE led to better deviations than those obtained in the parameter estimation, showing the quality and strength of our proposal. Analyzing the AAD, we have found that the atomic contribution Wada's atomic model is able to accurately predict the studied speeds of sound, with results compatible to, or better than, those obtained in the literature with correlative models.

4. Conclusions

In this work we have gathered literature data for speed of sound and densities of n-alkanes, branched alkanes, n-alkenes, aromatics, alcohols, ethers and esters, including short acetates, saturated and unsaturated FAMES and FAEEs and analyzed the data in the light of the Wada's constant.

Wada's constants for the major n-alkanes and some branched alkanes are estimated within experimental uncertainty with a linear model depending only on the number of carbons. However, Wada's constants of some position isomers present deviations significantly larger than the experimental uncertainty. First order group contribution methods are not able to distinguish between those isomers, and atomic contribution methods are also unable to distinguish them. Only second order group contribution methods can provide different results for these isomers. Due to the scarcity of data for branched molecules, the second order group contribution method was discarded, and the atomic contribution method was preferred to the first order group contribution, since the former method is simpler to use, demanding less parameters than the second.

The proposed model was used to correlate speed of sound of n-alkanes, n-alkenes, aromatics compounds, alcohol, ethers, saturated esters and acetates, with a root-mean-square deviation of 6.7 m/s and overall AAD of 0.47%, which are comparable to, or better than, those obtained in the literature with other correlative models. The extrapolation to unsaturated FAME, saturated and unsaturated FAEE led to deviations smaller than that obtained in the parameter estimation, showing the quality and strength of our proposal.

Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at <http://dx.doi.org/10.1016/j.fluid.2013.08.014>.

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