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Determination of CO_2 solubility in *Perna perna* mussel and analysis of the suitability of the ideal and non-ideal gas models

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ABSTRACT

In *SGS* (*Soluble Gas Stabilization*) processes, the carbon dioxide (CO_2) is dissolved into the food product under controlled temperature, pressure, and gas/product ratio. The prediction of CO_2 solubility can be achieved using a computational code using equations of state from experimental data on CO_2 concentration in food. In this work, the solubility of CO_2 in *Perna perna* mussels was obtained using Ideal Gas law and Virial, Van der Waals, Soave-Redlich-Kwong, and Peng-Robinson equations. The SGS process was performed at varying system pressure (200–600 kPa), temperature (0–6 °C), and gas/product (g/p) (mussels) ratio (1:1–5:1) in the cooked and shucked mussels for 65 h. A total of 11 experiments, arranged in a 2^3 experimental design, with triplicate runs at the central point, were performed. The compressibility factor indicated that the Ideal Gas state is a good approximation only for experiments 1, 2, 5, and 6. It was observed that the pressure and the gas/product ratio exert a more significant influence on the CO_2 solubilization process in the mussel. Visual Basic for Applications (VBA) to perform thermodynamic calculations showed to be a great resource regarding complex calculations.

1. Introduction

Soluble gas stabilization (SGS) is a process proposed by Sivertsvik et al. [1] where the CO_2 is solubilized into non-respiring foods before packaging as an alternative to modified atmosphere packaging (MAP). During the SGS process, the CO_2 is dissolved into the liquid phase of food until it reaches equilibrium. Although, studies of the solubility of CO_2 in water and non-respiring food have been done to avoid the package collapse due to the prior dissolution of CO_2 into the food product [2–4,1,5,6]. After the dissolution of CO_2 into the food reaches its equilibrium, it decreases the concentration gradient between the food and CO_2 at the gaseous phase, which may cause the package to collapse [7].

Then, the prior dissolution of CO_2 is used as an alternative method to reach equilibrium and maintain package integrity before the decreasing concentration gradient begins to influence gaseous flow. According to Esmaeilian et al. [8], SGS is a new technology aligned with sustainable objectives. It increases packaging efficiency, reduces distribution costs, decreases the number of plastic materials used for packaging, extends food shelf life, reduces food loss, and opens new opportunities for related industries.

The CO_2 absorption mechanism considers ideal gas law, during SGS in *Perna perna* mussel, through several conditions of pressure, temperature, and gas to product (g/p) ratio was evaluated by Lima et al. [9]. This phenomenon of CO_2 diffusion in a solid matrix is more complex than diffusion in a liquid or a gas, as the diffusion of CO_2 in the solid matrix is apparent [10]. For this matter, it is considered that the CO_2 can be dissolved in the water content of the food to form carbonic acid (H_2CO_3), which is dissociated into bicarbonate (HCO_3^-), carbonate (CO_3^{2-}) and hydrogen (H^+) [11]. From this reaction, there are changes in pH, which is the base for a theory that states the decrease in the respiratory rate of microorganisms as the main factor to the CO_2 bacteriostatic effect [10].

Lima et al. [9] determined CO_2 solubility in cooked mussels (*Perna perna*) through different gas-product ratios (g/p 5:1, 3:1, and 1:1), temperatures (0, 3, and 6 °C), and pressures (200, 400 and 600 kPa), considering an ideal gas situation through ideal gas law (Eq. (1)). In addition, the same authors used a system with constant volume (526 cm^3). They considered the absorption of CO_2 through the mass variation in the

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gaseous medium as a function of the pressure variation (in the same way as in rigid packages) based on the equation described by this situation by Simpson et al. [10]. The condition of higher pressure (600 kPa) and higher g/p rate (5:1), combined with lower temperature (0 °C), showed more CO_2 impregnation in the water content of the cooked mussels.

Lima et al. [9] modeled this distribution phenomenon under ideal conditions using Henry's Law. This theory of modern thermodynamics is documented in the literature for its experimental determination and significance in air-water systems [12].

It is known that the CO_2 solubility processes become faster under higher pressure conditions [13,14] in this low-temperature range [1]. However, due to the non-ideal behavior under these conditions, the ideal gas law fails to predict the CO_2 solubility. Thus, some Equations of State (EOS) could be used to correct the prediction of CO_2 solubility for experiments where the gas has a non-ideal behavior. The Equations of State chosen to perform calculations in this work were: Van der Waals (Eq. (2)) – [30]; Virial (Eq. (3)) – Onnes [15]; Soave-Redlich-Kwong (Eq. (4)) – Soave [16]; and Peng-Robinson (Eq. (5)) – Peng & Robinson [17].

$$P \cdot V = n \cdot R \cdot T \tag{1}$$

$$\left(P + \frac{a}{V^2}\right)(V - b) = RT \tag{2}$$

$$\frac{PV}{RT} = 1 + \frac{B(T)}{V} + \frac{C(T)}{V^2} + \frac{D(T)}{V^3} + \ldots \tag{3}$$

$$P = \frac{RT}{V} - \frac{\alpha \cdot a}{V(V + b)} \tag{4}$$

$$P = \frac{RT}{V - b} - \frac{\alpha \cdot a}{V(V + b) + b(V - b)} \tag{5}$$

where P is pressure, V is volume, n is the number of moles, R is the universal gas constant, T is temperature, and the other letters are parameters of each equation.

Solubility can be determined using Eqs. (1), 2,3,(4), and (5) from experimental data on CO_2 concentration in mussels using a computational code. Microsoft Excel is a prevalent mathematical tool that allows Visual Basic for Application (VBA) programming. It has emerged as an alternative to simplify simulation processes and take computer operations to a more accessible and friendly platform [18,19].

It is known that the VBA is not a state-of-art programming language, even for thermodynamics. However, it has shown to be a great resource regarding complex calculations involving a high amount of data, which several authors have also reported in the last years [20–22,18,23,19]. Still, the approach taken by this paper through the development of a VBA code is another step to optimize problem-solving and bring calculation program users to the awareness of the technology resources available.

Therefore, this work aimed to calculate the CO_2 solubility in *Perna Perna* mussel using Equations of State through developing a VBA code valid for both ideal and non-ideal gas conditions verifying the compressibility factor of the experimental tests.

2. Material and methods

2.1. Sample preparation

The *Perna perna* mussels were washed and cleaned, cooked at 100 °C for 6 min to open the shells, cooled with iced water at 10 °C for 10 min, and manually peeled before being submitted to the SGS process.

According to Lima et al. [9], the apparent specific gravity of *Perna perna* mussels obtained by fluid misplacement was 1040 kg m^{-3}.

2.2. Experimental apparatus

The SGS process was performed in a stainless-steel cylindrical vessel (526 cm^3). The mussels were introduced into the apparatus, and carbon dioxide - CO_2 (Linde, 0.999-mole fraction purity, Brazil, CAS number 124-38-9) was injected for 65 h, meanwhile temperature was controlled by a jacketed system linked to a thermostatic bath (variation of ±0.5 °C) (Quimis, 6214m^2, Brazil), according to Lima et al. [9].

The cylindrical vessel consisted of two thermocouples J type (Salvi Casagrande – Brazil) used to measure product and gas temperatures (variation of ±0.4 °C). Gas inlet and outlet were performed by needle-type valves (Swagelok, Brazil) connected to a CO_2 cylinder (Linde, 0.999-mole fraction purity, Brazil, CAS number 124–38–9) and a gas analyzer (Checkmate II, PBI-Dansensor, Denmark) respectively. The adjustment of the gas analyzer allowed a continuous determination of the gas composition. A pressure transducer (Warme WTP-4010, 0–10 V, Brazil) allowed obtaining the total pressure on the system (pressure was measured in V(volts) - the potential difference given by the pressure transducer connected to the data acquisition system, with $1 \cdot 10^{-3}$ V accuracy). An acquisition data system collected data every 30 s of the experiment (Agilent, Data Acquisition 34970A, USA) through Benchlink Data Logger 3.0 software.

The application of the model is necessary to obtain the experimental data, since the apparatus detailed in the methodology mentions the conditioning of the cooked mussels, kept at the temperatures predicted by the experimental design and these mussels are subjected to different pressures of pure CO_2 in the system.

Experimental development consists of two steps: (i) cooking the mussels; and (ii) exposing them to an environment rich in carbon dioxide. Then, data on the partial pressure of CO_2 in the headspace of the system is experimentally collected. It is important to emphasize that the results are obtained in millivolts and then converted to pressure, as mentioned earlier.

The execution of the experimental procedure is not enough to directly obtain the CO_2 concentration in the system. Therefore, the pressure data collected are submitted to the calculation procedure, in which the experimental pressure data are used to obtain the other answers, as illustrated in the flowchart of Fig. 1. The mathematical adjustment and data programming of this study was performed in VBA Excel 2016, which allows getting the answers even if the system is not in ideal condition. It is noteworthy that the program, entitled ATM_SOLUB, was registered at the National Institute of Industrial Property (INPI - Brazil, registration number 512018051784-6).

During the experimental tests in the hermetically closed system, the initial fraction of carbon dioxide added to the apparatus, expressed by the variation of the total pressure in the CO_2 gas phase during the period, was determined. The experimental data were collected until the total pressure reached stability. In this condition, the CO_2 solubilization is in thermodynamic equilibrium. The molar fraction of CO_2 also needs to be calculated indirectly. Because this is necessary using the Equations of State with the pressure data given by the experiment.

2.3. Solubility of CO_2 in mussels

The mass balance for the determination of carbon dioxide dissolved into the water followed some considerations taken by Lima et al. [9]: i) hermetically sealed system; ii) N_2 and O_2 flow and secondary reactions products can be neglected, considering only CO_2 dissolution as the main proceeding; iii) ideal gas for low pressures and non-ideal gas behavior for high pressures; iv) water steam pressure can be despised (low temperatures range); v) total pressure variation yields CO_2 mass variation on gaseous phase [4,1,5].

Considering the stated, rearrangements made by Sivertsvik et al. [1,5] resulted in an equation able to calculate absorbed CO_2 at equi-

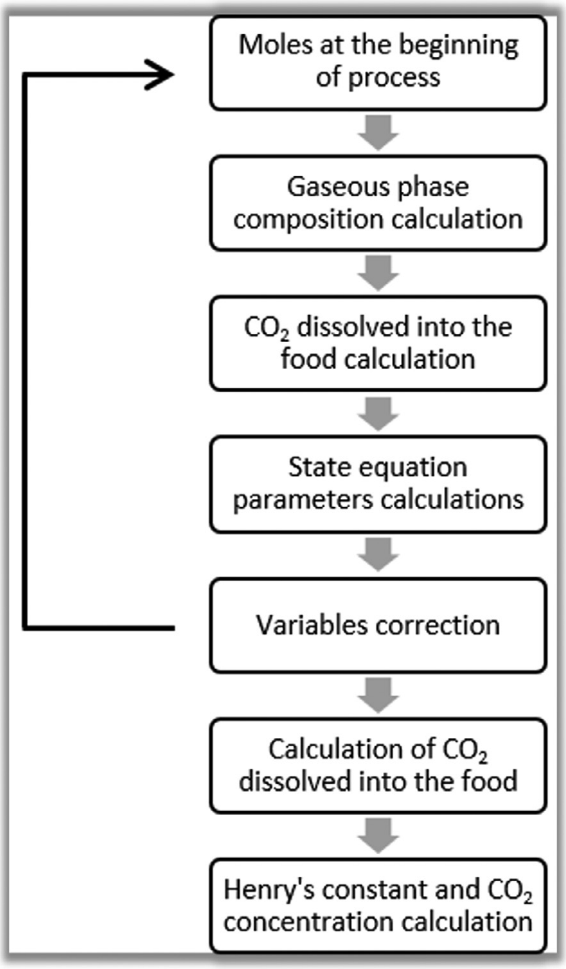

Fig. 1. Data programming flowchart to obtain CO_2 concentration from SGS experiments.

librium:

$$C^{t=\infty}_{pred\ CO_2} = \frac{\frac{g}{p} \cdot \left(P^{t=0}_{CO_2} - P^{t=\infty}_{CO_2}\right) \cdot M_{w_{CO_2}}}{RT\rho_p} \quad (8)$$

where $\frac{g}{p}$ represents gas to product ratio (volume base), $P^{t=0}_{CO_2}$ and $P^{t=\infty}_{CO_2}$ are pressure at the beginning and at equilibrium, $M_{w_{CO_2}}$ is the molecular weight (kg kmol^{-1}) of CO_2, R is the universal gas constant (J mol^{-1} K^{-1}), T is the temperature (K), and ρ_p is the density of mussels (kg m^{-3}).

Still, Henry's law can be used to express dissolved CO_2 at equilibrium according to Eq. (9) – Sivertsvik et al. [1,5] According to Carroll et al. [24], this equation relates Henry's constant with the CO_2 concentration absorbed by the water during exposure to the gas. It can be identified by the variation of the partial pressure of carbon dioxide from the initial period of the experiment until reaching thermodynamic equilibrium (stabilization of CO_2 concentration).

$$P^{t=\infty}_{CO_2} = H_{CO_2} \cdot C^{t=\infty}_{CO_2} \quad (9)$$

where H_{CO_2} is Henry's constant of CO_2 (Pa.ppm^{-1}) in the liquid phase (water) and $C^{t=\infty}_{CO_2}$is the concentration of CO_2 dissolved into the liquid phase of the food at equilibrium (ppm), which can be obtained from the moles of difference between initial and final moles of CO_2 in the system according to Eq. (10).

$$n^D_{CO_2} = n^i_{CO_2} - n^f_{CO_2} \quad (10)$$

where $n^D_{CO_2}$ is the number of moles of CO_2 dissolved into the liquid phase of mussels, $n^i_{CO_2}$ and $n^f_{CO_2}$ are the numbers of moles of CO_2 available at the headspace at the beginning and the equilibrium, respectively. The number of moles of CO_2 from both periods can be obtained from Eq. (11).

$$PV^G = Zn_{CO_2}RT \quad (11)$$

where V^G is the volume of gas, Z is the compressibility factor (dimensionless), and n_{CO_2} is the CO_2 number of moles.

Eq. (12) optimizes Henry's constant according to Rotabakk et al. [25], which consider that the dissolution of CO_2 in the SGS process is exclusively performed in the water content of the food. This can be assumed because of the low-fat content of the mussel's tissue [25].

$$H_{CO_{2,p}} = \frac{H_{CO_2}}{X_w} \quad (12)$$

where H_{CO_2} is CO_2 Henry's constant in water, X_w is the moisture content of the food (moisture -% in wet basis), and $H_{CO_{2,p}}$ represents a correction to the Henry's constant for the product according to the moisture content.

As CO_2 concentration is dependent on the ideality or non-ideality range of the experiments, it should be clear that, for the Ideal Gas state, $Z = 1$ on Eq. (11). About the compressibility factor, it is well known that at moderate temperatures, its value is usually <1, though, at elevated temperatures, it may be >1; at low pressure, Z approaches 1, and at moderate pressures, Z decreases roughly linearly with pressure [26]. So, for experiments where pressure is considerably higher ($Z \neq 1$), the concentration of CO_2 is expressed through the molar fraction of gas into a liquid and gaseous phase in the system, as described by Eq. (13).

$$y_{CO_2}\varphi^v_{CO_2}P = x_{CO_2}H_{CO_2} \quad (13)$$

where y_{CO_2} and x_{CO_2} are CO_2 molar fractions in the gaseous and liquid phase, $\varphi^v_{CO_2}$ is the fugacity coefficient of CO_2 in the gaseous phase, P is pressure, and H_{CO_2} is Henry's constant in the liquid phase (water).

Eq. (13) addresses the need to correct non-ideality conditions, using the fugacity concept to correct the value of partial pressure of CO_2 in the system. It assumes a validity of Henry's Law for the solubility in a gas-liquid binary system for the lightest component, allowing correspondent correlation or Equations of State (EOS) to describe the non-ideal gas behavior. Carroll et al. [24] researched the restrictions on applying Henry's Law to the solubility of CO_2 in water in the food literature. The authors proposed a model based on Henry's Law that correlates data to pressure (below 1 MPa) based on these data. The authors consider the equality of fugacity between solvent and solute, with some simplifications.

The fugacity coefficient of CO_2 in the system and mussels Henry's constant were obtained according to Lima et al. [9]. Based on Dalmolin et al. [13], iterative calculations from each initial and final pressure were obtained and inserted into the program to obtain CO_2 solubility. Calculations considering ideal gas law (Eq. (1)) and the four Equations of State (Eqs. (2) to (5)) were performed in this work. The pressure values used in this work were 200, 400, and 600 kPa, temperatures used were 0, 3, and 6 °C, and gas/product ratios were 1:1, 3:1, and 5:1 (volume ratio) in a 2^3 experimental design according to Table 1.

2.4. VBA routines

The VBA routines consider the Ideal Gas equation and four other state equations (Virial, Van der Waals, Soave-Redlich-Kwong, and Peng-Robinson) to determine CO_2 solubility in a food product. It consists of thermodynamic equations used to calculate the number of mols involved in a gas-liquid equilibrium process, considering that the dissolution of CO_2 occurs only in the aqueous phase of the product.

To calculate the solubility, in addition to the molar mass of CO_2 (g/mol), it is necessary to provide the data of the medium in which the gas dissolves (mussels), such as i) water content (moisture -% in wet basis) and product density (kg/m^3); ii) temperature (K) and pressure (initial and final) of the process (kPa); iii) proportion of product and gas in

Table 1
Range of variables to CO_2 solubility determination in *Perna perna* mussels (Adapted from [9]).

Trial	Pressure (kPa)	Temperature (°C)	g/p ratio (v/v)
1	200	0	1
2	200	6	1
3	600	0	1
4	600	6	1
5	200	0	5
6	200	6	5
7	600	0	5
8	600	6	5
9	400	3	3
10	400	3	3
11	400	3	3

Table 2
Compressibility factor results for the different equations used in the study.

Trial	Virial	Van der Waals	Soave Redlich Kwong	Peng Robinson
1	0.9865	0.9895	0.9869	0.9870
2	0.9874	0.9900	0.9877	0.9879
3	0.9595	0.9679	0.9598	0.9604
4	0.9623	0.9696	0.9625	0.9630
5	0.9865	0.9895	0.9869	0.9870
6	0.9874	0.9900	0.9877	0.9879
7	0.9595	0.9679	0.9598	0.9604
8	0.9623	0.9696	0.9625	0.9630
9	0.9740	0.9794	0.9744	0.9747
10	0.9740	0.9794	0.9744	0.9747
11	0.9740	0.9794	0.9744	0.9747

the medium (g/p ratio); iv) thermodynamic constants of each equation; and v) the constant volume of the medium in which the process occurs. All this information was provided in the Excel Worksheet table created to work together with the VBA routines. Once the data is specified, the user can run each routine separately (for each interest equation) since each spreadsheet is linked to a unique code. The CO_2 concentration results are given in the subsequent columns to the input data from the execution.

3. Results and discussion

3.1. Compressibility factor

As previously stated, the VBA code developed in this work allows the determination of the concentration of CO_2 considering Ideal Gas law, Virial, and cubic equations (Van der Waals, Soave-Redlich-Kwong, and Peng-Robinson). It is essential to know the compressibility factor results for each of the trials of the experimental design (Table 1).

Through the Equations of State, it is possible to obtain the compressibility factor (Z) value and correct the calculations in cases of non-ideality. The virial equation is applied to predict the properties in the vapor phase, and if truncated in the second term (more usual), it can be used for low and moderate pressures ($P \leq 1.01$ MPa). It also presents a generalized form, allowing the adjustable parameters to be calculated through the critical properties of the substances.

The Equation of Soave-Redlich-Kwong was proposed by Soave [16] to improve the Redlich-Kwong Equation of State and is widely used in simulation and thermodynamic modeling of processes. The Peng Robinson equation has applicability for calculating the vapor-liquid equilibrium of various mixtures, including hydrocarbons and gasses such as hydrogen sulfide and carbon dioxide.

The Thermodynamic models with Equation of State are good tools to evaluate the solubility behavior at higher pressures. The thermodynamic models with Equations of State are good tools to evaluate the solubility behavior at higher pressures. These equations accurately predict the solubility of CO_2 in aqueous solutions [27].

The results for the compressibility factor are listed in Table 2.

The Ideal Gas state is a reasonable approximation to reality when the value of Z is close to 1. Based on this, Table 2 suggests that the Ideal Gas state is a good approximation only for experiments 1, 2, 5, and 6. Consequently, the need for equations that provide more reliable results is now clear, unlike the Ideal Gas Law.

3.2. CO_2 solubility in mussels and a comparison to ideal gas law

The results for CO_2 solubility obtained in the VBA code developed in this work for Ideal Gas law, Virial, Van der Waals, Soave-Redlich-Kwong, and Peng-Robinson equations are presented in Fig. 2.

As expected, for experiments 1, 2, 5, and 6, the results for all equations are within the error range, which means that the Ideal Gas Law could be a good approximation to obtain the solubility of CO_2 in mussels under the circumstances of this study. In general, the results of CO_2 solubility are similar (within the error range) for Virial and the three cubic equations of state under evaluation (Van der Waals, Soave-Redlich-Kwong, and Peng-Robinson).

As reported by Lima et al. [9], the highest dissolved CO_2 concentration in mussels was obtained at the highest g/p ratio (5:1) and pressure condition (600 kPa) for treatments 7 and 8. Under these conditions, there were significant differences between the Ideal Gas condition and the other equations; besides, the Virial equation presented the highest deviations compared to Ideal Gas. For the experimental conditions used in this study (pressure, temperature, and g/p ratio), the Ideal Gas state is not a reliable approximation for experiments using higher pressures (experiments 3, 4, 7, and 8), which presented higher deviations compared to the other EOS. The slightest deviations were achieved in the lower pressures when comparing Ideal Gas and other EOS.

Analyzing the thermodynamic equations involved in this phenomenon, Smith et al. [26] describe that the PVT behavior of gasses under near ambient conditions for T and P is contemplated by the Ideal Gas Law, and for higher pressures and lower temperature conditions, pronounced deviations occur. The cubic Equations of State (often also called semi-empirical Equations of State) can be appropriately used, considering the critical compressibility factor Zc equal for all substances. The same authors emphasize that Zc data are obtained through experimental values of Tc, Pc, and Vc, resulting in different values found for different equations.

Based on Fig. 2, all the equations led to similar CO_2 concentration results, except for higher pressure conditions (where the Ideal Gas Law is not a good approximation to obtain the solubility of CO_2 in mussels under the circumstances of this study). Thus, experimental data obtained with Soave-Redlich-Kwong model were subjected to a multiple regression to fit an empirical model.

In this regression, the independent variables were transformed into the dimensionless form according to Eq. (14) for pressure, Eq. (15) for g/p ratio and Eq. (16) for temperature. The analysis of regression parameters was performed at a 5% significance level in a Student's t-test.

$$X_1 = \frac{P[kPa] - 400}{200} \tag{14}$$

$$X_2 = \frac{g/p\left[m^3/m^3\right] - 3}{2} \tag{15}$$

$$X_3 = \frac{T[K] - 276.15}{3} \tag{16}$$

Eq. (17) represents the fitted equation with the variables that had a statistically significant effect on the responses for the experimental data using Soave-Redlich-Kwong Equation of State ($R^2 = 0.9970$). The residual analysis of this regression shows that the residuals are independently and identically distributed according to a normal distribution with mean zero and fixed variance.

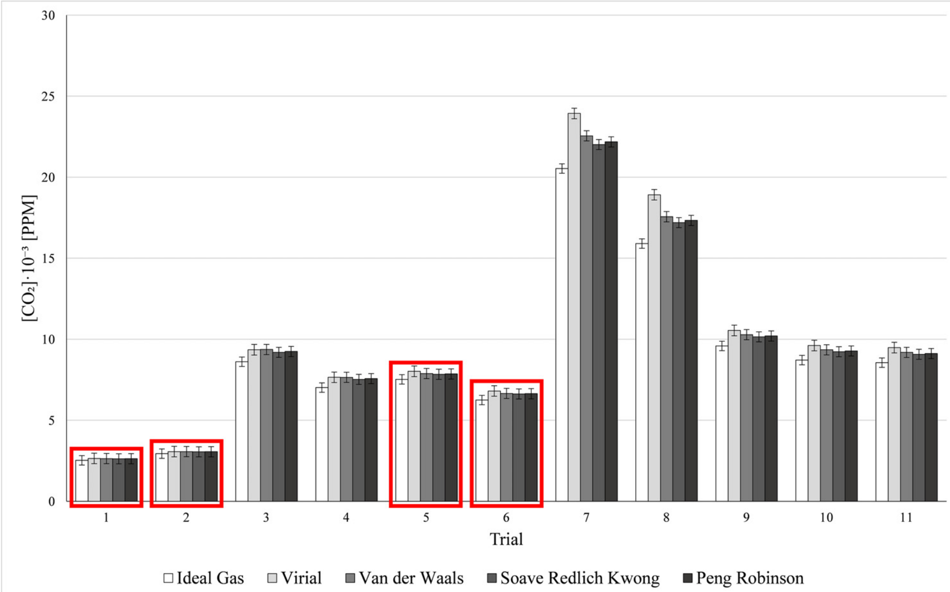

Fig. 2. Calculated CO_2 solubility using the VBA code. The indices from 1 to 11 on the abscissa axis refer to the experimental conditions presented in Table 1.

Table 3
Responses for the 2^3 experimental design in terms of CO_2 concentration dissolved at equilibrium using the Soave-Redlich-Kwong Equation of State.

Trial	$[CO_2]$ calculated (mg $CO_2 \cdot kg^{-1}$)	$[CO_2]$ predicted (mg $CO_2 \cdot kg^{-1}$)
1	2623.50	2430.00
2	3054.99	3234.00
3	9193.60	9376.00
4	7525.71	7332.00
5	7839.44	8022.00
6	6623.65	6430.00
7	22,013.47	21,820.00
8	17,197.51	17,380.00
9	10,152.27	9503.00
10	9233.12	9503.00
11	9073.73	9503.00

$$CO_2^{t=\infty} = 9503 + 4474 \cdot X_1 + 3910 \cdot X_2 - 909 \cdot X_3 + 1713 \cdot X_1 \cdot X_2 - 712 \cdot X_1 \cdot X_3 - 599 \cdot X_2 \cdot X_3 \quad (17)$$

Table 3 presents the responses of CO_2 concentration dissolved at equilibrium for the 2^3 experimental design using the Soave-Redlich-Kwong Equation of State.

The predicted values were obtained by evaluating the difference in process performance caused by changing from the low (−1) to the high (+1) level of the corresponding factor. The aforementioned R^2 value indicated that 99.7% of the CO_2 concentration dissolved at equilibrium using the Soave-Redlich-Kwong Equation of State was explained by Eq. (17).

The CO_2 solubility in a food product depends on the process variables (pressure, temperature, g/p ratio) and characteristics of the food product, such as moisture and lipid content, pH, and porosity. Sivertsvik et al. [5] achieved a CO_2 concentration of 2654 mg CO_2 kg^{-1} for raw salmon fillets at 0 °C, 150 kPa, and g/p of 3.84. For a cooked meat sausage, an average concentration of 1533 mg $CO_2 \cdot kg^{-1}$ was found in a SGS process performed from 100 to 200 kPa, 0 to 8 °C, and a g/p ratio from 1.7 to 3.9 [4]. Chicken drumsticks were able to absorb 567 mg CO_2 kg^{-1} at atmospheric pressure, 3 °C, and a g/p of 3:1 [28], a considerable low value compared to CO_2 solubility in mussels and salmon, for example, which is a result of both sample singularities and process variables. These studies have been considered only the ideal conditions.

Lima et al. [9] observed that the lower the temperature, the greater is CO_2 dissolved into the mussels, showing a behavior inversely proportional to CO_2 solubility in the liquid phases with the temperature [14,29]. However, the efficiency of packaging under a modified atmosphere can be increased in the non-respiring products, especially seafood, for an adequate gas-product (g/p) ratio, expressed on a mass basis. Thus, it is possible to guarantee the bacteriostatic effect of CO_2 and prevent the collapse of packaging. For seafood, it is recommended a g/p ratio of 2:1 to 3:1 [6].

4. Conclusion

In this paper, a VBA code was proposed to solve complex thermodynamic calculations involving estimating the solubility of CO_2 in *Perna Perna* mussel, using the Ideal Gas equation and four other EOS (Virial, Van der Waals, Soave-Redlich-Kwong, and Peng-Robinson). Using a generalized correlation within the Excel spreadsheet, the compressibility factor was calculated for all experimental conditions, and the Ideal Gas state is a good approximation only for experiments 1, 2, 5, and 6. The mean deviation of CO_2 concentration between the Ideal Gas equation and Soave-Redich-Kwong equation for experiments 1, 2, 5, and 6 was 4.35%. In comparison, the mean deviation for the other trials was 6.74%, confirming that the compressibility factor calculus is an essential contribution to the developed VBA code.

Among the conditions evaluated, the highest solubility values obtained in mussels occurred in experimental conditions 7 and 8, demonstrating the most significant influence of pressure and gas/product ratio in the solubilization of CO_2 in this product.

The VBA routines showed to be an excellent resource for the complex calculations of this study, as it presents a friendly language and generates rapid and reliable results. The development of the VBA in the well-known Microsoft Excel may be a facilitator point regarding its use in food industries to improve processes, implement optimization study cases, and production planning and control of operation units.

Declaration of interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

Danylo de Oliveira Silva, Laura Luiza Ferreira Cavalcanti, Marieli de Lima has patent "ATM_SOLUB" issued to Computer Program Application in Brazil. Registration number: 512018051784-6, registration data:

08/09/2018, Institution of registration: INPI - National Institute of Industry Property.

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