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**DEVELOPMENT OF A VBA CODE FOR HENRY'S CONSTANT
DETERMINATION IN *Perna perna* MUSSELS SOLUBILITY STUDIES**

PATOS DE MINAS

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Perna perna MUSSELS SOLUBILITY STUDIES*

Trabalho de Conclusão de Curso apresentado à disciplina de Trabalho de Conclusão de Curso II do curso de graduação em Engenharia de Alimentos da Faculdade de Engenharia Química da Universidade Federal de Uberlândia.

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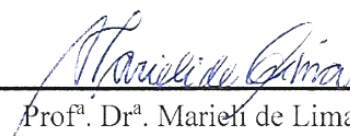
**DEVELOPMENT OF A VBA CODE FOR HENRY'S CONSTANT
DETERMINATION IN *Perna perna* MUSSELS SOLUBILITY STUDIES**

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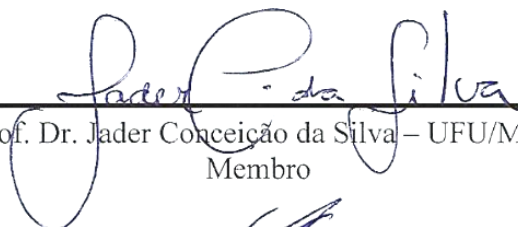
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ABSTRACT

Dissolution of carbon dioxide (CO₂) into food products is dependent of several parameters of process to be greatly performed. A novel process that has been developed to avoid packaging collapse during application of Modified Atmosphere Packaging (MAP) consists on the prior dissolution of CO₂ into the food under controlled temperature, pressure and gas/product ratio. This process is denominated *SGS (Soluble Gas Stabilization)*, and it aims to increase shelf life of products under MAP. In this paper, routines in Excel using VBA language are developed in order to obtain Henry's constant and CO₂ concentration in *Perna perna* mussels under a combination of parameters of temperature (0, 3 and 6°C), pressure (200, 400 and 600 kPa), and gas/product ratio (1:1; 3:1 and 5:1). Routines are developed for ideal gas law and four state equations (Virial, Van der Waals, Soave-Redlich Kwong and Peng-Robinson) calculations. Results show that pressure and g/p are variables that proportionally influenced CO₂ into the mussels during SGS process. Ideal gas law presented the best fit for the data and parameters used in this work, correlating to the considerably low values of pressure. VBA codes present a great resource for complex calculations as it generate rapid results, and is settled in the well-known Microsoft Excel, which may be a facilitator point regarding its use.

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1. INTRODUCTION

Modified atmosphere packaging (MAP) is a food conservation method that has gained attention from the food industry for both its performance in extending the shelf life and its capacity of maintaining the sensorial aspects of the product, such as appearance, texture and taste, as well as the nutritional value of the food (Embleni, 2013). MAP works with the replacement of the natural air composition in a package by a specific gas or a mixture of gases at a determined gas to product (g/p) ratio in a volume base (Silliker & Wolfe, 1980). For non-respiring foods, the use of CO₂ at headspace of packages has an important inhibitive effect on bacterial growth mainly through pH changes, and depends on initial microorganism load, CO₂ concentration and gas/product ratio, storage temperature, and nature of the food (Embleni, 2013; Genigeorges, 1985; Sivertsvik et al., 2004; Soccol & Oetterer, 2003).

The bacteriostatic effect of CO₂ lands on the exponential phase, at which the growth rate is decreased and the development of microorganisms is retarded (Farber, 1991; Reddy et al, 1992). Daniels et al (1985) describe premises by which CO₂ could act on bacterial cells, such as alterations in cell membranes, inhibition of enzymes, changing in the intracellular pH and, consequently, modification in physicochemical properties of proteins. The concentration of the gas influences directly on the quality of the process, as certain CO₂ amounts in the headspace may lead to a packaging collapse (Parry, 1993). The collapse of the package happens with the dissolution of CO₂ in wet food. Considering that dissolved CO₂ occupies less volume than gaseous CO₂, once the gas is dissolved and trapped into the food, the decrease on the volume of the headspace tends to shrink the package (Sivertsvik et al, 2004). For this reason, g/p ratio in which gaseous phase is at least 50% of the package is used in MAP with wet and fatty food products to keep CO₂ bacteriostatic effect and to avoid package collapse (Embleni, 2013; Sivertsvik et al, 2004), even though this parameter does not completely guarantee the integrity of the package for long periods.

Sivertsvik et al (2004) proposed an alternative atmosphere packaging for non-respiring foods in which CO₂ is dissolved into the food product before packaging at different temperatures and pressures. This novel method is denominated soluble gas stabilization (SGS), and it aims to avoid the package collapsing through the prior dissolution of CO₂ into the food product (Sivertsvik et al, 2004). Once the dissolution of CO₂ into the food reaches its equilibrium, the gradient of concentration between the food and CO₂ at gaseous phase decreases, which may cause the package collapse. Then, the prior dissolution of CO₂ is used as

an alternative method to both reach equilibrium and maintain package integrity before the decreasing gradient of concentration begins to influence gaseous flow.

Lima (2014) evaluated the CO₂ absorption mechanism during SGS in *Perna perna* mussel through several conditions of pressure, temperature, and g/p ratio. For this matter, it is considered that the CO₂ can be dissolved in the water content of the food to form carbonic acid (H₂CO₃), that is dissociated into bicarbonate (HCO₃⁻), carbonate (CO₃²⁻) and hydrogen (H⁺) (Knoche, 1980). From this reaction, there are changes in pH, which is the base for a theory that states the decrease on the respiratory rate of microorganisms as the main factor to CO₂ bacteriostatic effect (Simpson et al., 2009).

Lima et al (2015) determined CO₂ solubility through several conditions of g/p, temperature, pressure considering an ideal gas situation through ideal gas law (Eq. (1)). Some other state equations would also help to predict CO₂ solubility for experiments in which the gas has a non-ideal behavior. The other state equations chosen to perform calculations in this work were Van der Waals (Eq. (2)), Virial (Eq. (3)), Soave-Redlich Kwong (Eq. (4)) and Peng-Robinson (Eq. (5)) (Smith et al., 2013).

$$P \cdot V = n \cdot R \cdot T \quad (1)$$

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

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

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

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

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

In order to obtain CO₂ solubility from these equations, computer routines can be developed to perform the requested iterative equations, since several parameters on the stated equations are interdependent and do not have analytical solution. For example, Virial is a cubic state equation that is usually used by its second term as follows in Eq. (6):

$$Z = 1 + \frac{BP}{RT} \quad (6)$$

From Eq. (6), where P is pressure, R is universal gas constant, T is temperature and B is second term of Virial equation, Z (compressibility factor) is obtained and then used to calculate number of moles through Eq. (7).

$$n = \frac{PV}{ZRT} \quad (7)$$

where V is volume.

Number of moles obtained from Eq. (7) is compared to a supposed number of moles until the two are as close as possible, which characterizes the iterative process for Virial equation.

One practical, rapid, and flexible alternative to program this kind of data is Microsoft Excel through its programming tool VBA (Visual Basic for Application). The simplicity of its language, its friendly layout, easy learning and flexibility have made Microsoft Excel a very popular mathematical tool. In this matter, VBA programs have emerged as an alternative to facilitate simulation processes and to take computer operations to a more accessible and friendly platform (Norton & Tiwari, 2013; Wojeicchowski & Praxedes, 2015).

Le Roux & Brodalka (2004) created a routine in VBA for analysis of fluids velocity and sedimentation profiles from parameters as fluid density and dynamic viscosity, roughness and inclination of the container. Onofri (2005) developed a VBA program to run non-linear regressions from herbicides data to adjust ideal dosages to meet legislation needs and demands of the local vegetation. Heat transfer on potatoes high-pressure freezing was modeled by a VBA routine created by Norton & Tiwari (2013) from which a significant prediction of temperature profile was obtained.

Golman & Julklang (2014) simulated an exhaust gas recovery from spray dryer by a VBA routine based on mass and energy balance, and obtained 50% of energy recovery from recirculation of drying air. Wojeicchowskii & Praxedes (2015) simulated parameters adjustment from different models of an alcoholic fermentation process through VBA. The authors created a friendly program in which the user selects one of the models available on literature and its parameters, and obtains as results microorganism, product and substrate concentration throughout the process. Biglia & other authors (2017) also developed a VBA routine based on mass and energy balance, but seeking to model a cocoa thermal processing considering non-stationary steam tanks.

Considering the range of applications briefly described, it is recognizable that VBA is able to perform innumerable calculations as long as the user is able to handle the inputs. For this matter, developer and user must be clear on purposes so both the program and the inputs converges to a trustworthy result.

The objective of this paper is to develop a VBA code to determine Henry's constant in a CO₂ solubility study applied to *Perna perna* mussels. VBA routines considers ideal gas law and other four state equations to obtain Henry's constant, which is used to determine CO₂ solubility through the samples. The obtained results are compared to a model created by Sivertsvik et al. (2004) to simulate the accuracy of equations and routines and the effectiveness of the process according to the selected parameters.

2. METHODOLOGY

2.1 Sample preparation

The mussels were cleaned with water, steam cooked at 100°C for 6 minutes to get the shells opened, cooled with iced water at 10°C for 10 minutes, and manually peeled before submitted to SGS process.

Its apparent specific gravity was determined by volume displacement in a beaker. 50g of mussels were placed into a beaker filled with 300 mL of water, and the volume displaced was measured to be used on the calculation (mass/volume).

2.2 Experimental apparatus

A stainless steel cylindrical vessel (526 cm³) was developed to perform SGS process. The mussels were introduced into the apparatus and CO₂ (Linde, 99.9% purity, Brazil) injected for 65 h, meanwhile temperature was controlled by a jacketed system linked to a thermostatic bath (Quimis, 6214m2, Brasil), according to Fig. 1 (Lima, 2015).

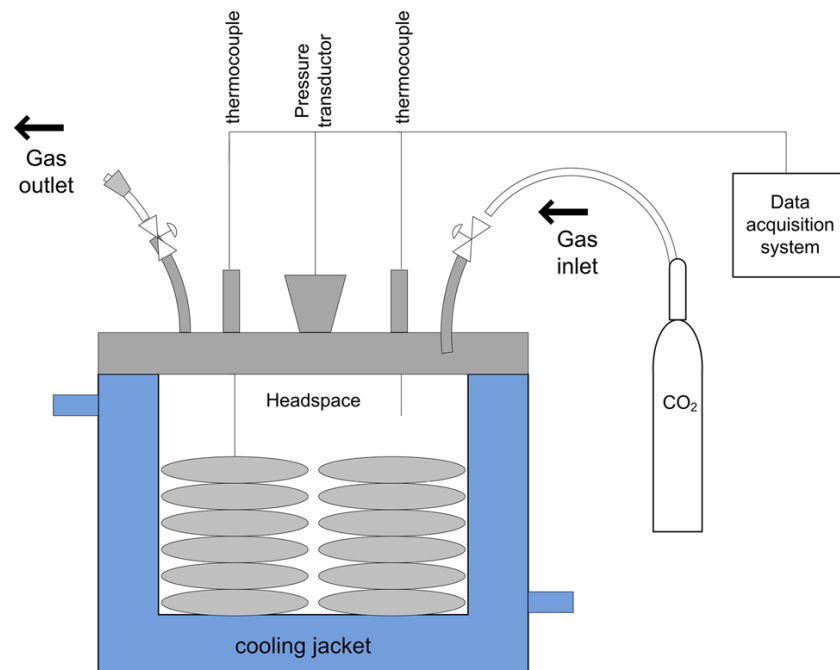


Fig. 1. SGS treatment apparatus (Lima, 2015).

Two thermocouples J type (Salvi Casagrande – Brazil) were used to measure product and gas temperatures. Gas inlet and outlet were performed by needle type valves (Swagelok, Brazil) connected to a CO₂ cylinder (Linde, 99.9% purity, Brazil) and to a gas analyzer (Checkmate II, PBI-Dansensor, Denmark) respectively. Gas analyzer was set to continuously determine gas composition. A pressure transducer (Warme WTP-4010, 0-10V, Brazil) was used to obtain total pressure on the system. An acquisition data system collected data at each 30 seconds of experiment (Agilent, Data Acquisition 34970A, USA) through the aid of the software Benchlink Data Logger 3.0 (Agilent, 2009).

2.3 Thermodynamic studies and predictive equation

In order to perform calculations, some considerations were taken by Lima (2015): hermetically sealed system; N₂ and O₂ flows and secondary reactions products can be neglected, considering only CO₂ dissolution as main proceeding; ideal gas for low pressures and non-ideal gas for high pressures; total pressure variation yields CO₂ mass variation on gaseous phase (Sivertsvik et al., 2004a; Sivertsvik et al., 2004b; Sivertsvik & Jensen, 2005).

Considering the stated, rearrangements made by Sivertsvik et al. (2004a, 2004b) resulted in an equation able to calculate absorbed CO₂ at equilibrium:

$$C_{pred\ CO_2}^{t=\infty} = \frac{g/p \cdot (P_{CO_2}^{t=0} - P_{CO_2}^{t=\infty}) \cdot M_{wCO_2}}{RT\rho_p} \quad (8)$$

where g/p represents gas to product ratio (volume base), $P_{CO_2}^{t=0}$ and $P_{CO_2}^{t=\infty}$ are pressure at the beginning and at equilibrium, M_{wCO_2} is the molecular weight (g.mol⁻¹) of CO₂, R is the universal gas constant (J.mol⁻¹.K⁻¹), T is temperature (K), and ρ_p is density of mussels (g.cm⁻³).

Still, Henry's law can be used to express dissolved CO₂ at equilibrium according to Eq. (9).

$$P_{CO_2}^{t=\infty} = H_{CO_2} \times C_{CO_2}^{t=\infty} \quad (9)$$

where H_{CO_2} is Henry's constant of CO₂ (Pa. ppm⁻¹) and $C_{CO_2}^{t=\infty}$ is the concentration of CO₂ 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 CO₂ in the system according to Eq. (10).

$$n_{CO_2}^D = n_{CO_2}^i - n_{CO_2}^f \quad (10)$$

where $n_{CO_2}^D$ is the number of moles of CO₂ dissolved into the liquid phase of mussels, and $n_{CO_2}^i$ and $n_{CO_2}^f$ are the number of moles of CO₂ available at the headspace at the beginning and at equilibrium. The number of moles of CO₂ 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 compressibility factor (unitless) and n_{CO_2} is CO₂ number of moles.

Eq. (12) optimizes Henry's constant according to Rotabakk et al. (2010), which considers that the dissolution of CO₂ in SGS process is exclusively performed into the water content of the food.

$$H_{CO_2,p} = \frac{H_{CO_2,H_2O}}{X_w} \quad (12)$$

where H_{CO_2,H_2O} is CO₂ Henry's constant in water and X_w is the moisture content of the food.

As CO₂ concentration is dependent of ideality or non-ideality range on the experiments, it should be clear that, for ideal gases, $Z = 1$ on Eq. (11). For experiments where pressure are considerable higher, $Z \neq 1$ (Smith et al., 2013), and, in this case, CO₂ concentration is expressed by means of molar fraction of gas into liquid and into gaseous phase in the system, as described by Eq. (13).

$$y_1\phi_1^vP = x_1H_1 \quad (13)$$

where y_1 and x_1 are CO₂ molar fractions into gaseous and liquid phase, ϕ_1^v is the fugacity coefficient of CO₂ in the gaseous phase, P is pressure and H_1 is Henry's constant.

Fugacity coefficient of CO₂ in the system and mussels Henry's constant were obtained by Lima (2015) based on Dalmolin et al. (2006) iterative calculations, from each initial and final pressure were obtained and inserted into the program in order to obtain CO₂ solubility. Calculations considering ideal gas law (Eq. (1)) and the four state equations (Eq. (2) to Eq. (5)) were performed in this work. The values of pressure used in this work were 200, 400 and 600 kPa, temperatures used were 0, 3 and 6°C and gas/product ratio were 1:1, 3:1 and 5:1 (volume ratio), in a 2³ experimental design according to Table 1.

Table 1.Range of variables to CO₂ solubility determination in *Perna perna* mussels (Adapted from Lima, 2015).

Experiment	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

The flow chart illustrated by Fig. 2 describes the steps taken during the data programming in VBA Excel 2016.

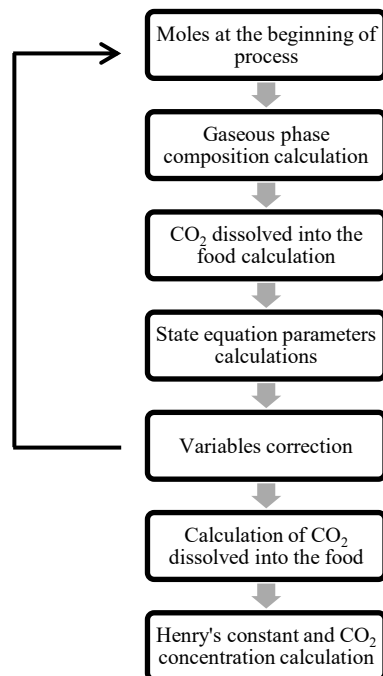


Fig. 2. Flow chart to data programming to obtain Henry's constant and CO₂ concentration from SGS experiments.

Percentage error between experimental and predicted Henry's constant and CO₂ calculations were estimated by Eq. (14) to evaluate CO₂ dissolution in the liquid phase of mussels.

$$error(\%) = 100 \times \frac{Var_{calc} - Var_{pred}}{Var_{calc}} \quad (14)$$

where Var_{calc} is the calculated variable and Var_{pred} is the predicted variable.

3. RESULTS AND DISCUSSIONS

3.1 Sample characterization

The apparent specific gravity of *Perna perna* mussels obtained by fluid misplacement was 1040 kg.m^{-3} (1.04 g.cm^{-3}), which is a result of a porous structure that allows a high amount of water and gases to permeate into the product.

3.2 CO₂ dissolution into mussels during SGS process

CO₂ concentrations were determined from ideal gas law, Virial, and cubic equations Van der Waals, Soave-Redlich Kwong and Peng-Robinson through VBA routines. The results that best fitted on the data or presented the lower percentage error on mussels for each experiment are listed on Table 2.

Table 2.
Experimental and predicted CO₂ concentration

Experiment	[CO ₂] _{exp} (mg CO ₂ .kg ⁻¹) ^[1]	[CO ₂] _{pred} (mg CO ₂ .kg ⁻¹) ^[2]	Error (%) ^[3]	Eq. ^[4]
1	2,530.67	2,437.77	3.67	IG
2	2,940.16	2,827.32	3.84	IG
3	8,055.97	8,282.72	-2.81	V
4	6,667.60	6,746.53	-1.18	VDW
5	7,181.16	7,248.95	-0.94	VDW
6	6,177.17	6,052.80	2.01	V
7	19,535.47	19,447.99	0.45	PR
8	15,545.84	15,092.51	2.92	SRK
9	9,496.95	9,200.10	3.13	V
10	8,611.36	8,367.22	2.84	V
11	8,434.59	8,212.68	2.63	V

^[1] From Eq. (7); ^[2] From Eq. (8); ^[3] From Eq. (14); ^[4] Description of better fitted equation (IG = ideal gas; VDW = Van der Waals; V = Virial; PR = Peng-Robinson; SRK = Soave-Redlich Kwong).

The highest CO₂ concentrations can be detected on experiments 7 and 8 (19,535.47 mg CO₂.kg⁻¹ and 15,545.84 mg CO₂.kg⁻¹), which were performed at the higher pressure (600 kPa) and at the higher g/p ratio (5:1); between these two experiments, the one that presented the higher CO₂ concentration was the one at lower temperature (0°C). Pressure and g/p were variables that positively influenced CO₂ into the mussels during SGS process, the first one

confirming Henry's law statement. Comparison between the experiments shows that the lower is the temperature the greater is CO₂ dissolved into the mussels, which matches the inversely proportional CO₂ solubility behavior into liquid phases according to the temperature (Diamond & Akinfiev, 2003; Simpson et al., 2001).

CO₂ solubility into a food product is dependent of variables of the process (pressure, temperature, g/p ratio) and characteristics of the samples (moisture content, pH, porosity, etc.) Dissolution of CO₂ in oysters at the same temperatures, pressures and g/p ratios as the ones used by Lima (2015) also yielded higher rates for high temperature and g/p ratio (Soares, 2013). Sivertsvik et al. (2004) achieved a CO₂ concentration of 2654 mg.CO₂.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 CO₂.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 (Sivertsvik & Jensen, 2005). Chicken drumsticks were able to absorb 567 mg CO₂.kg⁻¹ at atmospheric pressure, 3°C and a g/p of 3:1 (Al-Nehlawi et al., 2013), a considerable low value compared to CO₂ solubility into mussels and salmon, for example, which is a result of both samples singularities and process variables.

3.3 Solubility of CO₂ in mussels through Henry's constant determination

Experimental and predicted Henry's constants in mussels obtained from Eq. 9 combined to Eq. 12 according to experimental and predicted CO₂ concentrations are listed on Table 3.

Table 3.
Experimental and predicted Henry's constant in *Perna perna* mussels

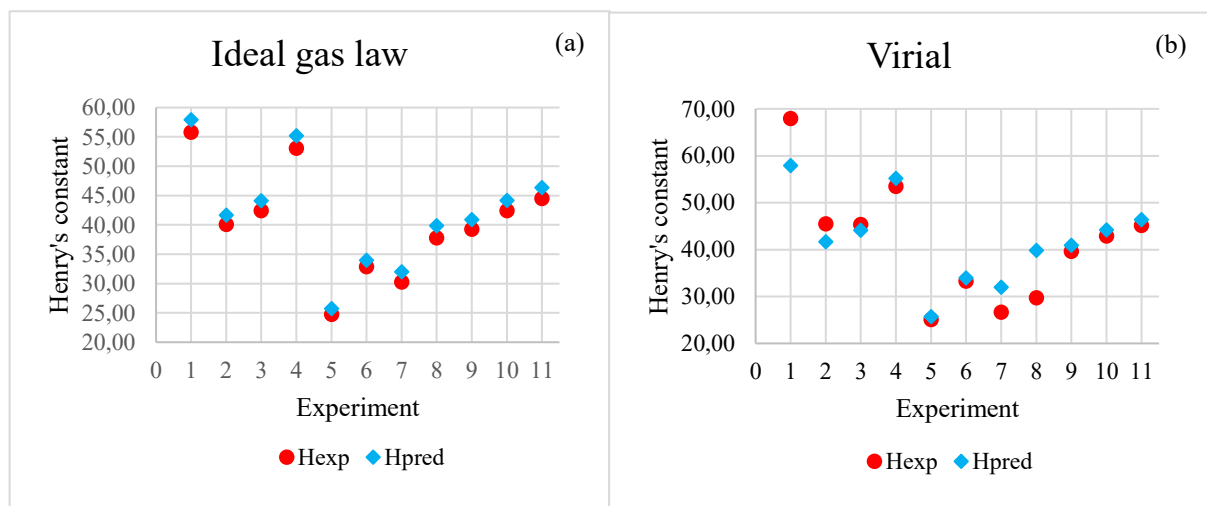
Experiment	H _{exp} (Pa/ppm)	H _{pred} (Pa/ppm)	Error (%) ^[1]	Eq. ^[2]
1	55.78	57.90	-3.81	IG
2	40.08	41.68	-3.99	IG
3	45.35	44.11	2.74	V
4	55.83	55.17	1.17	VDW
5	24.76	25.71	-3.94	IG
6	32.90	33.94	-3.17	V
7	32.10	31.99	-0.45	SRK
8	38.67	39.83	-3.00	SRK
9	39.62	40.89	-3.23	V
10	42.93	44.18	-2.92	V
11	45.14	46.36	-2.70	V

^[1] From Eq. (14); ^[2] Description of better fitted equation (IG = ideal gas; VDW = Van der Waals; V = Virial; PR = Peng-Robinson; SRK = Soave-Redlich Kwong)

The lowest Henry's constant values observed were yielded by experiments 5, 6, 7 and 8 (24.76, 32.90, 32.10 and 38.67), which is related to a high solubility of CO₂ into mussels. These experiments were performed at the higher g/p ratio (5:1), which endorses the positive effect of the amount of gas into the chamber during CO₂ dissolution into mussels. Experiments 5 and 6 did not presented considerably high values of CO₂ dissolution when compared to other experiments, which can be directly related to the low pressure (200 kPa) and to the significant influence of pressure in during SGS process. The higher values of Henry's constant are inversely related to low CO₂ concentrations, as it is observed in experiments 1 and 2, following Henry's law.

Perna perna mussels Henry's constant had not been reported in literature, so analyses were conducted considering related food products. Sivertsvik et al. (2004) obtained Henry's constants of 54.3 Pa.ppm⁻¹ and 57.9 Pa.ppm⁻¹ for codfish and salmon, respectively. In 2010, Rotabakk et al. reported chicken fillets' Henry's constant as 42.8 Pa.ppm⁻¹. Sivertsvik & Jensen (2005) reached Henry's constant values of 64.9 Pa.ppm⁻¹ for cooked ham and 87.5 Pa.ppm⁻¹ for meat sausage. The divergence between literature and values listed on Table 4 is related to food structure and composition as well as to process parameters (pressure, temperature and g/p).

Considering the four state equations and ideal gas law used in the calculations, ideal gas law was the equation that presented the lower average error (%) and deviation considering experimental and predicted Henry according to Fig. 3.



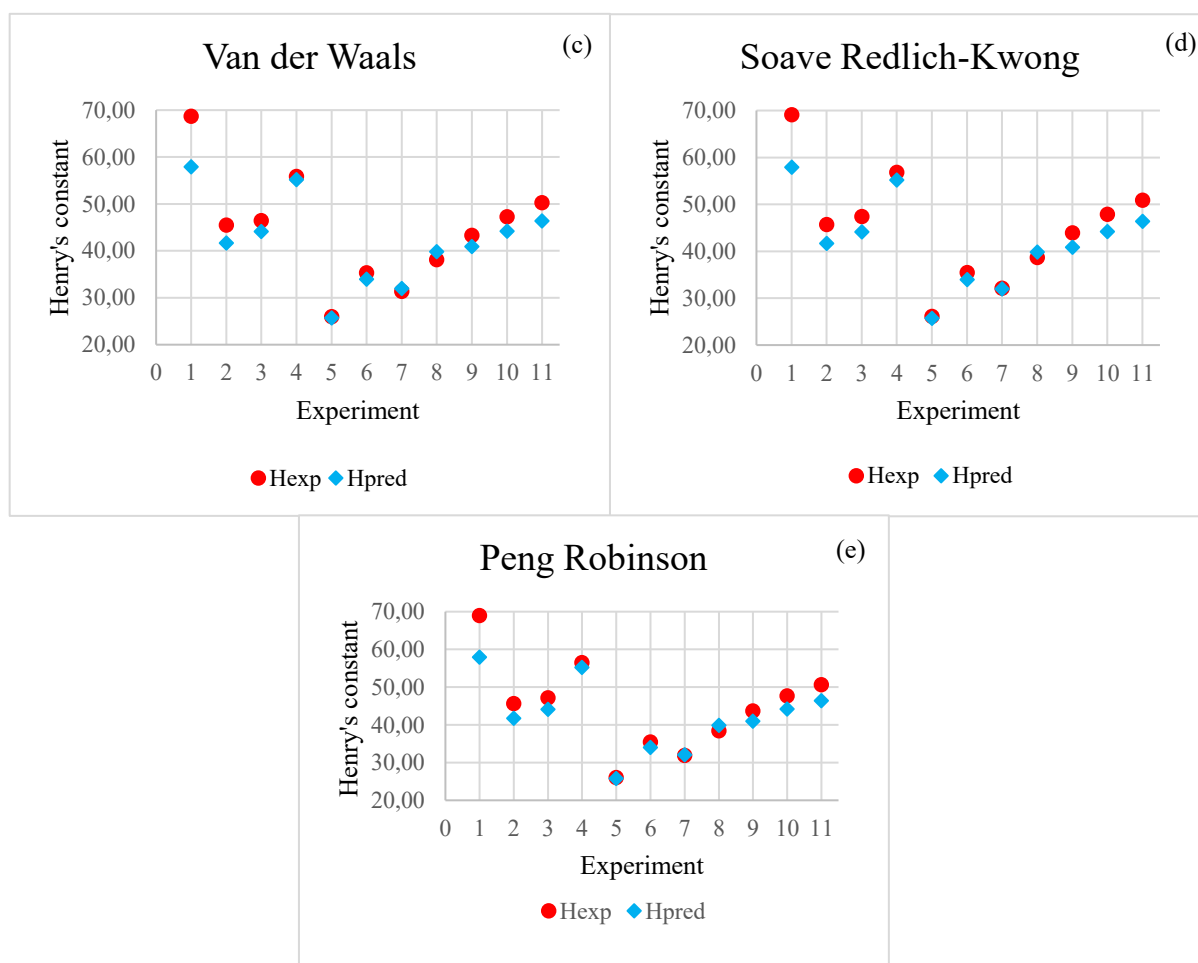


Fig. 3. Experimental and predicted Henry's constant for ideal gas law and each state equation.

Fig. (3a) shows that gas ideal law yielded the lower deviation (0.72) throughout the 11 experiments, as well as the lower average error (%) between experimental and predicted Henry's constant. The low pressures used in the process were not sufficient to overcome the barrier of ideality and, for this reason, ideal gas law has fitted greatly into the data from the whole process. A simulation was performed on the ideal gas law routine using pressures above 50 atm, and, as expected, the obtained errors were significantly high (60% up), reinforcing the validity range of ideal gas law.

Virial was the state equation that presented the lowest fit to experimental data (Fig. (3b)), which may be a result of parameters adjustment and stopping of equation. Even though the other four state equations presented low average errors, for the parameters used in this work, ideal gas law is an equation that requires fewer inputs and still presents a satisfactory performance.

The use of a VBA code to perform thermodynamic calculations showed to be a great resource regarding complex calculations involving a high amount of data, which has also been reported by several authors in the last 14 years (Biglia et al., 2017; Golman & Julklang, 2014; Le Roux & Brodalka, 2004; Onofri, 2005; Norton & Tiwari, 2013; Wojeicchowskii & Praxedes, 2015). Still, the approach taken by this paper through the development of a VBA code is another single step to optimize problem solving and to bring calculation program users to the awareness of technology resources. Data programming in VBA presented an accessible language combined to rapid results, which validates the service of technology to users' advantage.

4. CONCLUSION

In this paper, a VBA code is proposed to solve complex thermodynamic calculations involving Henry's constant determination through ideal gas law and other four state equations. Even though the five routines showed great fit to the predicted data, ideal gas law yielded the lowest average error (%). This result can be analyzed as associated to the low range of pressure used in the experiment, which may have not been enough to achieve non-ideal gas stage. VBA routines showed to be a great resource for complex calculations as it presents a friendly language, generate rapid and reliable results, and is settled in the well-known Microsoft Excel, which may be a facilitator point regarding its use.

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