Infinite dilution activity coefficient of solvents in poly-3-hydroxybutyrate from inverse gas chromatography

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A B S T R A C T

Over the past few years, there has been an increase in the production of biopolymers, including poly(3-hydroxybutyrate) P(3HB). However, finding compatible solvents for these new materials can be a challenging task. The infinite dilution activity coefficient (IDAC) is a thermodynamic property that indicates the level of interactions between two substances and can be determined from experiments of inverse gas chromatography (IGC). In this work, IGC was used to determine IDAC of 12 solvents in P(3HB). The substances studied were 1,1,1,3,3,3-hexafluoro-2-propanol (HFIP), 1,2-dichloroethane, 2,2,2-trifluoroethanol, 2-butanone, 2-heptanone, benzene, chloroform, cyclohexane, dimethyl carbonate, ethyl acetate, isooctane and toluene. HFIP was found to be the most compatible solvent with P(3HB) with IDAC values smaller than 1. Isooctane presented the highest IDAC value, in agreement with the well-known incompatibility between hydrocarbons and P(3HB). In addition, P(3HB) crystallinity was determined through IGC technique, enabling the calculation of the IDAC of amorphous phase only, where vapor-liquid equilibrium can be assumed. The degree of crystallinity obtained with HFIP analysis in P(3HB) was 68%, a value close to that previously reported in the literature.

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1. Introduction

The consumption of plastics, mainly in the form of disposable products, has highly increased in recent years. Non-biodegradable polymers, from petrochemical industry, have high resistance to degradation, a characteristic which has made them used in large scale [1,2]. As a result of this, concerns about solid waste management and environmental issues have grown worldwide. In this scenario, biopolymers are being increasingly studied as an alternative to common plastics. Amongst them, poly(3-hydroxybutyrate) (P(3HB)) is a strong candidate due to its biodegradability and also because it has mechanical properties similar to polypropylene [3,4]. Moreover, it can be produced by biological routes from renewable carbon sources derived from agriculture or industry [5].

However, there are several difficulties to overcome in order to allow the production of P(3HB) on a large scale [3,5]. The polymer extraction from the culture medium is an important step of P(3HB) production, and a suitable solvent for P(3HB) is necessary, preferably environmentally friendly. In this context, the infinite dilution activity coefficient (IDAC) is an interesting property to study, since it indicates the level of interaction between two substances and how close to ideality a binary mixture is.

Among the existent techniques for measuring IDAC, the inverse gas chromatography (IGC) is an effective method for the study of solvents in polymers. In IGC, the material of interest is packed into the column to be used as stationary phase [7,8], and its interactions with different mobile phases are measured as different retention volumes. The study of polymers using this technique provides good approximation to conditions of processing and purification, opposed to methods that use dilute polymer solutions [9].

In available literature, there are many reports about the determination of IDAC in polymers and solvent mixtures using IGC [10–16]. All cited articles used similar procedures and materials to that used in this study. Lichtenthaler et al. [10] studied poly(dimethylsiloxane)-hydrocarbon systems; Galin and Rupprecht [11] investigated the thermodynamic interaction between linear or branched polystyrene and solutes, and also the adsorption
phenomena in IGC analyses; Schuster et al. [12] determined partial molar sorption and other mixing functions for polystyrene and non-polar solvents; Price et al. [13] measured thermodynamic data for several probe molecules in three polymers, poly(dimethylsiloxane) (PDMS), polyisobutylene (PIB) and ethylene-propylene rubber (EPR); Du et al. [14] investigated the interactions among 9 hydrocarbon polymers and 43 solvents; Zeng et al. [15] provided data of solvents in poly(vinyl alcohol) and cross-linked poly(vinyl alcohol) at several different temperatures; Papadopoulou and Panayiotou [16] calculated the thermodynamic properties of poly(2,2,2-trifluoroethyl methacrylate) (PFEMA) in 15 solvents. However, to the best of our knowledge, just a few equilibrium data are available for biopolymers, and none for P(3HB).

Therefore, this research aims to obtain IDAC values for solvents in P(3HB) through the inverse gas chromatography technique. P(3HB) is used as stationary phase and various solvents as volatile samples in the inert mobile phase. Additionally, this research intends to study possible adsorption effects during IGC analysis due to P(3HB) polarity and to determine the polymer degree of crystallinity.

2. Methodology

2.1. Materials

Poly(3-hydroxybutyrate) (P(3HB)) was purchased from Sigma-Aldrich (Lot STBB9669V). The glass transition temperature and the melting point of P(3HB) are approximately 278 K and 453 K, respectively [4,17]. No data regarding molecular weight (M_0) was provided. Polar and nonpolar solvents were used as probes for IGC analysis. The solvents selection aimed at the study of biopolymer interactions with different chemical families, such as alkane, ketone, alcohol, esters, organic halides. Solvents known to be linked poly(vinyl alcohol) at several different temperatures; Papadopoulou and Panayiotou [16] calculated the thermodynamic properties of poly(2,2,2-trifluoroethyl methacrylate) (PFEMA) in 15 solvents. However, to the best of our knowledge, just a few equilibrium data are available for biopolymers, and none for P(3HB).

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2.2. Column preparation and inverse gas chromatography setup

Column packing containing from 20% to 25% (w/w) of the stationary phase (biopolymer) was prepared by coating the solid support, Chromosorb P, with a solution of 2,2,2-trifluoroethyl methacrylate (PTFEMA) in 15 solvents. However, to the best of our knowledge, just a few equilibrium data are available for biopolymers, and none for P(3HB).

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2.3. Theory

Retention time data were used to calculate the IDAC of tested solvents in P(3HB). At infinite dilution, interactions between the solvent molecules are avoided and solvent retention inside the column is mainly governed by interactions with the stationary phase [25]. The net retention volume \( V_R \) is calculated from the following equation [11,16]:

\[
V_R = (t_R - t_M) \frac{P_g T}{T_g} Q
\]

where \( t_R \) and \( t_M \) are the retention times of solvent and air, respectively, \( Q \) is the carrier gas flow rate measured at column outlet pressure (atmospheric pressure) \( P_{out} \) and room temperature \( T_o \).\( T \) is the column temperature and \( J^2 \) is the James and Martin factor used to correct carrier gas compressibility, defined as [26]:

\[
J^2 = \frac{\left( \frac{P_{in}}{P_{out}} \right)^2 - 1}{\left( \frac{P_{in}}{P_{out}} \right)^3 - 1}
\]

where \( P_{in} \) and \( P_{out} \) are column inlet and outlet pressure, respectively.

The specific retention volume \( V_0^s \) is the property used to obtain several thermodynamic properties from IGC and it is calculated in terms of \( V_R \) as [8,16]:

\[
V_0^s = \frac{V_R T_{273.15}}{m_p T}
\]

where \( T_{273.15} \) is the temperature of 273.15 K and \( m_p \) is the polymer weight inside the column.

When studying polymers, the mass-based infinite dilution activity coefficient \( \Omega^\infty \) is more convenient than the molar quantity \( \gamma^\infty \) because polymer molecular weight can be unknown or poorly defined [27]. Based on vapor–liquid equilibrium achieved during the IGC analysis between polymer (liquid — stationary phase) and solvent (vapor — mobile phase) \( \Omega^\infty \) is calculated by Refs. [23,28]:

\[
\Omega^\infty = \frac{R T_{273.15}}{v_0^s} M_1 f_1
\]

where \( R \) is the universal gas constant, \( M_1 \) is the solvent molecular mass and \( f_1 \) is solvent fugacity coefficient [29]:

\[
f_1 = \frac{P_{sat} T}{P_{in}} \exp \left( \frac{P_{sat} (B_{11} - v_1)}{RT} \right)
\]

being \( P_{sat} \) the solvent vapor pressure at temperature \( T \), \( B_{11} \) its pure second virial coefficient, that can be obtained from correlations available in the literature [30]; and \( v_1 \) the solvent liquid molar volume. Sources and values of \( B_{11} \) and \( v_1 \) used in this study are presented as Supplementary material.

However, when using IGC for crystalline and/or polar stationary phases, like P(3HB), interactions other than only VLE must be taken into account and corrected values of retention volume must be applied to Equation (4). Due to the relevance of these effects in the present study they are further discussed in the following sections.

2.3.1. Adsorption contribution

The specific retention volume \( V_0^s \) experimentally obtained is represented by sum of two contributions [31]:

\[
V_0^s = V_{gb}^s + V_{gas}^s
\]

where, \( V_{gb}^s \) is the retention volume regarding vapor—liquid/polymer interactions, generally called as the bulk contribution; and \( V_{gas}^s \) is the retention volume due to physical surface adsorption, which includes vapor adsorption in the inert solid, in the polymeric crystals and in the liquid layer.

According to Galin and Rupprecht [11] and Courval and Gray [32], Equation (6) can be rewritten as

\[
V_0^s = V_{gb}^s + K_a \frac{S}{W}
\]

with \( K_a \) representing adsorption contributions in the analysis, \( S \) the column inert support weight and \( W \) the polymer weight. As only bulk contributions should be taken into account for \( \Omega^\infty \) determination, \( V_{gb}^s \) can be obtained by the linear coefficient of a regression of experimental \( V_0^s \) and the quantity \( \frac{S}{W} \) measured using at least three columns with different polymer loading. In a plot of \( V_0^s \) versus \( \frac{S}{W} \), the lower the slope of experimental data, the smaller is the surface adsorption contribution tending to a horizontal line for nonpolar amorphous polymers.

It is important to mention that surface contribution vary according to the pair polymer/solvent. For a polar stationary phase, such as P(3HB), adsorption contribution can be significant since both nonpolar and polar solvents can present high adsorption in polar stationary phases [5,31].

2.3.2. Degree of crystallinity

IGC technique is a way of determining crystallinity of the stationary phase. Braun and Guillet [33] showed that the crystallinity fraction \( X_c \) is obtained by comparing retention volumes measured below \( T_m \) (\( V_0^{f1} \)) and linear extrapolation of retention volumes measured above the melting temperature (\( V_0^{f2} \)), according to the equation:

\[
X_c = 1 - \left( \frac{V_0^{f1}}{V_0^{f2}} \right)
\]

To determine P(3HB) crystallinity, analyses above its melting
temperature were carried out at 453 K, 463 K and 473 K, using HFIP in the mobile phase. Such narrow temperature range was used to avoid P(3HB) degradation inside the column, expected to be around 473 K, very close to its melting point. Only HFIP was used in this step because it has well known better compatibility with P(3HB). Chen and Al-Saigh [34] and Camacho et al. [35] also suggested the use of compatible solvents for experiments with poly(vinylidene fluoride), and polyethylene and EVA copolymers, respectively. In order to confirm the constant polymer mass inside the column, column weight was checked before and after experiments.

Table 2
Experimental retention volumes calculated for different solvents at 373 K and 383 K.

<table>
<thead>
<tr>
<th>Compounds</th>
<th>373 K</th>
<th>383 K</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( V_0 ) exp.</td>
<td>( V_0^0 )</td>
</tr>
<tr>
<td>HFIP</td>
<td>31.24 ± 2.40</td>
<td>22.63 ± 3.96</td>
</tr>
<tr>
<td>1,2-dichloroethane</td>
<td>12.02 ± 1.13</td>
<td>5.64 ± 1.36</td>
</tr>
<tr>
<td>2,2,2-trifluoroethanol</td>
<td>12.77 ± 1.12</td>
<td>6.70 ± 1.45</td>
</tr>
<tr>
<td>2-butane</td>
<td>7.38 ± 0.71</td>
<td>5.02 ± 0.40</td>
</tr>
<tr>
<td>2-heptane</td>
<td>41.42 ± 3.58</td>
<td>27.50 ± 1.10</td>
</tr>
<tr>
<td>Benzene</td>
<td>7.58 ± 0.73</td>
<td>3.42 ± 1.37</td>
</tr>
<tr>
<td>Chloroform</td>
<td>7.65 ± 0.49</td>
<td>6.35 ± 0.79</td>
</tr>
<tr>
<td>Cyclohexane</td>
<td>3.52 ± 0.37</td>
<td>1.43 ± 0.78</td>
</tr>
<tr>
<td>Dimethyl carbonate</td>
<td>10.00 ± 0.98</td>
<td>4.33 ± 2.00</td>
</tr>
<tr>
<td>Ethyl acetate</td>
<td>6.29 ± 0.66</td>
<td>2.60 ± 1.31</td>
</tr>
<tr>
<td>Isooctane</td>
<td>3.60 ± 0.41</td>
<td>0.95 ± 0.68</td>
</tr>
<tr>
<td>Toluene</td>
<td>13.47 ± 1.21</td>
<td>7.88 ± 0.28</td>
</tr>
</tbody>
</table>

Standard uncertainty \( u(T) = 1 \) K.
Values after ± correspond to expanded uncertainties, calculated with a coverage factor \( k = 2 \).

Table 3
Experimental retention volumes calculated for different solvents at 393 K and 403 K.

<table>
<thead>
<tr>
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<th>393 K</th>
<th>403 K</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( V_0 ) exp.</td>
<td>( V_0^0 )</td>
</tr>
<tr>
<td>HFIP</td>
<td>14.16 ± 1.11</td>
<td>8.82 ± 1.47</td>
</tr>
<tr>
<td>1,2-dichloroethane</td>
<td>6.86 ± 0.62</td>
<td>3.62 ± 1.06</td>
</tr>
<tr>
<td>2,2,2-trifluoroethanol</td>
<td>6.60 ± 0.56</td>
<td>3.63 ± 0.70</td>
</tr>
<tr>
<td>2-butane</td>
<td>4.34 ± 0.34</td>
<td>2.98 ± 0.72</td>
</tr>
<tr>
<td>2-heptane</td>
<td>20.72 ± 1.93</td>
<td>10.67 ± 4.38</td>
</tr>
<tr>
<td>Benzene</td>
<td>4.50 ± 0.41</td>
<td>2.15 ± 0.71</td>
</tr>
<tr>
<td>Chloroform</td>
<td>4.51 ± 0.37</td>
<td>3.28 ± 0.96</td>
</tr>
<tr>
<td>Cyclohexane</td>
<td>2.27 ± 0.20</td>
<td>1.10 ± 0.20</td>
</tr>
<tr>
<td>Dimethyl carbonate</td>
<td>5.62 ± 0.49</td>
<td>3.23 ± 1.08</td>
</tr>
<tr>
<td>Ethyl acetate</td>
<td>3.53 ± 0.32</td>
<td>1.89 ± 0.69</td>
</tr>
<tr>
<td>Isooctane</td>
<td>2.21 ± 0.21</td>
<td>0.90 ± 0.25</td>
</tr>
<tr>
<td>Toluene</td>
<td>7.82 ± 0.72</td>
<td>3.65 ± 1.19</td>
</tr>
</tbody>
</table>

Standard uncertainty \( u(T) = 1 \) K.
Values after ± correspond to expanded uncertainties, calculated with a coverage factor \( k = 2 \).
3. Results and discussion

3.1. Degree of crystallinity

When using IGC for polymers studies, with the polymer like stationary phase, one can expect a sharper transition in the retention diagram around its melting point. In this work, it was possible to see such behavior for P(3HB) using HFIP as probe as shown in Fig. 1.

Retention data above and below P(3HB) melting temperature were fitted to Equation (7) and can be seen in Fig. 2(a). Correlation, angular and linear coefficients data of Fig. 2(a) are presented in Table S2 of Supplementary material.

As can be seen in the results of Fig. 2(a), adsorption influence is observed in the whole temperature range analyzed. Experimental data slopes ($K_a$) are higher than 10% of linear coefficients ($V_0^{gb}$) showing that adsorption between stationary and mobile phase is relevant in this investigation and must be disregarded in order to calculate crystallinity degree.

Using $V_0^{gb}$ values, crystallinity of P(3HB) was calculated with Equation (8). The extrapolation performed for $V_0^{gb}$ estimation is illustrated in Fig. 2(b) and a crystallinity fraction value of 0.68±0.08 was obtained in the temperature range analyzed. This result was expected since P(3HB) has a well known high crystallinity degree [36–38].

3.2. Specific retention volume

Experimental retention volumes for all analyzed solvents were calculated using Equation (3). Retention volumes of bulk contribution ($V_0^{gb}$) were obtained through linear data regression of Equation (7). In order to take into account only interactions between vapor and liquid amorphous polymer, P(3HB) mass inside the column was determined subtracting the crystalline portion of

### Table 4

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<thead>
<tr>
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<th>373 K</th>
<th></th>
<th></th>
<th></th>
<th>383 K</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\Omega^\infty$</td>
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<td></td>
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<td></td>
</tr>
<tr>
<td>HFIP</td>
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<td>0.48 ± 0.09</td>
<td></td>
<td>1.32 ± 0.11</td>
<td>2.02 ± 0.46</td>
<td>0.65 ± 0.15</td>
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</tr>
<tr>
<td>1,2-dichloroethane</td>
<td>12.10 ± 1.25</td>
<td>25.58 ± 8.15</td>
<td>8.27 ± 1.99</td>
<td></td>
<td>12.81 ± 1.28</td>
<td>22.75 ± 7.96</td>
<td>7.36 ± 2.57</td>
<td></td>
</tr>
<tr>
<td>2,2,2-trifluoroethanol</td>
<td>7.17 ± 0.67</td>
<td>13.58 ± 2.93</td>
<td>4.39 ± 0.95</td>
<td></td>
<td>7.81 ± 0.67</td>
<td>11.62 ± 2.30</td>
<td>3.76 ± 0.74</td>
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<tr>
<td>2-butane</td>
<td>24.10 ± 2.44</td>
<td>35.15 ± 2.71</td>
<td>17.30 ± 6.64</td>
<td></td>
<td>25.63 ± 2.24</td>
<td>39.93 ± 10.55</td>
<td>12.92 ± 3.41</td>
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<tr>
<td>2-heptane</td>
<td>26.97 ± 2.31</td>
<td>36.57 ± 1.42</td>
<td>11.83 ± 0.47</td>
<td></td>
<td>27.43 ± 2.40</td>
<td>48.88 ± 14.28</td>
<td>15.81 ± 4.62</td>
<td></td>
</tr>
<tr>
<td>Benzene</td>
<td>22.89 ± 2.39</td>
<td>50.33 ± 20.10</td>
<td>16.28 ± 4.08</td>
<td></td>
<td>24.53 ± 2.50</td>
<td>49.59 ± 18.87</td>
<td>16.04 ± 4.64</td>
<td></td>
</tr>
<tr>
<td>Chloroform</td>
<td>8.55 ± 0.60</td>
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<td>9.14 ± 0.72</td>
<td>12.21 ± 2.75</td>
<td>3.95 ± 0.89</td>
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<td>Cyclohexane</td>
<td>47.57 ± 5.20</td>
<td>115.71 ± 63.10</td>
<td>37.43 ± 20.41</td>
<td></td>
<td>47.68 ± 4.36</td>
<td>86.06 ± 13.83</td>
<td>27.84 ± 4.47</td>
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</tr>
<tr>
<td>Dimethyl carbonate</td>
<td>19.25 ± 2.03</td>
<td>44.07 ± 20.35</td>
<td>14.26 ± 6.58</td>
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<td>19.76 ± 1.77</td>
<td>32.63 ± 8.90</td>
<td>10.55 ± 2.88</td>
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<td>Ethyl acetate</td>
<td>21.90 ± 2.36</td>
<td>51.60 ± 26.05</td>
<td>16.69 ± 8.43</td>
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<td>22.95 ± 1.79</td>
<td>29.15 ± 7.22</td>
<td>9.43 ± 2.33</td>
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<td>Isocyanate</td>
<td>57.97 ± 7.14</td>
<td>215.83 ± 153.70</td>
<td>69.81 ± 40.72</td>
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<td>57.31 ± 5.66</td>
<td>120.30 ± 37.87</td>
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<td>14.16 ± 0.51</td>
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<td>25.69 ± 2.47</td>
<td>46.23 ± 16.44</td>
<td>14.95 ± 5.32</td>
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Standard uncertainty u(T) = 1 K.
Values after ± correspond to expanded uncertainties, calculated with a coverage factor k = 2.

### Table 5

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<th>Compounds</th>
<th>393 K</th>
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<th>403 K</th>
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<td>$\Omega^\infty$</td>
<td>$\Omega^\infty$</td>
<td>$\Omega^\infty$</td>
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<td>2.56 ± 0.14</td>
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<td>1,2-dichloroethane</td>
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<td>7.69 ± 0.71</td>
<td>13.89 ± 2.69</td>
<td>4.49 ± 0.87</td>
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<td>7.54 ± 0.69</td>
<td>13.49 ± 1.68</td>
<td>4.36 ± 0.54</td>
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<td>2-butane</td>
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<td>35.66 ± 8.58</td>
<td>11.53 ± 2.78</td>
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<td>24.21 ± 2.33</td>
<td>47.57 ± 2.19</td>
<td>15.38 ± 0.71</td>
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<td>2-heptane</td>
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<td>47.52 ± 19.49</td>
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<td>27.75 ± 2.55</td>
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<td>Benzene</td>
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<td>Cyclohexane</td>
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<td>Dimethyl carbonate</td>
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<td>36.59 ± 4.99</td>
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<td>Ethyl acetate</td>
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<td>49.99 ± 4.03</td>
<td>13.26 ± 1.30</td>
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<tr>
<td>Isocyanate</td>
<td>56.66 ± 5.94</td>
<td>137.85 ± 38.15</td>
<td>44.39 ± 12.34</td>
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<td>54.30 ± 5.61</td>
<td>126.98 ± 14.19</td>
<td>41.07 ± 4.59</td>
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<td>Toluene</td>
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<td>54.35 ± 17.75</td>
<td>17.58 ± 5.74</td>
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<td>24.49 ± 2.56</td>
<td>54.29 ± 8.31</td>
<td>17.56 ± 2.69</td>
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</table>

Standard uncertainty u(T) = 1 K.
Values after ± correspond to expanded uncertainties, calculated with a coverage factor k = 2.
the total mass [34], considering a crystallinity degree of 68%. All retention volumes along with experimental expanded uncertainties, are listed in Tables 2 and 3. Small retention volumes indicate high IDAC values and, consequently, lower compatibility between the solvent and P(3HB).

As can be observed, significant smaller values of $V^\Omega_b$ are obtained when compared to raw experimental ones, indicating an important adsorption contribution for all chemicals investigated [31]. Disregarding the crystalline polymer inside the column, retention volumes increase considerably due to the smaller polymer amount available to interact with solvent molecules. The retention volume values in Tables 2 and 3 for toluene can be visually compared in Fig. 3.

### 3.3. Infinite dilution activity coefficients – $\Omega^\infty$

IDAC values were determined using Equation (4) at 373 K, 383 K, 393 K and 403 K. Results for twelve solvents are listed in Tables 4 and 5.

High IDAC values indicate that the mixture of P(3HB) and solvent exhibit a strong positive deviation from the Raoult’s law, while low values of IDAC mean strong compatibility and interactions. According to Açikses et al. [39] IDAC values less than 5, indicate good compatibility between polymer and solvent. Such fact was observed in this work for organohalogenates (HFIP, 1,2-dichloroethane, 2,2,2-trifluoroethanol, 2-butanone, benzene and isooctane in P(3HB)).

Fig. 4 shows the IDAC natural logarithm of $\Omega^\infty$ amorphous as a function of temperature for $\bullet$ HFIP, $\triangle$ 2,2,2-trifluoroethanol, $\times$ 1,2-dichloroethane, $\circ$ 2-butanone, $=$ benzene and $\ast$ isooctane in P(3HB).

### 4. Conclusion

Values of infinite dilution activity coefficient values (IDAC) were successfully determined for twelve selected compounds in poly(3-hydroxybutyrate) P(3HB) at four different temperatures (373 K–403 K) by inverse gas chromatography (IGC). It has been found that IDAC values mostly depend on the substances polarity and structure. Organo- and organohalogenates showed greater compatibility with P(3HB) and smaller IDAC values, with 1,1,1,3,3-hexafluoro-2-propanol (HFIP) being the solvent with the lowest IDAC value at all temperatures analyzed. As expected, alkanes presented higher IDAC values, showing that nonpolar compounds have low compatibility with P(3HB). The adsorption phenomena proved to be important for the calculation of IDAC. Inverse gas chromatography was used to determine the degree of crystallinity of P(3HB) in the stationary phase, the value found for pair P(3HB)–HFIP was 68%. The high crystallinity of P(3HB) reported in the literature was confirmed in this work.

### CRediT authorship contribution statement

**Anne C. Belusso:** Conceptualization, Investigation, Formal analysis, Writing - original draft. **Maria Lina Strack:** Conceptualization, Methodology, Validation, Investigation, Writing - original draft. **Lucas da S. Guadagnin:** Conceptualization, Methodology. **Debora J.L. Faccin:** Conceptualization, Resources. **Nilo S.M. Cardozo:** Conceptualization, Resources. **Rafael de P. Soares:** Conceptualization, Writing - review & editing. **Paula B. Staudt:** Conceptualization, Writing - review & editing, Supervision.

### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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### Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.fluid.2020.112742.

### References


