CO2 and O2 solubility and diffusivity data in food products stored in data warehouse structured by ontology
Valérie Guillard, Patrice Buche, Juliette Dibie-Barthelemy, Stéphane Dervaux, Filippo Acerbi, Estelle Chaix, Nathalie Gontard, Carole Guillaumé

To cite this version:
Valérie Guillard, Patrice Buche, Juliette Dibie-Barthelemy, Stéphane Dervaux, Filippo Acerbi, et al.. CO2 and O2 solubility and diffusivity data in food products stored in data warehouse structured by ontology. Data in Brief, Elsevier, 2016, 7, pp.1556-1559. 10.1016/j.dib.2016.04.044. hal-01357730

HAL Id: hal-01357730
https://hal-agroparistech.archives-ouvertes.fr/hal-01357730
Submitted on 27 May 2020

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
Data Article

CO₂ and O₂ solubility and diffusivity data in food products stored in data warehouse structured by ontology

Valérie Guillard a,* , Patrice Buche a , Juliette Dibie b , Stéphane Dervaux b , Filippo Acerbi a , Estelle Chaix a , Nathalie Gontard a , Carole Guillaume a

a UMR IATE, University of Montpellier – INRA, 2 place Pierre Viala, F-34060 Montpellier Cedex 1, France
b AgroParisTech & INRA UMR MIA 518, 16, rue Claude Bernard, F-75 231 Paris Cedex 05, France

Abstract

This data article contains values of oxygen and carbon dioxide solubility and diffusivity measured in various model and real food products. These data are stored in a public repository structured by ontology. These data can be retrieved through the @Web tool, a user-friendly interface to capitalise and query data. The @Web tool is accessible online at http://pfl.grignon.inra.fr/atWeb/.

2016 The Authors. Published by Elsevier Inc. This is an open access article under the CC BY license (http://creativecommons.org/licenses/by/4.0/).

Specifications Table

<table>
<thead>
<tr>
<th>Subject area</th>
<th>Biochemistry</th>
</tr>
</thead>
<tbody>
<tr>
<td>More specific subject area</td>
<td>Food science and food engineering</td>
</tr>
<tr>
<td>Type of data</td>
<td>Table, links</td>
</tr>
</tbody>
</table>

* Corresponding author.
E-mail address: guillard@univ-montp2.fr (V. Guillard).

http://dx.doi.org/10.1016/j.dib.2016.04.044
2352-3409/© 2016 The Authors. Published by Elsevier Inc. This is an open access article under the CC BY license (http://creativecommons.org/licenses/by/4.0/).
How data was acquired
Chemical titration (for CO₂ quantification) and luminescence-based detection (for O₂ detection) implemented in dedicated experimental set-ups

Data format
Analyzed, ready to use

Experimental factors
Samples considered are model and real food products without any pre-treatment except addition of sodium azide to avoid microbial growth

Experimental features
Solubility is measured by quantifying the concentration of dissolved gas in a sample in equilibrium with a fixed and controlled partial pressure. Diffusivity is identified from an experimental diffusion kinetic curve by using a mathematical model and appropriate numerical treatment (algorithm of optimization).

Data source location
University of Montpellier, FR-34060, France

Data accessibility
Data is within this article.

Value of the data
- A unique set of CO₂ solubility and diffusivity data indispensable in food engineering to model CO₂ gas transfer in food.
- A unique set of O₂ diffusivity values within synthetic oils as a function of temperature.
- O₂ diffusivity data could be used to predict oxidation of O₂-sensitive compounds in foods.
- These data could serve as benchmark for other researchers coping with research on gas transfer in food for numerous simulation.

1. Data

Data shared with this article are more than 100 data of solubility and diffusivity of gases (O₂ and CO₂) in food samples. These data are stored in a data warehouse called @Web in which the data management is guided by ontology.

All data are available for uploading at the URL specified below and recalled in the table hereafter with the details about the nature and amount of data available at each URL.

<table>
<thead>
<tr>
<th>Data type</th>
<th>Table URL (copy/paste the URL in your Internet browser)</th>
<th>Amount of data</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO₂ solubility</td>
<td>pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2775&amp;ridDoc=1335&amp;rid=35272672</td>
<td>34</td>
</tr>
<tr>
<td></td>
<td>pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2776&amp;ridDoc=1335&amp;rid=35305550</td>
<td>21</td>
</tr>
<tr>
<td></td>
<td>pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2777&amp;ridDoc=1335&amp;rid=35245144</td>
<td>48</td>
</tr>
<tr>
<td></td>
<td>pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2778&amp;ridDoc=1335&amp;rid=35320430</td>
<td>16</td>
</tr>
<tr>
<td>CO₂ diffusivity</td>
<td>pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2779&amp;ridDoc=1346&amp;rid=35346176</td>
<td>12</td>
</tr>
<tr>
<td></td>
<td>pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2780&amp;ridDoc=1346&amp;rid=35361064</td>
<td>11</td>
</tr>
<tr>
<td></td>
<td>pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2781&amp;ridDoc=1346&amp;rid=36350532</td>
<td>16</td>
</tr>
<tr>
<td></td>
<td>pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2782&amp;ridDoc=1346&amp;rid=35333312</td>
<td>11</td>
</tr>
<tr>
<td></td>
<td>pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2783&amp;ridDoc=1346&amp;rid=35320430</td>
<td>12</td>
</tr>
</tbody>
</table>
2. Experimental design, materials and methods

**O₂.** Oxygen optical sensors (Presens GmbH, Regensburg, Germany) were used to monitor O₂ partial pressure. This measurement is based on dynamic luminescence quenching. Due to an excitation flash emitted through an optical fibre, the luminophore contained in the sensor goes into an excited state and thus emits fluorescence backscatter signal, which is detected by the optical fibre. If the luminophore is in contact with an oxygen molecule, the backscatter signal is changed due to a dynamic quenching of luminescence. The change in the backscatter signal permits to detect the O₂ partial pressure in the medium. Two different set-ups exist (1) an invasive O₂-sensitive optical sensor made of a syringe probe (micro-sensors, Presens GmbH, Regensburg, Germany) connected to the optical fibre and oxygen metre (Oxy-4 micro, Presens) and (2) a non-invasive oxygen sensor made of a dot of 5 mm of diameter that can be stuck on the wall of a transparent container and measurement is then made through the transparent container. Oxygen sorption kinetics were measured at fixed temperature value when imposing a controlled partial pressure of O₂ in the surrounding of the sample. The mono-directional O₂ ingress into the sample was measured locally at the bottom or in the middle of the thin layer of food material previously free of O₂ using one of the aforementioned sensors. More details on the experimental set-up could be found in [1–3].

**CO₂.** The solubility of CO₂ was measured at equilibrium by quantification of the gas dissolved in the sample using chemical titration [4,5]. This measurement was done in a set-up where the sample is in a controlled chamber (controlled temperature, relative humidity, CO₂ gas composition).

The diffusion of CO₂ was characterised by (1) imposing a gradient of CO₂ to a piece of material of simple geometry (cylinder or plane sheet), (2) measuring the CO₂ sorption kinetic in the sample and (3) identifying diffusivity values by adjusting a dedicated mathematical model to the experimental kinetic. Two types of kinetic could be obtained: (1) CO₂ space-dependent profile in the cylindrical sample after its slicing and CO₂ quantification in each slice or (2) CO₂ time-dependent profile after CO₂ quantification in each thin slice (one slice corresponding at one time of kinetic) [4,6].

Numerical treatment. For both O₂ and CO₂, diffusivities are identified by fitting a dedicated mathematical model to the experimental kinetic curve (space-dependent profile or time-dependent profile). This identification step is performed using a routine (“lsqnonlin”) of Matlab® software.

**Acknowledgements**

Part of the data presented here were acquired in the framework of the Map’Opt project (ANR-10-ALIA-002 2011 to 2015) funded by the French National Research Agency, whose title is “Equilibrium gas composition in modified atmosphere packaging and food quality.”
Appendix A. Supplementary material

Supplementary data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.dib.2016.04.044.

References