



HAL
open science

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

Valérie V. Guillard, Patrice Buche, Juliette Dibie-Barthelemy, Stéphane Dervaux, Filippo Acerbi, Estelle Chaix, Nathalie N. Gontard, Carole Guillaume

► **To cite this version:**

Valérie V. 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*, 2016, 7, pp.1556-1559. 10.1016/j.dib.2016.04.044 . hal-01357730

HAL Id: hal-01357730

<https://agroparistech.hal.science/hal-01357730v1>

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.



ELSEVIER

Contents lists available at ScienceDirect

Data in Brief

journal homepage: www.elsevier.com/locate/dib

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 Dibia ^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

ARTICLE INFO

Article history:

Received 19 March 2016

Received in revised form

15 April 2016

Accepted 19 April 2016

Available online 26 April 2016

Keywords:

Diffusivity

Solubility

Data

Data warehouse

Ontology

Food

O₂CO₂

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

Subject area	Biochemistry
More specific subject area	Food science and food engineering
Type of data	Table, links

* 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	<i>Chemical titration (for CO₂ quantification) and luminescence-based detection (for O₂ detection) implemented in dedicated experimental set-ups</i>
Data format	<i>Analyzed, ready to use</i>
Experimental factors	<i>Samples considered are model and real food products without any pre-treatment except addition of sodium azide to avoid microbial growth</i>
Experimental features	<i>Solubility is measured by quantifying the concentration of dissolved gas in a sample in equilibrium with a fix 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).</i>
Data source location	<i>University of Montpellier, FR-34060, France</i>
Data accessibility	<i>Data is within this article.</i>

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.

Data type	Table URL (copy/paste the URL in your Internet browser)	Amount of data
CO ₂ solubility	pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2775&idDoc=1335&id=35272672	34
	pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2776&idDoc=1335&id=35305550	21
	pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2773&idDoc=1335&id=35245144	48
	pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2732&idDoc=1332&id=34354344	3
	pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2780&idDoc=1346&id=35361064	12
CO ₂ diffusivity	pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2826&idDoc=1346&id=36350532	11
	pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2779&idDoc=1346&id=35346176	11
	pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2778&idDoc=1346&id=35333312	12
	pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2777&idDoc=1346&id=35320430	16

	pfl.grignon.inra.fr/atWeb/TableServlet? viewTable=2733&idDoc=1332&id=34367074	11
O ₂ diffusivity	pfl.grignon.inra.fr/atWeb/TableServlet? viewTable=2764&idDoc=1342&id=35103704	24
	pfl.grignon.inra.fr/atWeb/TableServlet? viewTable=2755&idDoc=1342&id=34742706	30
	pfl.grignon.inra.fr/atWeb/TableServlet? viewTable=2754&idDoc=1342&id=34730102	10
	pfl.grignon.inra.fr/atWeb/TableServlet? viewTable=2765&idDoc=1342&id=35116534	44
	pfl.grignon.inra.fr/atWeb/TableServlet? viewTable=2910&idDoc=1342&id=40225446	2

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

- [1] E. Chaix, C. Guillaume, N. Gontard, V. Guillard, Performance of a non-invasive methodology for assessing oxygen diffusion in liquid and solid food products, *J. Food Eng.* 171 (2016) 87–94. <http://dx.doi.org/10.1016/j.jfoodeng.2015.10.014>.
- [2] C. Pénicaud, S. Guilbert, S. Peyron, N. Gontard, V. Guillard, Oxygen transfer in foods using oxygen luminescence sensors: influence of oxygen partial pressure and food nature and composition, *Food Chem.* 123 (2010) 127–1281 (<http://www.sciencedirect.com/science/article/B6T6R-5051PS2-2/2/923ab815d46f428626b86c9b60f335b5>).
- [3] E. Chaix, C. Guillaume, V. Guillard, Oxygen and carbon dioxide solubility and diffusivity in solid food matrices: a review of past and current knowledge, *Compr. Rev. Food Sci. Food Saf.* 13 (2014) 261–286. <http://dx.doi.org/10.1111/1541-4337.12058>.
- [4] E. Chaix, C. Guillaume, N. Gontard, V. Guillard, Diffusivity and solubility of CO₂ in dense solid food products, *J. Food Eng.* 166 (2015) 1–9. <http://dx.doi.org/10.1016/j.jfoodeng.2015.05.023>.
- [5] F. Acerbi, V. Guillard, C. Guillaume, N. Gontard, Impact of selected composition and ripening conditions on CO₂ solubility in semi-hard cheese, *Food Chem.* 192 (2016) 805–812. <http://dx.doi.org/10.1016/j.foodchem.2015.07.049>.
- [6] F. Acerbi, V. Guillard, C. Guillaume, M. Saubanere, N. Gontard, An appraisal of the impact of compositional and ripening parameters on CO₂ diffusivity in semi-hard cheese, *Food Chem.* 194 (2016) 1172–1179. <http://dx.doi.org/10.1016/j.foodchem.2015.08.020>.