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## CO<sub>2</sub> and O<sub>2</sub> solubility and diffusivity data in food products stored in data warehouse structured by ontology

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## Data in Brief

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## Data Article

# CO<sub>2</sub> and O<sub>2</sub> solubility and diffusivity data in food products stored in data warehouse structured by ontology



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## 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/>.

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## Specifications Table

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

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How data was acquired	<i>Chemical titration (for CO<sub>2</sub> quantification) and luminescence-based detection (for O<sub>2</sub> 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 CO<sub>2</sub> solubility and diffusivity data indispensable in food engineering to model CO<sub>2</sub> gas transfer in food.
- A unique set of O<sub>2</sub> diffusivity values within synthetic oils as a function of temperature.
- O<sub>2</sub> diffusivity data could be used to predict oxidation of O<sub>2</sub>-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 (O<sub>2</sub> and CO<sub>2</sub>) 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 <sub>2</sub> solubility	<a href="http://pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2775&amp;idDoc=1335&amp;id=35272672">pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2775&amp;idDoc=1335&amp;id=35272672</a>	34
	<a href="http://pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2776&amp;idDoc=1335&amp;id=35305550">pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2776&amp;idDoc=1335&amp;id=35305550</a>	21
	<a href="http://pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2773&amp;idDoc=1335&amp;id=35245144">pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2773&amp;idDoc=1335&amp;id=35245144</a>	48
	<a href="http://pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2732&amp;idDoc=1332&amp;id=34354344">pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2732&amp;idDoc=1332&amp;id=34354344</a>	3
	<a href="http://pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2780&amp;idDoc=1346&amp;id=35361064">pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2780&amp;idDoc=1346&amp;id=35361064</a>	12
CO <sub>2</sub> diffusivity	<a href="http://pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2826&amp;idDoc=1346&amp;id=36350532">pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2826&amp;idDoc=1346&amp;id=36350532</a>	11
	<a href="http://pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2779&amp;idDoc=1346&amp;id=35346176">pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2779&amp;idDoc=1346&amp;id=35346176</a>	11
	<a href="http://pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2778&amp;idDoc=1346&amp;id=35333312">pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2778&amp;idDoc=1346&amp;id=35333312</a>	12
	<a href="http://pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2777&amp;idDoc=1346&amp;id=35320430">pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2777&amp;idDoc=1346&amp;id=35320430</a>	16

	<a href="http://pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2733&amp;idDoc=1332&amp;id=34367074">pfl.grignon.inra.fr/atWeb/TableServlet? viewTable=2733&amp;idDoc=1332&amp;id=34367074</a>	11
O <sub>2</sub> diffusivity	<a href="http://pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2764&amp;idDoc=1342&amp;id=35103704">pfl.grignon.inra.fr/atWeb/TableServlet? viewTable=2764&amp;idDoc=1342&amp;id=35103704</a>	24
	<a href="http://pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2755&amp;idDoc=1342&amp;id=34742706">pfl.grignon.inra.fr/atWeb/TableServlet? viewTable=2755&amp;idDoc=1342&amp;id=34742706</a>	30
	<a href="http://pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2754&amp;idDoc=1342&amp;id=34730102">pfl.grignon.inra.fr/atWeb/TableServlet? viewTable=2754&amp;idDoc=1342&amp;id=34730102</a>	10
	<a href="http://pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2765&amp;idDoc=1342&amp;id=35116534">pfl.grignon.inra.fr/atWeb/TableServlet? viewTable=2765&amp;idDoc=1342&amp;id=35116534</a>	44
	<a href="http://pfl.grignon.inra.fr/atWeb/TableServlet?viewTable=2910&amp;idDoc=1342&amp;id=40225446">pfl.grignon.inra.fr/atWeb/TableServlet? viewTable=2910&amp;idDoc=1342&amp;id=40225446</a>	2

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## 2. Experimental design, materials and methods

**O<sub>2</sub>.** Oxygen optical sensors (Presens GmbH, Regensburg, Germany) were used to monitor O<sub>2</sub> 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 O<sub>2</sub> partial pressure in the medium. Two different set-ups exist (1) an invasive O<sub>2</sub>-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 O<sub>2</sub> in the surrounding of the sample. The mono-directional O<sub>2</sub> ingress into the sample was measured locally at the bottom or in the middle of the thin layer of food material previously free of O<sub>2</sub> using one of the aforementioned sensors. More details on the experimental set-up could be found in [1–3].

**CO<sub>2</sub>.** The solubility of CO<sub>2</sub> 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, CO<sub>2</sub> gas composition).

The diffusion of CO<sub>2</sub> was characterised by (1) imposing a gradient of CO<sub>2</sub> to a piece of material of simple geometry (cylinder or plane sheet), (2) measuring the CO<sub>2</sub> 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) CO<sub>2</sub> space-dependent profile in the cylindrical sample after its slicing and CO<sub>2</sub> quantification in each slice or (2) CO<sub>2</sub> time-dependent profile after CO<sub>2</sub> quantification in each thin slice (one slice corresponding at one time of kinetic) [4,6].

Numerical treatment. For both O<sub>2</sub> and CO<sub>2</sub>, 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<sup>®</sup> software.

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## 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>.

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