Carbon Dioxide Diffusion Loss from PET Bottle

Introduction

An interesting case is the diffusion of CO_2 (Carbon Dioxide) through the wall of a PET (Polyethylene Terephthalate) bottle that contains soft or alcoholic drinks. You can think of Cola or beer. Reason for putting gaseous CO_2 in drinks is taste. The gas gives a sparkling feeling and a reduction in tasted sweetness. You can imagine that diffusion of CO_2 through the wall is a problem because of loss of these features in time; in other words, a loss of quality in time.

It is obvious from the tabled gas figures on the website, that PET is - compared to other commonly used plastics - one of the best barriers against various gases. However, the overpressure of the gas in combination with thin bottle walls manufactured of partially amorphous PET[1], may lead to a considerable loss of CO_2. Below we assess the loss by diffusion of CO_2 from a 1.5 litre PET bottle for Cola.

Graphical Analysis

The following assumptions are reasonable for a bottle of Cola stored at room temperature:

- Concentration of CO_2 in a closed bottle: 7 gram / litre
- Pressure of CO_2 in a closed bottle: 3 bar
- Temperature: 24 degrees Celsius
- Thickness of the PET bottle wall: ~270 micrometer
- Total diffusion surface of standardized 1.5 litre PET bottle: 0.07 m^2

Solubility and diffusion properties of CO_2 in PET evaluated in initial conditions are:

- Solubility: 1×10^4 gram CO_2 /m^3 polymer at 3 Bar (1.7 m_{stp}^3 / m^3 x bar)
- CO_2 Diffusion coefficient: 2×10^{-13} m^2/s
- Activity of CO_2 in Cola: 0.97

Now let us look at the amount of CO_2 that is lost from the bottle during the first 40 hours and 2 years after production. See next page.

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[1] PET that is used for drink bottles contains a larger amorphous fraction than the almost completely crystalline PET that is evaluated in the solubility and diffusion table on the website. Practical applications of polymers nearly always require customized adaptation of the properties because of transparency, mechanical stability, etc. The difference in the physical properties of the PET on respectively the website table and this case are:
PET density: 1.48 / 1.35 gram/m^3,
CO_2-PET solubility: 1.4 / 1.7 m_{stp}^3 / m^3 x bar,
CO_2-PET diffusivity: 5.4 10^{-14} / 2 10^{-13} m^2/s.

Initial Loss of Carbon Dioxide from PET Bottle for Cola
CO2 Activity: 97% | Temperature: 24 degrees Celsius | Init. Gas Pressure: 3 bar

Figure 1. Initial loss expressed in grams.

Flux of Carbon Dioxide through PET Bottle Surface
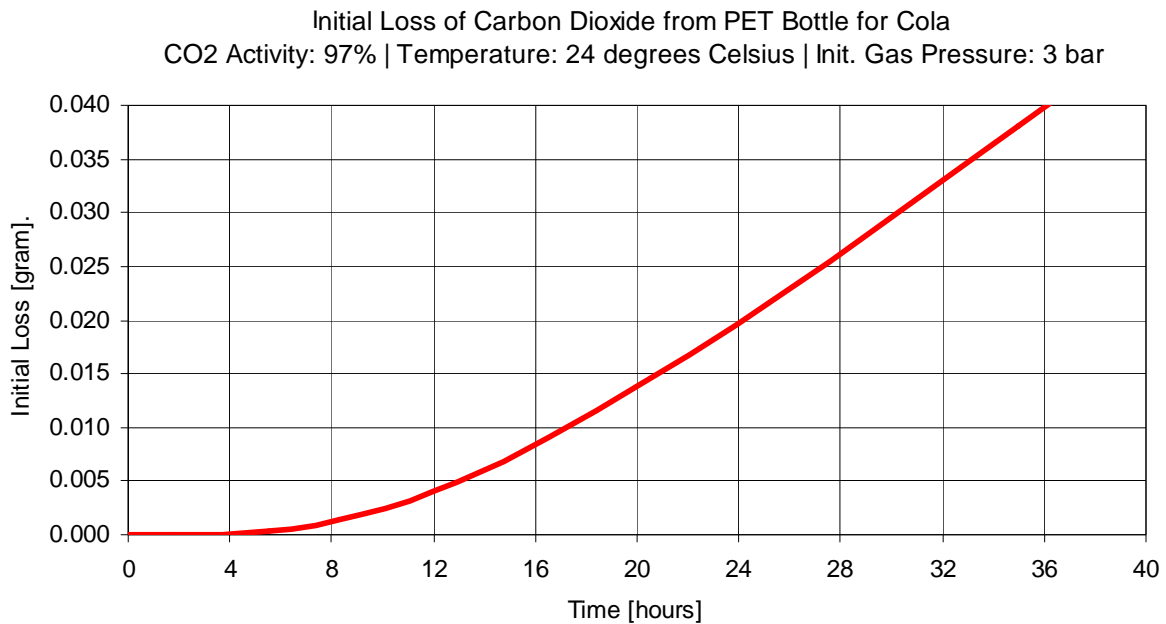#### CO2 Activity: 97% | Temperature: 24 degrees Celsius | Init. Gas Pressure: 3 bar
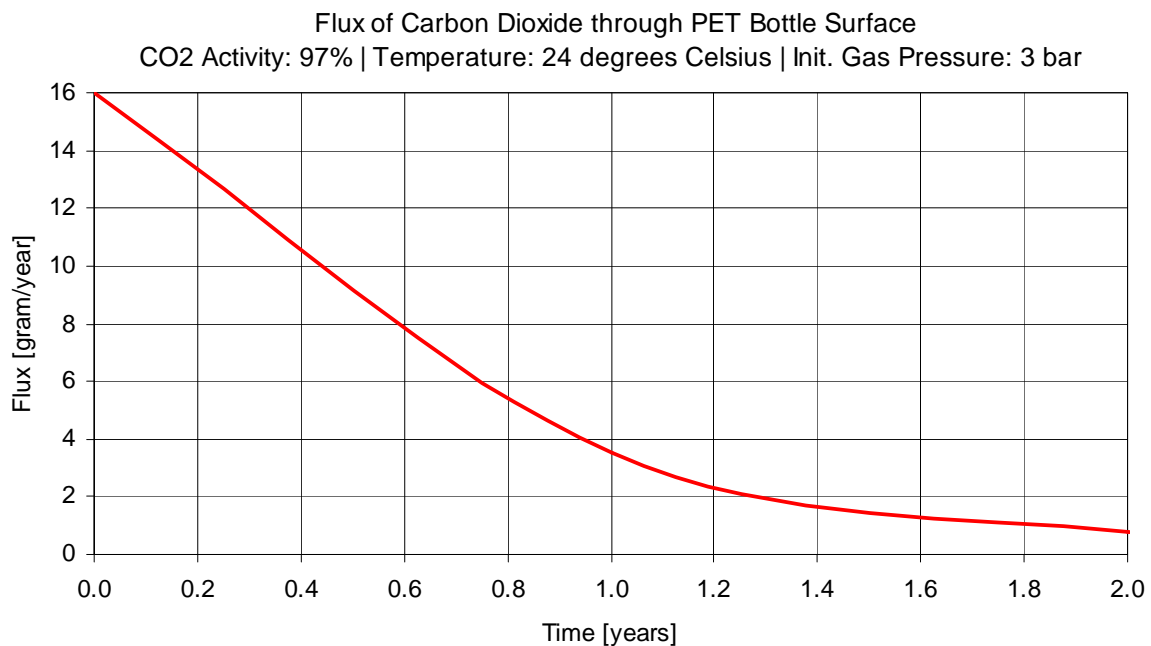

Figure 2. Loss during shelf life, expressed in flux.

Explanation

From figure 1 one can see that the time lag is relative short: after 4 hours the first CO_2 molecules escape from the bottle. From figure 2 it becomes clear that the loss reduces in the first year almost linearly and then slowly bends to a flux of zero. Reason for the loss reduction in time is the disappearance of CO_2 in the bottle and the related reduction of CO_2 pressure. After 1 year only 25% of the original amount of CO_2 is left, after 2 years less than 10%.