From oxygen concentration to oxygen flux

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Summary: In a closed oxygraph chamber, the oxygen concentration declines over time as a result of respiratory processes. The time derivative, therefore, is a negative number. Why is then the 'rate of oxygen consumption' not expressed as a negative value? Why is the term 'oxygen flux' used in this context of chemical reactions? The rationale is based on fundamental concepts of physical chemistry and non-equilibrium thermodynamics.

1   Oxygen concentration in the chamber of the Oxygraph

Concentration, c_B, is the expression of the amount of substance B per unit of volume, V. The amount of elemental oxygen dissolved per volume of the Oxygraph chamber is the oxygen concentration, c_{O2}, measured by the polarographic oxygen sensor (POS) as an electric current, I [A]. This current is converted and amplified into a voltage [V], which is recorded as the raw signal, R_t, at any time t [s]. The raw signal is calibrated and converted into oxygen concentration $c_{O2,t}$.

Since the oxygen concentration in pure water at equilibrium with air at standard barometric pressure of 100 kPa is 254.8 to 207.3 µmol/litre between 25 to 37 °C, it is most practical to express oxygen concentration in units µmol/litre.

$$1 \text{ µmol/litre} = 1 \text{ µmol/dm}^3 = 1 \text{ µM} = 1 \text{ nmol/ml} = 1 \text{ nmol/cm}^3$$

In the 'open' Oxgraph chamber, in which the aqueous medium is in equilibrium with a gas phase (such as air), the partial oxygen pressure, p_{O2} [kPa] is identical in the gas phase and aqueous phase. The oxygen concentration, however, is very different in air and water at equilibrium. At equilibrium, the gas concentration in the gas phase is much higher the the gas concentration in aqueous solution. The dissolved oxygen concentration is proportional to the partial oxygen pressure at constant temperature and composition of the aqueous medium. This proportionality constant is the oxygen solubility, S_{O2} [µM/kPa]. In pure water at 25 °C (37 °C), the oxygen solubility is 12.56 (10.56) µM/kPa.

2   Oxygen concentration as a function of time in the closed Oxygraph chamber

Cell respiration is the exergonic metabolic process in living cells or organisms, by which molecular oxygen is consumed, organic substances are oxidised, energy is converted, and carbon dioxide, water or other oxidised products are formed by the cell. In the 'closed' Oxygraph chamber, which is sealed against any exchange of oxygen across the chamber walls and sealings, all chemical reactions which consume oxygen (such as mitochondrial respiration) lead to a decline of oxygen concentration with time. If the oxygen consuming process is activated, then the oxygen concentration falls off more quickly or steeply over time. In contrast, when all oxygen consuming processes are fully inhibited, then the oxygen concentration remains constant over time.

3   Rate of reaction: Oxygen flux in the closed Oxygraph chamber

A linear negative slope, i.e. a constant fall of oxygen concentration with time in the closed Oxygraph chamber, is the result of a constant rate of the chemical

reaction. The faster the reaction rate, the steeper is the negative slope. Defining the reaction as

$$\text{Substrate(s)} + O_2 = \text{Product(s)} \tag{1}$$

then the oxygen consumption rate per unit volume (= oxygen flux, volume-specific) is proportional to the negative slope of oxygen concentration with time.

In mathematical terms, we may consider the difference of oxygen concentration between two time points,

$$\Delta t = t_2 - t_1 \tag{2a}$$

$$\Delta c_{O2} = c_{O2,2} - c_{O2,1} \tag{2b}$$

The slope between these points is the rate of concentration change,

$$r_{O2} = \Delta c_{O2} / \Delta t \tag{3}$$

whereas the rate of reaction [Eq 1] is the negative slope (the negative sign is due to the stoichiometric number of oxygen of −1 in Eq 1),

$$J_{O2} = -(\Delta c_{O2} / \Delta t) \tag{4}$$

In differential form (when the time difference is taken infinitesimally small), the expression becomes

$$J_{O2} = -(dc_{O2} / dt) \tag{5}$$

With the differential form [Eq 5], gradual changes of oxygen flux can be evaluated, in contrast to the assumption of linearity in the difference form [Eq 4].

4 Reference

Gnaiger E (1993) Nonequilibrium thermodynamics of energy transformations. *Pure & Appl. Chem.* 65: 1983-2002.