A chance to work with Dr. Pijpers' data

(Connects to Figure 3B)

In Figure 3B, the Solar-to-Fuel efficiency of the artificial leaf was determined as follows. Students can use the raw data, provided by Dr. Pijpers and used in his experiments, to recreate the figure.

To collect this data, the "leaf" (the wireless cell) was immersed in an electrolyte in a closed reactor vessel (so air from the outside could not get in) that was filled with nitrogen. The leaf was illuminated by a solar simulator (a lamp with the same color and intensity as sunlight). See the figure below for a diagram of the experimental conditions.

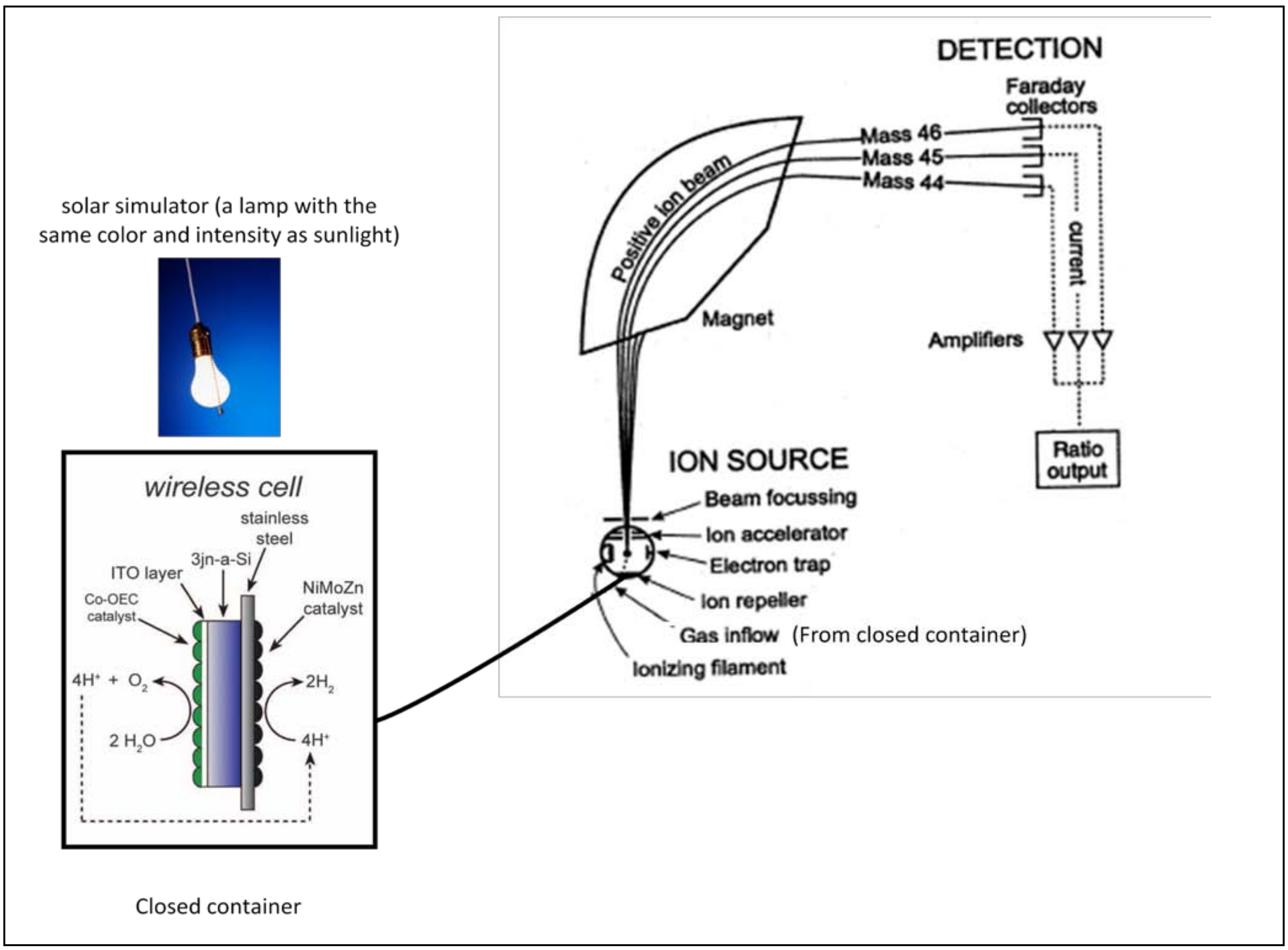
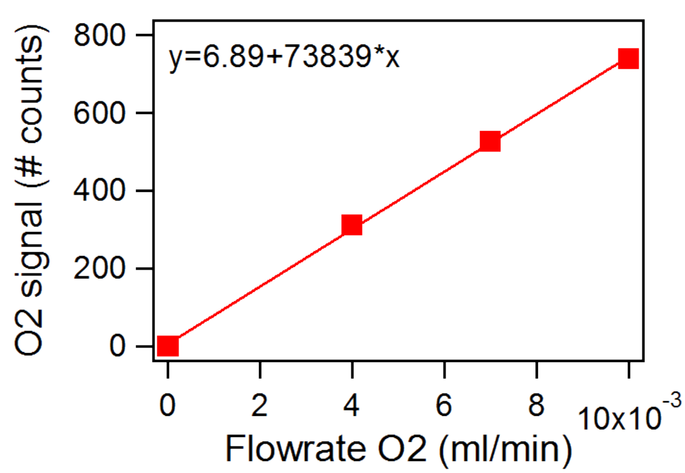


Figure is adapted from http://en.wikipedia.org/wiki/File:Mass_spectrometer_schematics.png and Reece *et al*. *Science* (2011) 334: 645-648.

As soon as the light is switched on, H_2 and O_2 evolve from the leaf and bubble into the headspace of the closed vessel. (Click here for a video of the wireless cell at work). From the headspace, the product gases were flown into a mass spectrometer. In this device, the inlet gas stream is ionized by an ion beam creating charged molecules. These charged species are led to a mass analyzer, which sorts the ions by their masses by applying electromagnetic fields. Charged species with different mass (e.g. charged H_2 and O_2) are deflected along a different pathway, so H_2 and O_2 species hit the detector at a different spot. The output of the detector is as "number of counts", i.e., the number of times that ionized H_2 or O_2 molecules hit the detector. This number is rather meaningless and this is why Dr. Pijpers converted it into a "Solar-to-Fuel" efficiency using the calibration method described below.

The solar simulator was switched on, causing the leaf to start bubbling. **This is indicated by time 0:00 on the excel spreadsheet.** The mass spectrometer signal in the data file (corresponding to the O_2 signal) started to rise until the concentration in the headspace was constant. After about 2 hours of operation, the lamp was switched off and the leaf stopped operating. Next, calibration gases with different compositions [i.e. with known O_2 contents, e.g., 1 ppm (parts per million) O_2 in N_2] were flown through the headspace of the reactor. In this configuration, the signal that the mass spectrometer detects originates from a gas flow with known O_2 concentration. Since Dr. Pijpers knows the flow rate of the calibration gas stream, he could construct the following calibration curve for a number of different calibration gas compositions (note: the raw mass spectrometer data for the calibration curve is not given in the spreadsheet):



The line through these data points is the calibration curve. Using this calibration curve, students can infer the O_2 flow rate (in ml O_2/min) for a given value of the MS signal (in number of counts).

The calculation below shows how students can convert the number on the left axis (in number of counts, O_2) (**found in columns C and G of the excel file**) into Solar-to-Fuel efficiency (in %):

The Solar to Fuel efficiency is subsequently obtained in a number of steps:

1. Convert [ml O_2/min] into [ml O_2/s] **(these numbers are found in column C and G of the excel file, corresponding to operation two different electrolytes).**

2. Convert [ml O_2/s] into [m3 O_2/s] **(there are 1,000,000 milliliters in 1 cubic meter)**

3. Convert [m3 O_2/ s] into [mol O_2/s] using the ideal gas law (pV = nRT, p = 108000 Pa, T = 295K, R = 8.314) **(please note: This is slightly different from the usual ideal gas law in that the units of V and n are m3/s and moles/s, respectively, because we are dealing with flow rates.)**

4. Convert [mol O_2/s] into the moles of electrons that you need to make this amount of O_2 [i.e., multiply (mol O_2/s) by 4, since the reaction equation is 2 $H_2O \rightarrow O_2 + 4H^+ + 4e^-$]

5. Convert [moles e^-/s] into current (Ampere) by multiplying with the Faraday constant [= 96485 Coulombs/mole}.

6. Convert the current into efficiency (eff = Current*1.23/0.15), where 1.23 is the potential that you store by water splitting (1.23 V), so the numerator is the power output by the leaf (P = I*V). The number in the denominator (0.15) is the power input by the lamp that is hitting the area of the leaf (0.15 W); the intensity of the lamp is 0.1 W/cm^2 (often taken as the standard intensity for sunlight), and the area of the leaf is 1.5 cm^2, so the leaf of this particular size is exposed to 0.15 W of light.