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A model of humidity behavior in CHUPS and dummy TPC and experimental test

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1. Model for water outgasing.

We have some volume with water partial pressure $P[ppb]$. This is the partial pressure which we are measuring at the exit of the volume. Let assume that at the inlet of the volume we have volume flux $Q\left[\frac{l}{\min}\right]$ and partial water pressure $P_1[ppb]$.

Let assume that the mass flux ($Q_w\left[\frac{ppb\cdot l}{\min}\right]$) of the water from the walls will be

$$Q_w = a \cdot (P_e - P), \tag{1}$$

where

$a\left[\frac{l}{\min}\right]$– coefficient,

$P_e[ppb]$– some equilibrium partial pressure, which will be in the volume without any flux after infinite time. Mass balance of the water in the system will be

$$V\frac{\partial P}{\partial t} = QP_1 - QP + a \cdot (P_e - P), \tag{2}$$

where $V[l]$is the system volume.

In this case the mass balance when nothing changes $\frac{\partial P}{\partial t} = 0$ will be:

$$QP_1 + a \cdot (P_e - P) = QP. \tag{3}$$

We can express P:

$$\begin{gathered} QP_1 + a \cdot P_e - a \cdot P = QP \\ P = \frac{QP_1 + a \cdot P_e}{Q + a} \end{gathered} \quad . \tag{4}$$

a is unknown parameter, P_1 is a parameter of the inlet gas (CHUPS itself), P_e– parameter of the volume (history of preparation, materials, surface quality and so on).

$$P = \frac{QP_1 + a \cdot P_e}{Q + a} \tag{5}$$

2. Experiment with the CHUPS water outgasing without any external volume.

We made the number of experiment when the external volume (dummy TPC) was cut off. The tests have been done at the different fluxes of the hydrogen (see fig. 1).

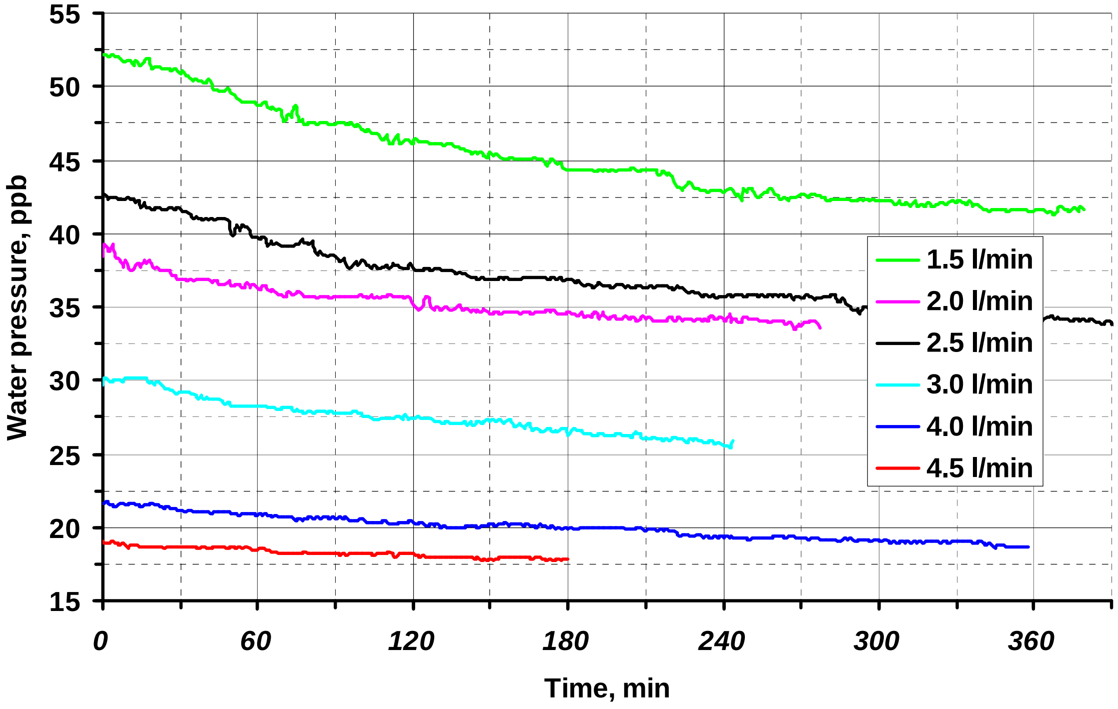

Fig. 1. Time dependence of the water partial pressure at the different fluxes without any external volume.

Analyses of these curves on base of simple exponential decay ($P = P_{end} + (P_0 - P_{end})e^{-\frac{t}{t_1}}$) gives the parameter P_{end} (see fig. 2). Fit of the experimental date on base of (5) gives

$P_e = 137 \pm 36\, ppb$ − pressure which will be in the closed system without hydrogen flux.

$P_1 = -1.7 \pm 4.2\, ppb$ − pressure after the last “cold part” of CHUPS. This is practical “0”.

$a = 0.67 \pm 0.32 \frac{l}{\min}$ − “effective” water flux from the walls.

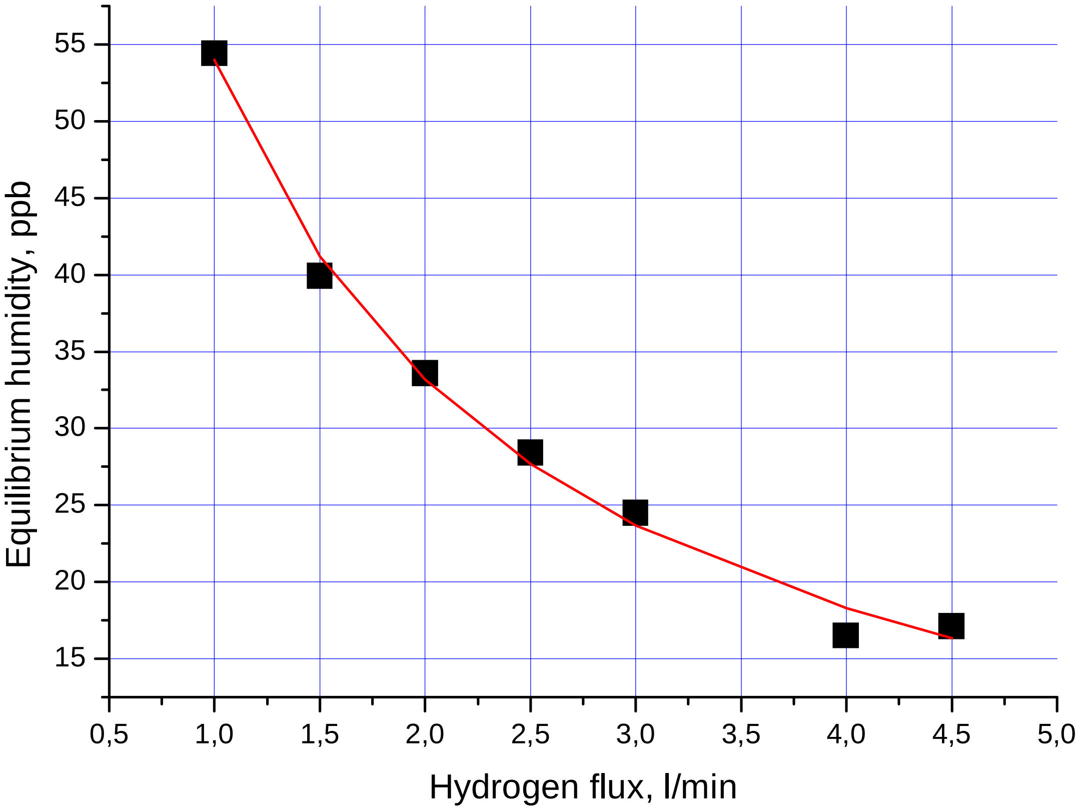

Fig. 1. Equilibrium humidity at the different fluxes without any external volume.

Main conclusions from this experiment are:

- after the last cold part of CHUPS we have virtually zero humidity;
- reserve volume “1”, 1 m stainless steal tubes, MFC and few valves give humidity at the flux 2 l/min (nominal flux) about 32 ppb;
- we did not see “drying” of this part of CHUPS elements during 7 days of operation at different fluxes. It means that “water capacity” of these elements is much bigger than “drying” velocity by the hydrogen flow at room temperature.
- “reasonable” parameters partly confirm the model of outgasing.

3. Experiment with the water outgasing with dummy TPC at room temperature.

We can solve differential equation (2) respect P

$$V\frac{\partial P}{\partial t}=\left(QP_1+aP_e\right)-P\left(Q+a\right),$$

$$V\frac{\partial\left(P-\dfrac{QP_1+aP_e}{Q+a}\right)}{\partial t}=-\left(Q+a\right)\left(P-\frac{QP_1+aP_e}{Q+a}\right),$$

$$P-\frac{QP_1+aP_e}{Q+a}=Ce^{-\frac{Q+a}{V}t}, \tag{6}$$

where C is a free constant defined by the starting pressure point P_{20}.

$$-C=\frac{QP_1+aP_e}{Q+a}-P_{20}. \tag{7}$$

Finally

$$P=\frac{QP_1+aP_e}{Q+a}-\left(\frac{QP_1+aP_e}{Q+a}-P_{20}\right)e^{-\frac{Q+a}{V}t}. \tag{8}$$

The "drying" process for dummy TPC at the hydrogen flux $2.5\frac{l}{\min}$ is shown in figure 3. The

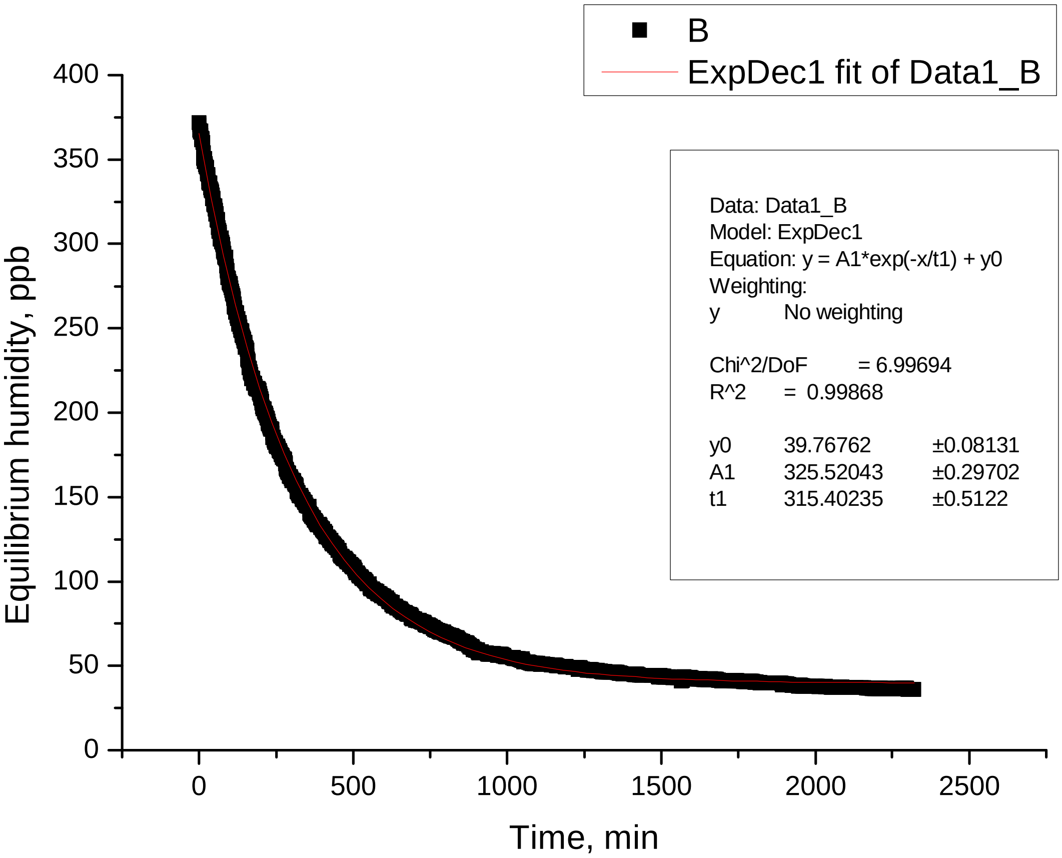

Fig. 3. Humidity dependence after dummy TPC at room temperature.

The final concentration of water is $39.8\pm0.1\,ppb$. It is only on $15\,ppb$ bigger than concentration without dummy. Parameter $t_1=315.4\pm0.5\min$ we can write from (8) as

$$t_1 = \frac{V}{Q+a} = \frac{260\,l}{2.5\frac{l}{\min}} = 104\min \tag{9}$$

this is 3 times faster then real exponent!!! We compare with "drying" curves of the humidity sensor itself and understand that this is own sensor drying time.

3. Experiment with the water outgasing with dummy TPC at with heating.

The aim of the experiment with dummy TPC heating was:

- define how much water we have on the inner dummy TPC surface;
- try to decrease the humidity in the system.

Heating has been done up to the $110 \pm 5C$. The humidity dependence is shown in figure 4.

A – time interval for dummy TPC heating from room temperature up $110 \pm 5C$;

B – interval when dummy TPC was at temperature $110 \pm 5C$;

C – interval of cooling down to the room temperature;

D – interval of "drying" of dummy TPC at room temperature.

E – this jump on the humidity line is visible in the both directions. This is connected with the internal calibration curve of the sensor (decades are not connected).

F – alarm situation connected with the liquid nitrogen level.

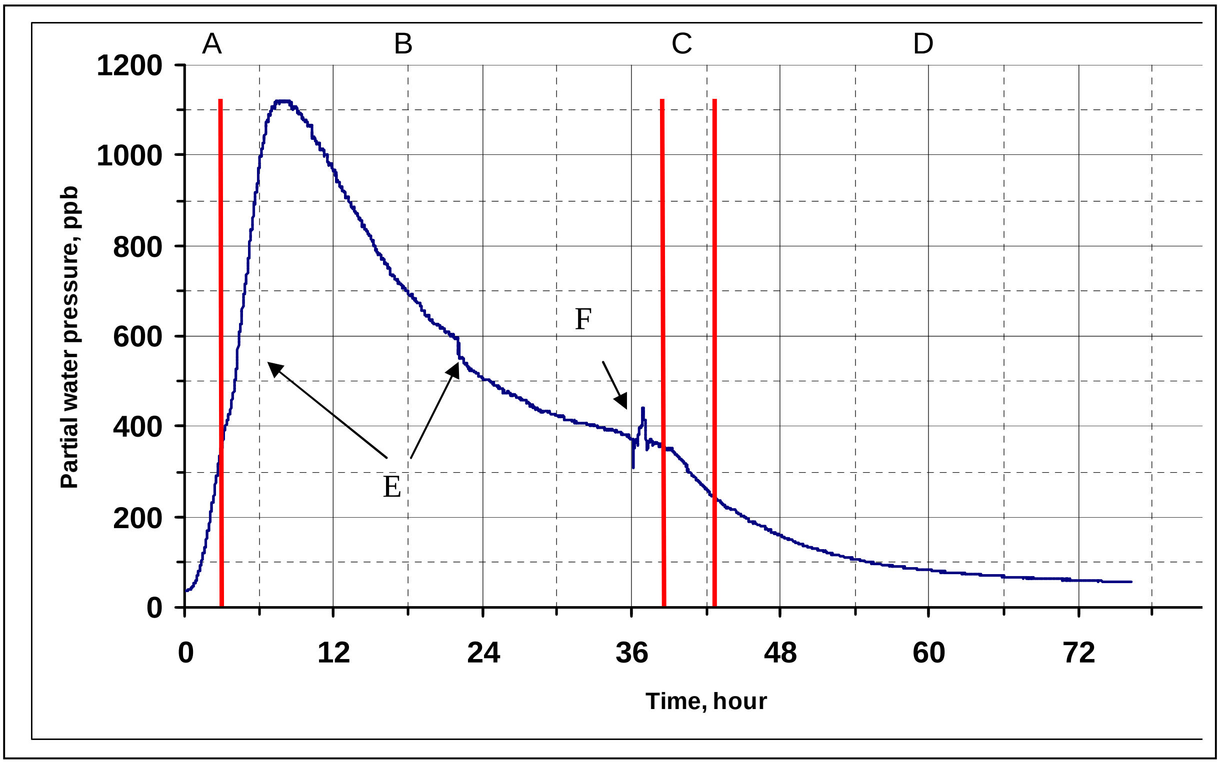

Fig. 4. Humidity during and after the heating of dummy TPC.

We have to analyze and compare two "drying" intervals: at high temperature and at room temperature. The parameters of exponent decay are done in table 1.

Table 1.

Experiment	P_e, ppb	t_1, min
Before heating	39.8 ± 0.1	315.4 ± 0.5
At $110 \pm 5C$	294.8 ± 1.5	658 ± 4
After heating	53.3 ± 0.1	536 ± 1

Parameters of the “drying” are not reproducible and we did not improve humidity situation in the system. We can not explain the decreasing of the “drying” velocity after heating. On base of these measurements we can make ONLY conclusions that: during heating we extract the water quantity much smaller then the total quantity of the water in dummy TPC.

Water flux from the system is

$$Q_{H_2O}\left[\frac{1}{\min}\right] = \frac{P_{H_2}[bar]\cdot P_{H_2o}[ppb]\cdot 10^{-9}\cdot Q_{H_2}\left[\frac{l}{\min}\right]\cdot N_A\left[\frac{1}{mole}\right]}{V_A\left[\frac{bar\cdot l}{mole}\right]} \tag{10}$$

The total water quantity extracted from the system during the experiment will be

$$N_{H_2O} = \int_o^{t_{end}} Q_{H_2O}(t)dt = \frac{P_{H_2}\cdot 10^{-9}\cdot Q_{H_2}\cdot N_A}{V_A}\int_0^{t_{end}} P_{H_2o}dt \tag{11}$$

During our experiment ($4579\min$) we extract

$$N_{H_2O} = \frac{P_{H_2}\cdot 10^{-9}\cdot Q_{H_2}\cdot N_A}{V_A}\int_0^{t_{end}} P_{H_2o}dt = \frac{10\cdot 10^{-9}\cdot 2.5\cdot 6.02\cdot 10^{23}}{22.4}\cdot 1685449 = 1.13\cdot 10^{21}\, molecules$$

This is $34mg$ of the water – really huge number!!!

Example. If we have the nominal flux $2\frac{l}{\min}$ and the partial water pressure $50\,ppb$ the water flux from the chamber will be

$$Q_{H_2O} = \frac{P_{H_2}\cdot P_{H_2o}\cdot 10^{-9}\cdot Q_{H_2}\cdot N_A}{V_A} = 2.69\cdot 10^{16}\left[\frac{molecules}{\min}\right] \tag{12}$$

“Drying” time for the water quantity which was extracted during the heating will be

$$t = \frac{N_{H_2O}}{Q_{H_2O}} = \frac{1.13\cdot 10^{21}}{2.69\cdot 10^{16}} = 42000\min \approx 1month \tag{13}$$

Water extraction from the surface is connected with the monolayers destruction. We can calculate the water in one monolayer.

Inner surface of Dummy TPS is

$$S_{Dummy} = \left[p\,(d-2t)\right]\cdot h + 2\left[p\,\frac{(d-t)^2}{4}\right], \tag{14}$$

Where *d* − outer diameter of the chamber;
t − thickness of walls;
h − height of the chamber.
By *d* = 0.22 m, *h* = 0.87 m and *t* = 0.005 m S_{Dummy} = 0.647 m^2.
Area per 1 molecule of H_20 is

$$S_{H_2O} = 1\cdot 10^{-15}\,cm^2 \qquad (15),$$

thus the total amount of water molecules inside the Dummy TPS (in assumption of monolayer) is

$$N_{H2O} = \frac{S_{Dummy}}{S_{H_2O}} = 6.466\cdot 10^{18} \tag{16}$$

During heating we destroy and pump $\frac{1.13\cdot 10^{21}}{6.466\cdot 10^{18}} = 175$ monolayers.

4. Conclusions.

1. After the last cold part of CHUPS we have practical zero humidity.
2. At the nominal flux of hydrogen $2.5\frac{l}{\min}$ the CHUPS elements (tubes, valves, MFC, reserve volume 1) increase humidity up to $26\,ppb$. During the experiment we did not see the changes in this value – surface water quantity is much bigger in comparison of the drying speed.
3. With dummy TPC we reached $40\,ppb$ humidity at hydrogen flux $2.5\frac{l}{\min}$.
4. Heating of dummy TPC up to $110C$ during about two days released from the surface $34\,mg$ of water. It corresponds to one month CHUPS operation at room temperature.
5. Heating experiment did not improve the final humidity in the system. We are going to repeat heating.
6. We have to discuss with all colleagues procedures of TPC drying before hydrogen filling.