

# CFD of the pressure distribution in the Nel electrolyzer during sudden start-up

Ahad Zarghami and Bert Vreman

## Introduction

A flexible electrolyser should be able to operate over a broad range of operating conditions and flow regimes. Any change of operating condition, such as flow velocity, in the system induces a change in pressure. The sudden startup of the electrolyser may cause flow transient and water hammer phenomena in the top part (collector) of the compartments that could result in too high pressure in the electrolyser. It is therefore important to estimate the mixture pressure buildup that can be expected.

A Nel electrolyser consists of 200 hydrogen and oxygen compartments located side-by-side (see Fig. 1). When the system is started up, a huge amount of gas is generated at the electroded and consequently, a large amount of electrolyte is moved out of the cells toward the collector (or head space) that may result in violent change of the pressure in the collector. In order to analysis the pressure distribution, some CFD tests on full-size geometry of the collector are done.



Fig 1: A Nel electrolyser.

## Simulation Setup

For doing simulations, we focus on the collector of the hydrogen. The schematic drawing of the cross-section of a Nel electrochemical cell is shown in Fig. 2. The size of the cross-section for

doing simulations is shown in Fig. 3, which have been approximated from the real-size cell. Also, the bottom-view of the selected geometry, that consists of 200 openings as the hydrogen inlets and 200 walls between the openings, is shown in Fig. 3, as well.

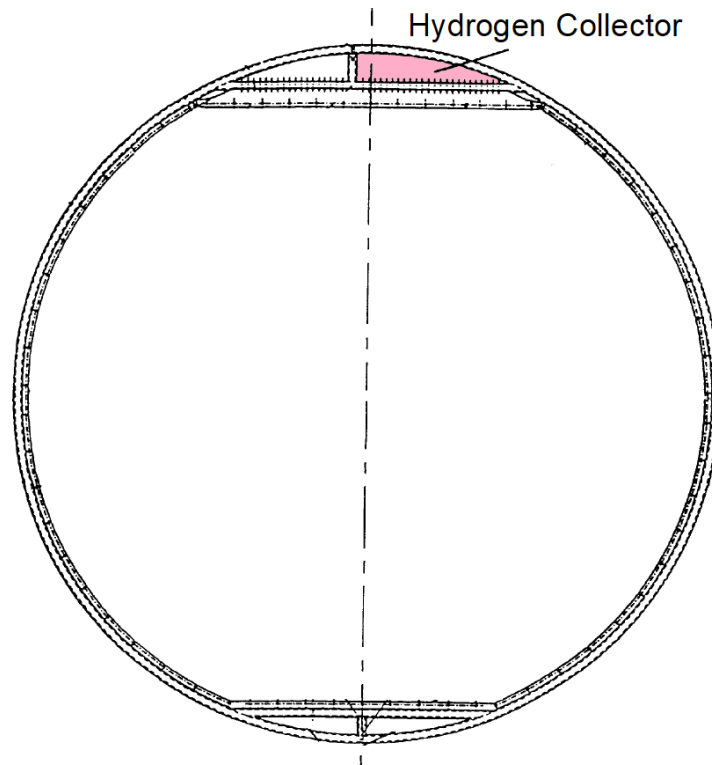


Fig. 2: The cross-section of an electrochemical cell.

The width of each hydrogen inlet and also the thickness of the wall between the inlets are set to 2 cm. For numerical stability issues, the last wall of the collector is enlarged and is considered equal to 50 cm. Hence, the total size of the collector is 8.5 m. When the system starts up, the gas is generated at the electrodes and the liquid, i.e. KOH-H<sub>2</sub>O, is pushed into the collector. Hence, only the liquid phase is considered as the flow inlet into the collector, since this expected to cause the largest possible pressure rise. The flow is modeled as a turbulent flow and the normal velocity-inlet boundary condition is applied for the inlets as the liquid phase enters to the collector with  $U_{in}=0.22$  m/s, which is equivalent to the superficial velocity of the gas through the outlet during normal continuous operation. The walls and outlet are modeled as no-slip and pressure-outlet boundary conditions, respectively.

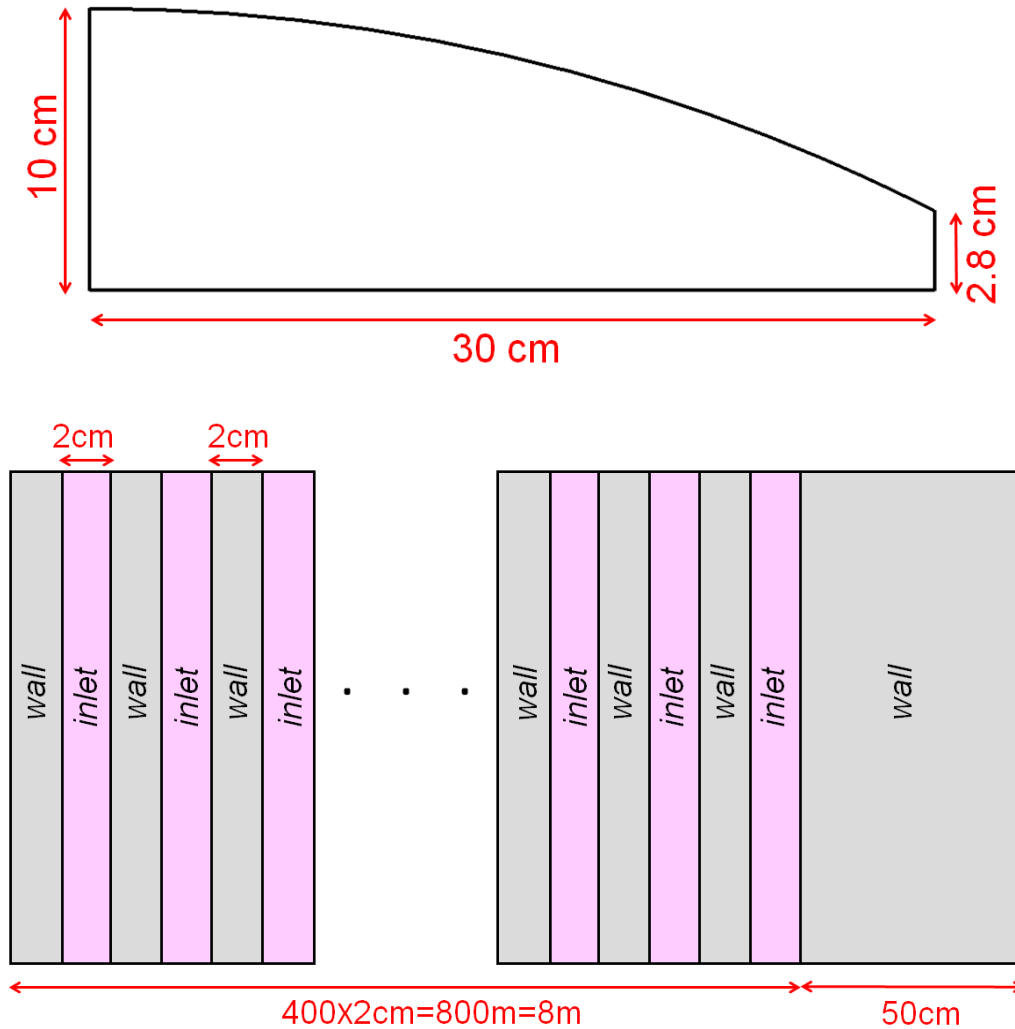


Fig. 3: Side-view cross-section (top panel) and bottom-view cross-section (bottom panel) of the hydrogen collector (head space).

## Results

The simulations are performed for three different mesh sizes, i.e. element size equal to 0.02, 0.01 and 0.005 m, by using ANSYS-Fluent 19.1. The pressure distributions one centimeter above the inlets and along the longitude cross-section of the collector for  $i=2000 \text{ A/m}^2$  are shown in Fig. 4. The results show that the maximum pressure happens above the first inlets. The pressure decreases monotonically as a function of the collector length as reaches zero at outlet. Also, it is clear that by increasing the mesh density, the pressure decreases slightly. The maximum value of the static pressure for the finest mesh is equal to 2.6 bar (2.6 bar higher than the pressure at the outlet of the collector). This large value indicates that the pressure variation in the collector during this startup condition is large. The static pressure contour in the collector is shown in Fig. 5.

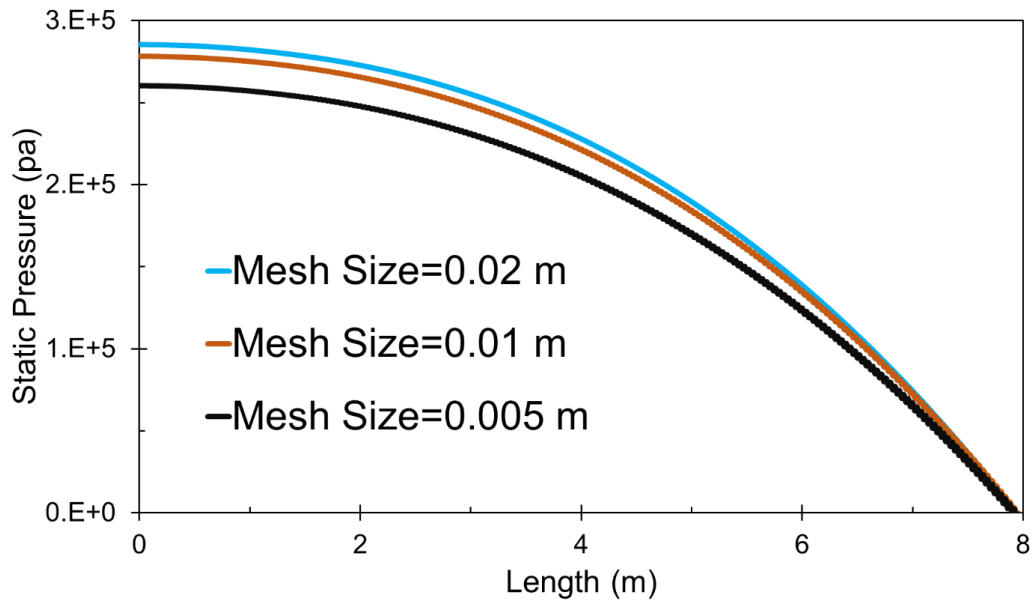


Fig. 4: The pressure distribution along the centerline in the collector.

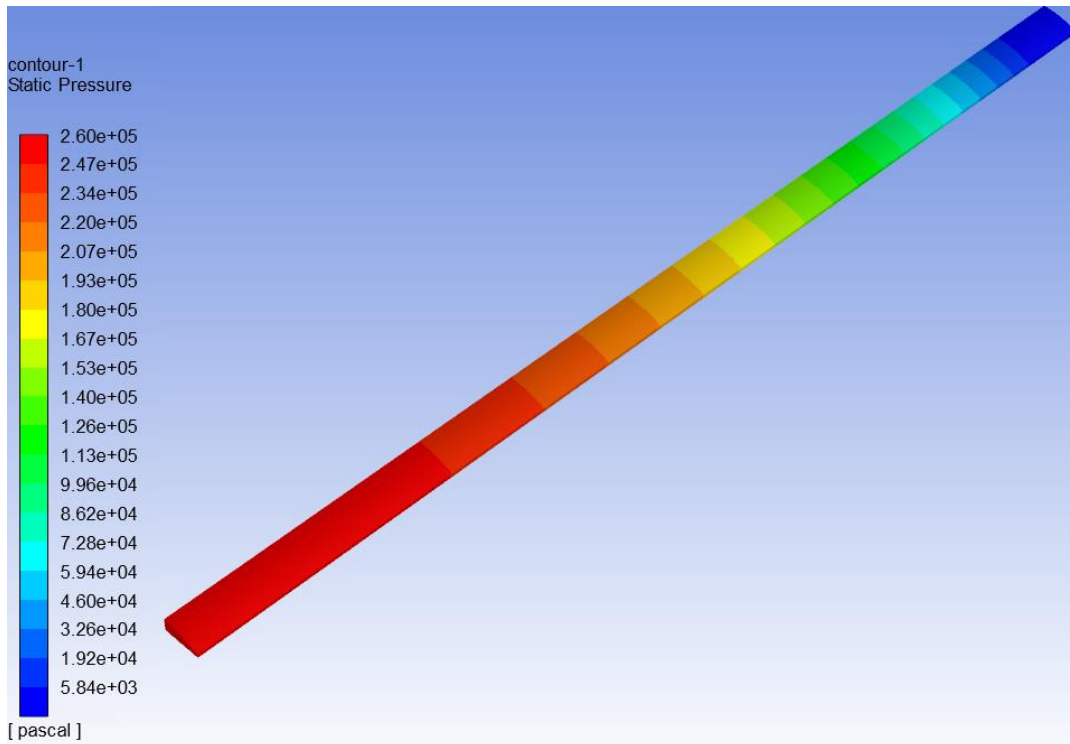


Fig. 5: The pressure distribution contour in the collector.

## Discussion and conclusion

For flexible operation of the Nel electrolyzer, it is important to estimate the increase of the pressure in the cells at sudden start-up. The pressure is not allowed to become too high (so-called blow-up of the electrolyzers should be prevented).

In the previous sections we considered 200 half-cells, in which the hydrogen is produced, in a stack. The current density was  $2000 \text{ A/m}^2$ . The electrolyte superficial velocity of  $0.3 \text{ mm/s}$  due to circulation of the electrolyte at normal operation is small compared to the electrolyte superficial velocity during start-up and is therefore neglected. At sudden start-up the maximum volumetric flow of liquid going from a hydrogen cell compartment into the collector above the compartments will not be larger than the volume of gas produced in the cell per second at atmospheric pressure, which is

$$2000 \text{ A/m}^2 * (\pi/4) * (2 \text{ m})^2 / (2 * 96485 \text{ mol/C}) * 1.35 * 0.03 \text{ m}^3/\text{mol} = 0.0013 \text{ m}^3/\text{s}.$$

The factor 1.35 accounts for the water vapor content in the gas and the  $0.03 \text{ m}^3/\text{mol}$  is the volume per mole of gas at  $80^\circ\text{C}$ .

The cross section of the outlet of the half-cell (the inlet of the collector) is assumed to be  $0.30 \text{ m} * 0.02 \text{ m} = 0.006 \text{ m}^2$ . Thus, the maximum velocity at the inlet of the collector is  $0.0013 / 0.006 = 0.22 \text{ m/s}$ .

If the electrolyte enters with a velocity of  $0.22 \text{ m/s}$  in each inlet of the collector, we deduce from the simulations in the previous section that the pressure drop in the collector is 2.6 bar.

### Effect of the communication between the cell inlets at the bottom of the cells

According to the computations in this report the pressure in the cell is a function of the axial coordinate of the collector. Since the cell inlets are connected through the distributor at the bottom, electrolyte from cells with higher pressure will start to flow to cells with lower pressure via the inlets of the cells. However, since the area of these inlets is much smaller than the area of the outlets (the inlets of the collector), the effect of flow interaction via the bottom distributor on the pressure in the cells might be relatively small.

### Effect of the increase of the pressure on the gas volume produced

Since the gas volume produced is reversely proportional with the pressure  $p$  in the cell, the velocity at the collector inlets will in fact not be the same for all inlet, but it can be described as

$$u = (p_0 / p) * 0.22 \text{ m/s}.$$

Due to this effect the pressure drop over the collector is expected to be substantially smaller than the computed 2.6 bar. The CFD simulation could be refined by a user-defined inlet condition according to the formula above. This is not trivial; the introduction of an underrelaxation factor in the application of such a dynamic pressure dependent velocity inlet condition might be necessary to obtain convergence.

### Effect of bars in the in the cell outlets (collector inlets)

In practice, there are bars in the cell outlets, which reduce the open area of these outlets and thereby reduce electric shunt currents. We have not specific information about these bars but suppose that they act like an orifice and reduce the open area by a factor  $f$ . The resistance

coefficient of an orifice can be estimated by  $2f^4$ . Thus, we estimate the pressure drop over the cell outlets by  $2 f^4 * 0.5 * 1200 \text{ kg/m}^3 * (0.22 \text{ m/s})^2 \approx 60 f^4 \text{ Pa} = 0.0006 f^4 \text{ bar}$ . This pressure drop equals 0.01 bar if  $f = 2$  and 0.15 bar if  $f=4$ .

### **Effect of liquid height in the gas-liquid separators**

The outlet of the collector is connected to a gas-liquid separator (hydrogen and oxygen have separate collectors and separators). Let us assume that before start-up the liquid level in the gas-liquid separator is just below the outlet of the collector. We also assume that during sudden start-up no liquid can leave the separator (extreme case). Then the liquid level will rise above the outlet of the collector and the pressure in the cell will increase by  $\rho gh$ , where  $\rho=1200 \text{ kg/m}^3$ ,  $g = 9.8 \text{ m/s}^2$  and  $h$  is the increase of the level.

Suppose the diameter of the gas-liquid evaporator is 1.5 m. Suppose the diameter of the electrolyzer is 2 m, the width of the hydrogen compartment  $w$ , and there are 200 compartments. Suppose the gas volume fraction during normal operation is  $v_f=0.4$ . If the electrolyzer is filled with electrolyte before start-up, the amount of liquid that is pushed out of the electrolyzer during start-up is

$$200 * v_f * w * 0.25 * \pi * 2^2 = 628 v_f * w.$$

Then the level in the gas liquid separator increases by

$$h = 628 * v_f * w / (0.25 * \pi * 1.5^2) = 355 * v_f * w.$$

Substituting  $v_f = 0.4$  and  $w=0.02 \text{ m}$  for the hydrogen compartment leads to  $h=2.8 \text{ m}$ , so that the pressure further increases by 0.34 bar.

### **Differences between hydrogen and oxygen sides**

At the oxygen side, the gas volume produced is less by a factor two, the cell outlet area is different, and the gas collector geometry is different. Also,  $v_f$  and  $w$  on the oxygen sides are probably not the same as on the hydrogen side. Thus, the pressure drop over the oxygen collector at sudden start-up and the increase of the liquid level in the oxygen separator are different from their hydrogen counterparts. This leads to several problems. One problem is that substantial pressure differences across the diaphragms separating the hydrogen and oxygen compartments will occur. This not allowed since these differences cause gas crossover through the diaphragms. Another problem is that the level control of the gas liquid separators can probably not handle fast and large level variations.

### **Conclusion**

CFD simulations of the flow in the head space (collector) of the electrolyzer during sudden start-up has been performed. A pressure drop of 2.6 bar was simulated, from which we conclude that the pressure in the cells upon sudden start-up can rise to 3.6 bar. We regard this estimate as a worst-case estimate. The estimate could be refined by several consideration, as discussed above. Overall, it is likely that the cell pressure during sudden start-up will be substantially lower than 3.6 bar. Nonetheless, we do include that in case of a sudden start-up, a large increase of the pressure in the cells of the electrolyzer can indeed occur.

