Considerations for modeling the fuel cell stack

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(Preliminary note: For clarity of language, in this document *cell* refers to an individual fuel cell, and *stack* means a collection of individual cells. This may differ from how the term "fuel cell" is used elsewhere.)

1. The maximum theoretical voltage (V_T, where the subscript T is short for thermodynamic) of a single cell is not attained in practice due to the voltage drop driving the reaction (ΔV) and due to resistance to electron and ionic "flow" through the components of the cell (V_Ω). The result is that the measured external voltage (V_E) is lower than V_T, with the complete relationship being $V_T = V_E + V_\Omega + \Delta V$.
2. The reaction rate of hydrogen at the anode is orders of magnitude faster than the oxygen reaction at the cathode. Thus, the oxygen side is used to model the cell performance. This rate expression is $i = i_0^* \cdot \varepsilon \cdot P_{O_2} \exp(\beta \cdot \Delta V)$, where i and i_0^* are current densities (i_0^* is a constant), ε is an effectiveness factor (reduced by accumulation of water on the surface of the catalyst at high reaction rates), P_{O2} is partial pressure of oxygen, β is a kinetic parameter, and ΔV is as identified above. Note that the rate expression includes the partial pressure of O_2 and that the reaction is voltage-driven because electrical potential (ΔV) is the driving force for overcoming the activation barrier in electrochemical reactions, just as temperature is in chemical reactions.
3. The UO lab "fuel cell" setup consists of 3 cells arranged in *series*, both electrically and with respect to gas flow[1]. As a result, the same current passes through each cell (current density is the same for each cell) and the total stack voltage is the sum of the individual cell voltages. In addition, oxygen and hydrogen are depleted as they flow from cell to cell. Consider the effects of the depletion of these gases on both net rate of flow and partial pressure: Since H_2 is pure gas (with some humidification), its partial pressure should not change significantly (barring gas crossover or side reactions), provided that it is not entirely consumed. However, the source for O_2 is air—a mixture that is at most 21% O_2 if it is humidified. Since the inert N_2 in air is not consumed, the partial pressure of O_2 drops from cell to cell as it is consumed. Note that the <u>total</u> pressure in the stack remains constant for each gas stream (H_2 and air) and is determined by the back pressure regulators (see operator's manual Figure 5B.2, p. 52), but the <u>net</u> rate of gas flow changes through the cells.

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[1] The reason for series arrangement is that it ensures that gas is always flowing through all cells to prevent cell reversal. If a cell is starved of gas, the cells on either side of it may drive it to react backwards, creating oxygen on the hydrogen side and creating hydrogen on the oxygen side. If enough H_2 and O_2 are present, a *burn* may occur where the Pt catalyst causes combustion between these gases.
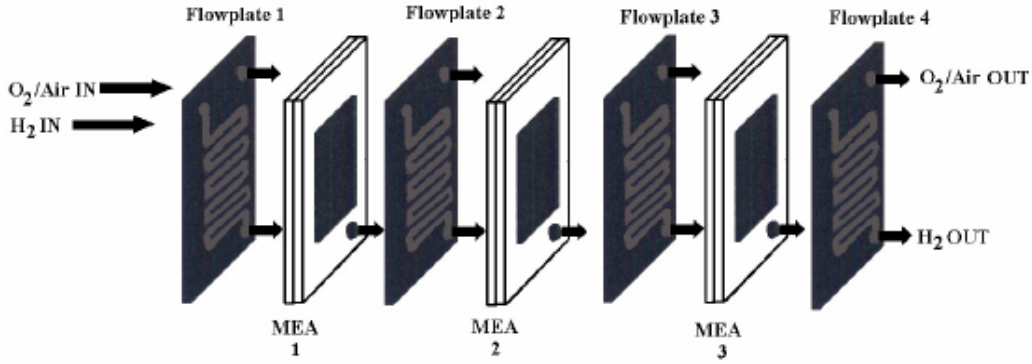
Figure 1. Illustration of series configuration of cells in the TVN Systems RU-2100 stack.

4. A relationship exists between current and reaction rate. Neglecting side reactions, the overall reaction stoichiometry is $2H_2 + O_2 \rightarrow 2H_2O$. Each mole of H_2 consumed involves a transfer of 2 moles of electrons, and each mol of O_2 involves 4 electrons. Current (I) is measured in amps, or coulombs per second (C/s). The charge on an electron is $1.602\ldots\times10^{-19}$ C. Faraday's constant (F) is the net charge of 1 mole of electrons, or 96485 C/mol. Thus, current (in C/s) can be used to obtain reaction rate (in mol/s), which gives $\dfrac{dn_{O_2}}{dt} = \dfrac{I}{4F}$ and $\dfrac{dn_{H_2}}{dt} = \dfrac{I}{2F}$.

Note that, because of the series configuration, if the current density is the same for each cell, then the reaction rate should also be the same for each cell. Also note that higher gas flow rates allow for higher maximum possible current densities.

5. $P_{O2} = y_{O2}*P_{tot}$. y_{O2} = (molar flow rate of O_2)/(total molar flow rate). Also, total material balances over each cell reveal that $flowO_{2,in} = flowO_{2,out} + rxnO_2$.

6. The RU-2100 operator's manual is confusing on the matter, but it seems to instruct that the entire stack can be modeled all at once using $i = i_0^* \cdot \varepsilon \cdot P_{O_2} \exp(\beta \cdot \Delta V)$. For the *entire* stack, $\Delta V_{stack} = 3V_T - V_{E,stack} - V_{\Omega,stack}$. However, as indicated above, the conditions vary from cell to cell, with each having a different partial pressure of O_2, temperature, degree of humidification, etc. Although more tedious, considering each cell separately (with $\Delta V_{cell} = V_T - V_{E,cell} - V_{\Omega,cell}$) is fundamentally more accurate and may provide insights regarding each cell's performance as O_2 pressure decreases, water accumulates, etc. Although analyzing the stack on a cell-by-cell basis has been successful, some have had difficulty getting the cell-by-cell method to work correctly with their data (probably because of operation at lower pressures). In such cases, it may be preferable to model the entire stack as one "cell," although again such a model does not truly consider what is happening. The most significant factor is using the incoming partial pressure of O_2 in computing $i = i_0^* \cdot \varepsilon \cdot P_{O_2} \exp(\beta \cdot \Delta V)$, while (as indicated above) this partial pressure is not constant from cell to cell. The value of V_T also depends on the partial pressure of O_2 and H_2, and the value of V_Ω is ~3 times larger for the whole stack versus individual cells. Hence, everything in the ΔV equation is approximately 3 times greater if the whole stack is used, and consequently β_{stack} is approximately 3 times smaller than β_{cell}.

7. Important note: Power density is equal to current density multiplied by the *external* voltage, V_E (<u>not</u> ΔV). It may be computed for either the entire stack (using $V_{E,stack}$) or on each cell at a time ($V_{E,cell}$), repeated 3 times, for reasons discussed above.