***Appendix***

**Physics-based semi-empirical PEMFC equations were used to generate Dataset1 [30]:**



where is the final fuel cell output voltage, is the fuel cell, refers to the fuel cell activation overpotential, ohmic overpotential, and concentration overpotential, respectively. is the fuel cell output current, is the membrane ohmic resistance, is the temperature of the fuel cell, represents the partial pressures of the hydrogen, oxygen, and saturation pressure of water vapor. are the empirical coefficients. Further, the equations given above are described below:

1. The net output of the fuel cell or terminal voltage is defined as the sum of reversible voltage, activation overpotential, ohmic overpotential, and concentration overpotential potentials;

2. Reversible voltage E is calculated by using the Nerst equation, adapting the thermodynamic values of the standard entropy change;

3. All the relevant overpotentials are defined by correlating operational current, resistance, and empirical constants which are determined by regressions based on the experimental data;

4 and 5. V0 and Va are dependent on the partial pressure of oxygen (slow cathode ORR rate), cathode operating pressure, saturation pressure, and fuel cell temperature. Saturation pressure is determined as a function of temperature; and

6. Then this equation is achieved by substituting equations 2-5 into 1 above.

**Dataset 1 (physics-based semi-empirical data):**

**A picture containing calendar

Description automatically generated**

**Dataset 2 (1-D CFD data) [31]:**

**Shape

Description automatically generated**

**Normalized Dataset 1 (physics-based semi-empirical data):**

**Chart

Description automatically generated**

**Normalized Dataset 2 (1-D CFD data):**

**A picture containing text, map, indoor

Description automatically generated**

**Chart

Description automatically generated**