

CHEMCAD
FUEL CELL SIMULATION

Contents

1.0	INTRODUCTION	3
2.0	THEORY	3
3.0	CHEMCAD MODEL	4
4.0	MODEL VALIDATION CHECK.....	6

1.0 INTRODUCTION

A fuel cell is an electrochemical device which brings together hydrogen and oxygen, or air in the midst of a catalyst to produce electricity, heat and water. (Fig. 2) or (Fig. 2a) The single cell fixture consists a single electrolyte sandwiched between electrodes. This inner sandwich is then placed in-between current collectors which usually serve as the poles of the cell. A fuel cell generates current by transforming (usually by using the catalyst in the electrodes) hydrogen gas into a mixture of hydrogen ions and electrons on the anode side of the cell. Because of the insulating nature of the electrolyte, the anions transfer through the electrolyte to the cathode side of the cell while the electrons are conducted to the current collectors and through a load to do work. The electrons then travel to the cathode side current collector where they disperse onto the electrodes to combine with incoming hydrogen anions, oxygen, or air in the presence of a catalyst to form water completing the circuit.

CHEMCAD FUEL CELL SIMULATION

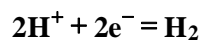
2.0 THEORY

1 Faraday = 96487 coulomb / mol. cell where coulomb = amp sec

1 mol/sec = 3.6 kmol/h = 96487 amp/cell



The number of Faradays that must pass through a circuit when one mol of a substance is produced or consumed is a whole number; for example at the anode two Faradays produce 1 mol of H₂ as shown below:



Total circuit resistance
$$\mathbf{R} = \mathbf{R}_i + \mathbf{R}_a$$

Total circuit current
$$\mathbf{I} = \mathbf{U}_0 / \mathbf{R}$$

Internal cell voltage
$$\mathbf{U}_i = \mathbf{R}_i \mathbf{I}$$

External voltage
$$\mathbf{U}_a = \mathbf{U}_0 - \mathbf{U}_i$$

Power
$$\mathbf{N} = \mathbf{U}_a \mathbf{I}$$

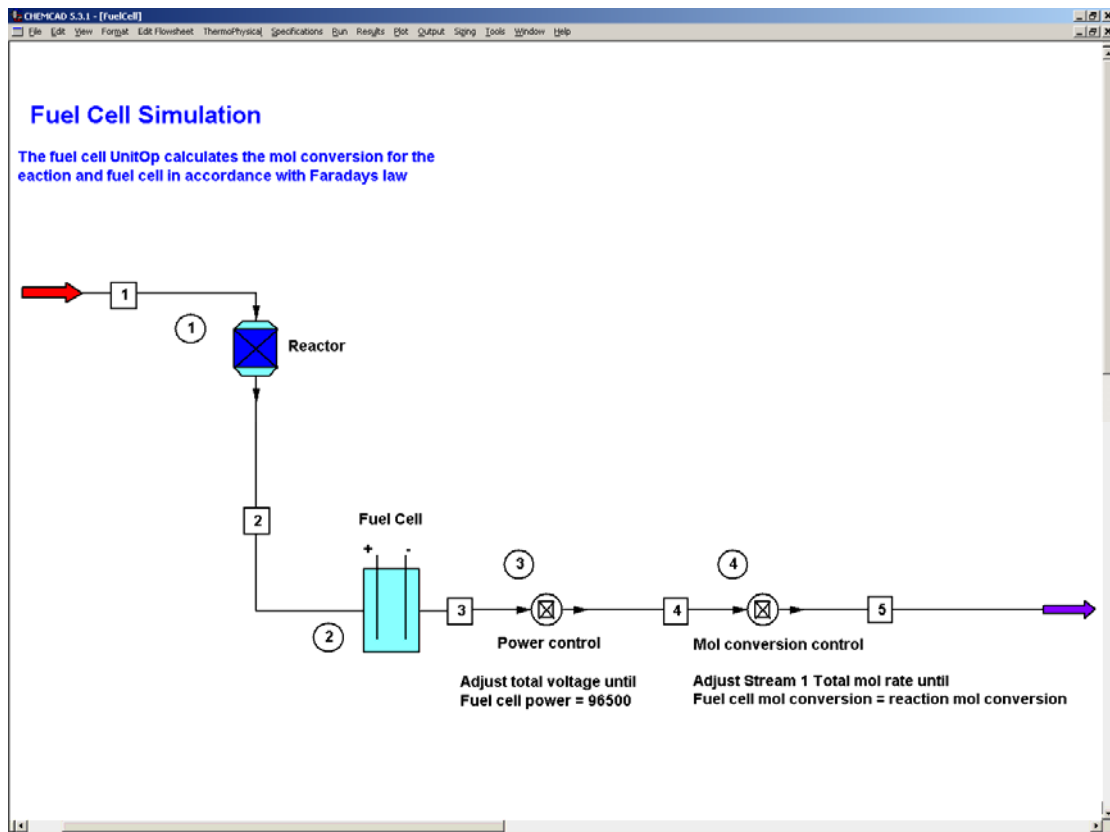
Cell Power
$$\mathbf{N}_{\text{cell}} = \mathbf{U}_0 / \mathbf{U}_{\text{cell}}$$

Mol conversion cell
$$\mathbf{MH} = (3.6 / 96487) (1 / 2) \mathbf{I} \quad \mathbf{N}_{\text{cell}} = 1.866\text{E}-05 \mathbf{I} \quad \mathbf{N}_{\text{cell}}$$

Mol reaction
$$\mathbf{MR} = (\mathbf{n}_{\text{H}_2\text{O}})_0 - (\mathbf{n}_{\text{H}_2\text{O}})_i$$

3.0 CHEMCAD MODEL

Excel UnitOp has been configured using Visual Basic to calculate the operational characteristics of a fuel cell circuit using the above theory.



- Stoichiometric Reactor (REAC) -

General Specifications More Components

ID: 1

Specify Thermal Mode:

1. Adiabatic
 2. Isothermal C
 3. Heat Duty MJ/h

Key Component
 Frac. Conversion
 Heat of Reaction kJ/kmol
 Reactor Pressure bar
 Calc H of Reac. kJ/kmol

Stoichiometric Coefficients:

Hydrogen	<input type="text" value="-1"/>	N/A	<input type="text"/>	N/A	<input type="text"/>
Oxygen	<input type="text" value="-0.5"/>	N/A	<input type="text"/>	N/A	<input type="text"/>
Water	<input type="text" value="1"/>	N/A	<input type="text"/>	N/A	<input type="text"/>

- Brennstoffzelle -

Brennstoffzelle (Fuel Cell)

Reaktor

Component ID# 1

InStream ID# 9

OutStream ID# 10

Molumsatz Reaktor [Kmol/h] 11

Molumsatz Zelle [Kmol/h] 2

Brennstoffzelle

Ri [Ohm] 4

Ua [V] 5

Ra [Ohm] 6

N [W] 7

Uo [V] 3

I [A] 8

Ucell 12

Ncell 13

Hinweise

See Calc2.txt for the code associated with this unitop,
 uspec index = var index + 1

4.0 MODEL VALIDATION CHECK

Input data required are U_O , U_{cell} , R_i and R_a

Example for

$U_O=108.08$ volts, $U_{cell} = 1.1$ volts, $R_i = 0.01$ ohm, and $R_a = 0.1$ ohm

$I = 108.08 / (0.1 + 0.01) = 982.54$ amp

$U_a = 108.08 - (0.01 \times 982.54) = 98.254$ volt

$N = 98.254 \times 982.54 = 96538$ watt

$N_{cell} = 108.08 / 1.1 = 98.254$

$MH = 1.866E-05 \times 982.54 \times 98.254 = 1.801$

$MR = 0.01833$