CFD Modeling of Gas-Liquid Flows in Water Electrolysis Units

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Abstract

This paper presents the results of computational fluid dynamics (CFD) modeling of gas-liquid flows in water electrolysis systems. CFD is used as a cost-effective design tool at Stuart Energy Systems Corporation (SESC) to optimize the performance of different water electrolysis units produced by SESC. General-purpose CFD software is used as a framework for analyzing the gas-liquid flow characteristics (pressure, gas and liquid velocities, gas and liquid volume fractions). The analysis is based on solving the coupled two-fluid conservation equations under typical and alternative operating conditions with appropriate boundary conditions, turbulence models and constitutive inter-phase correlations. Numerical results have been validated based on the experimental data available for a low-pressure cell.

Keywords: CFD modeling, SESC, gas-liquid flow, hydrogen, bubbles, cell

1. Introduction

The efficiency of water electrolysers depends on the proper design of system components (cells, cell stacks, gas-liquid separators, etc.). In particular, the gas-liquid circulation flow rate and the gas-liquid separation efficiency are important system parameters playing a significant role in overall performance of the units. These quantities, which are dependent on the gas-liquid flow patterns, could be calculated and analyzed using proper gas-liquid flow models and computer modeling tools.

To improve the designs of stacks and separators, the general-purpose CFD software, PHOENICS [1], has been used at SESC to model various two-phase gas-liquid flows in electrolysis units under typical and alternative conditions. The CFD simulation results have been used to properly design the system components (cells, cell stacks and gas-liquid separators). PHOENICS is a well-recognized general-purpose CFD software package that has been validated and successfully used around the world for more than 20 years. Its main features and capabilities have been described in [1]. The software serves as a cost-effective and convenient framework for modeling and design when a proper CFD model has been developed and validated for a particular application.

In this paper, the CFD modeling of gas-liquid flows using PHOENICS has been validated based on the published data [2] on a low-pressure rectangular electrolysis cell.

2. Modeling Approach

The modeling approach is based on applying the basic (built-in) two-fluid CFD models available in the PHOENICS software. The basic gas-liquid CFD model applied for the analyses of gas-liquid flows in the electrolysis units is based on the two-fluid inter-phase slip algorithm (IPSA), which is a built-in modeling option of the PHOENICS software [1]. IPSA enables to account for the differences (slips) in velocities and temperatures of gas and liquid and calculate 3-D distributions of pressure, velocity components, temperatures and volume factions of two phases. In IPSA, the coupled two-fluid conservation equations are solved under specified operating conditions with appropriate boundary conditions, turbulence models and constitutive inter-phase correlations. The drag force between liquid and gas phases is calculated using the built-in drag laws with specified average bubble diameter, D_B. A built-in 'spherical bubble' drag law was used in this paper to describe the drag between the gas and liquid phases.

Three geometrical sub-systems of the stack (the single hydrogen cell, the horizontal top channel with inlets from the cells and the gas-liquid separator) are considered separately. Also, an integrated CFD model, which includes both the stack and the separator, is being developed and tested at SESC. The primary task of the modeling is to create a cost-effective cell stack design tool. This paper describes only the simulation results obtained for a single hydrogen cell, which was tested in Reference [2].

Boundary conditions are needed at the cell/separator inlets and outlets. At the gas-liquid flow inlets, the liquid and gas flow rates, Q_L and Q_G, need to be specified. Their ratio, k, is specified at the gas-liquid inlet. Also, proper boundary conditions should be applied at the outlets. In this paper, the outlet boundary conditions are based on specified pressure values. The details of boundary conditions are shown in Table 1 below.

The LVEL turbulence model of PHOENICS was selected as a proper turbulence model. This model allows for both laminar and turbulent flow conditions to be considered. It computes a local Reynolds number in every computational cell and applies the local effective viscosity based on this number. The effective viscosity includes both laminar and turbulent components. This allows for accurate modeling of fluid flow conditions within the whole domain.

3. Input and Output Parameters

The list of primary input parameters involved in the CFD modeling of isothermal gas-liquid flows contains the following data.

- Cell/channel/separator geometry, i.e. the dimensions and locations of each CFD object, in particular, inlets, outlets and solid/porous blockages within the fluid domain and at its boundaries.
- Operating pressure and temperature.
- Physical properties of gas and liquid at operating pressure and temperature: densities, viscosities and diffusion coefficients.
- Gas production rate based on the current density and Faraday's law.
- Gas and liquid flow rates at the inlets.
- Pressure at the outlets.

- Average bubble size.

Table 1 below shows the input data used for CFD modeling of the electrolysis cell [2].

Table 1. Input Data List (Electrolysis Cell [2], H_2 Side)

Name	Symbol	Units	Value	Range
Cell Length	L	m	0.0254	
Cell Width	W	m	0.00461	
Cell Height	H	m	1.4732	
Liquid Inlet Location	(X_i, Y_i, Z_i)	m	(0,0,0)	
Liquid Inlet Area	A_{iL}=L*W	m^2	1.17E-4	
Gas Inlet Area (Cathode)	A_{iG}	m^2	2.322E-2	
G/L Outlet Location	(X_{oG},Y_{oG}, Z_{oG})	m	(0,0,1.4732)	
G/L Outlet Area	A_{oG}=L*W	m^2	1.17E-4	
Temperature	T	°C	27	27÷38
Operating Pressure	P	bar	1	
Liquid Density	ρ_L	kg/m^3	1210	
Liquid Viscosity	ν_L	m^2/s	7.025E-7	
Liquid Surface Tension	σ_L	N/m	0.09609	
Gas Density	ρ_G=0.0838(P/1)* 293.15/(T+273. 15)	kg/m^3	0.082	
Bubble Size Gas Production Rate	D_B Q_{Go}	mm NCMH/ kA	0.0635 0.4184	0.025÷0.152
Electric Current Density	i	kA/ m^2	3.5	1.94÷4.31
Normal Gas Flow Rate	$Q_{GN}= Q_{Go}$ i A_{iG}	NCMH	3.40E-2	
Actual Gas Flow Rate (Cathode) in CMH	$Q_{GA}= Q_{GN}$ /(P/1)* (T+273.15)/273.15	CMH	3.74E-2	
Gas Flow Rate in m^3/s	$Q_G= Q_{GA}/3600$	m^3/s	1.04E-5	
Inlet Velocity (Liquid)	V_L	m/s	0.091	0.091÷0.244
Inlet Gas Volume Fraction	α_G	m^3/m^3	0.0	
Liquid Flow Rate (Inlet)	$Q_L = V_L A_{iL}(1-\alpha_G)$	m^3/s	1.06E-5	
Relative Liquid Flow Rate	$k=Q_L / Q_G$	m^3/m^3	1.02	
Relative Outlet Pressure	$\Delta P_{oG}=P_{oG}-P$	Pa	0	

The list of output variables obtained from the CFD modeling of isothermal gas-liquid flows contains the following.

- 3-D distributions of pressure, gas and liquid velocity components and gas and liquid volume fractions within computational domain.
- Total gas and liquid flow rates at the outlets from the domain while using the pressure based outlet boundary conditions.

These quantities could be used to assess the efficiency of gas-liquid separation within separators. In particular, the CFD predictions of phase volume fractions, R1 and R2, are important for the analysis of separation efficiency. In the case of ‘complete’ separation, the values of gas volume fraction, R2, at the gas outlet would be equal to 1 (100%) and, as a result, the values of liquid volume fraction, R1, would be equal to 0 (0%). In the case of 'incomplete' separation, the values of R2 at the gas outlet are not equal to 1 and the values of R1 are not equal to 0. It means that a certain fraction of incoming liquid exits the gas-liquid separator via the gas outlet, i.e. there is some liquid carry-over at the gas outlet. The greater R1 is at the gas outlet the lower the gas-liquid separation efficiency.

Also, the predictions of 3-D distributions of gas volume fraction, R2, are useful for the analyses of hydrogen cell performance as the gas volume fraction distribution affects the flow circulation rate, the flow patterns and the electric current within the cell.

4. Results

In this section, results of CFD modeling of gas-liquid flow in the hydrogen cell [2] are described. The results were obtained with the basic CFD model, using a prescribed average bubble size for the whole cell. Also, the liquid flow rate and the gas volume fraction were specified at the cell inlet. Table 1 above shows the details of input parameters. A sensitivity study was conducted to analyze the effects of inlet liquid flow rate and current density on the hydrogen volume fraction distribution within the cell. Four cases were simulated to analyze the effects of liquid flow rate and current density. Table 2 shows the simulation cases considered and the results obtained. Sections 4.1 and 4.2 describe the details of the sensitivity study.

Table 2. Simulation Cases for Hydrogen Cell Tested in [2]

Case No.	Electric Current Density, i, kA/m^2	Gas Flow Rate, Q_G, m^3/s	Inlet Liquid Velocity, V_L (m/s)	Liquid Flow Rate, Q_L, m^3/s	Relative Liquid Flow Rate, $k=Q_L/Q_G$	Average Gas Volume Fraction at Symmetry Plane (%)	Average Gas Volume Fraction at Cell Outlet (%)
1	3.5	1.04E-5	0.091	1.06E-5	1.02	19.2	48.9
2	3.5	1.04E-5	0.244	2.84E-5	2.73	9.3	26.1
3	4.2	1.23E-5	0.091	1.06E-5	0.86	21.7	53.6
4	4.2	1.23E-5	0.244	2.84E-5	2.31	10.9	29.9

4.1. Effect of Liquid Flow Rate on Gas Volume Fraction

Cases 1 and 2 were used to analyze the effect of inlet liquid velocity on the 3-D distribution of gas volume fraction, R2. Table 2 shows that the predicted average gas volume fractions at the vertical symmetry plane and the horizontal outlet plane decrease significantly as the inlet liquid velocity increases from 0.091 m/s (the lowest value in [2]) to 0.244 m/s (the largest value in [2]). It is important to note that the predicted average gas volume fractions at the cell outlet (last column in Table 2) match well the experimental values [2] and the estimates based on the homogeneous model ($R2=1/(1+k)$), assuming the zero slips of phase velocities. This model was justified in [2] based on the experimental data.

Figures 1 and 2 illustrate the predicted distributions of hydrogen volume fraction, R2. The contour plots of R2 are shown at the bottom inlet, the top outlet, the vertical cathode plate and the vertical cross section (cell symmetry plane). The R2 probe value of 0.485 is shown for the probe location (see the red pencil at the top outlet plane) and the R2 average value of 0.192 is shown for the vertical cross section (cell symmetry plane). It can be seen that the gas volume fraction increases with height in both cases. R2 decreases with the increase of liquid velocity from 0.091 m/s (case 1) to 0.244 m/s (case 2).

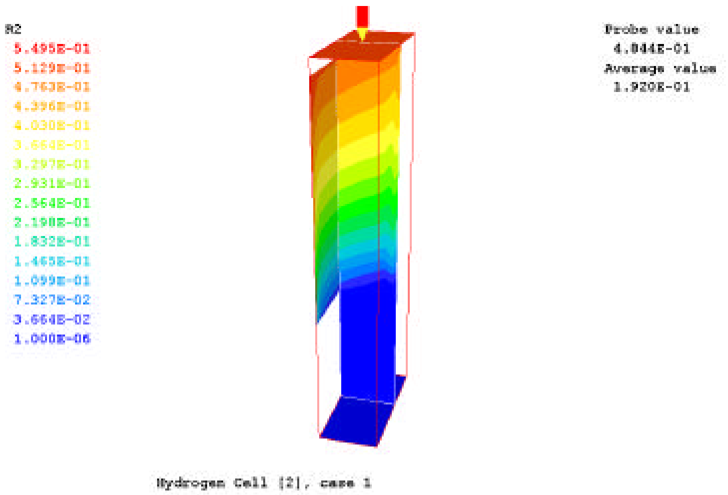

Fig. 1. Gas volume fraction in Case 1: V_L=0.091 m/s, i=3.5 kA/m^2.

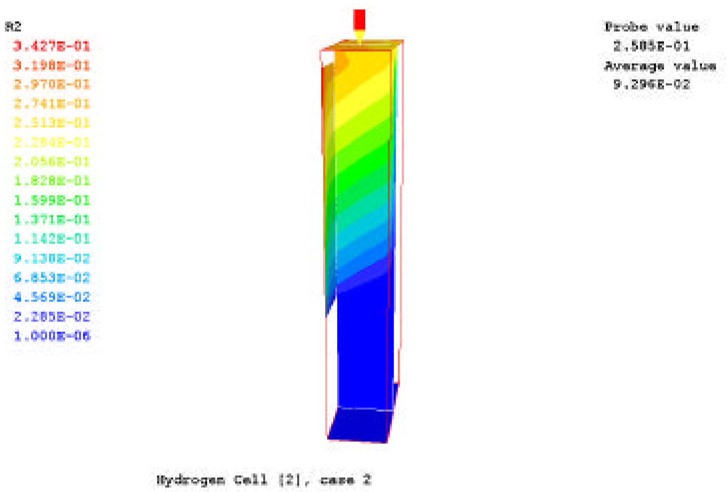

Fig. 2. Gas volume fraction in Case 2: V_L=0.244 m/s, i=3.5 kA/m^2.

4.2. Effect of Electric Current Density on Gas Volume Fraction

The effect of electric current density, i, on gas volume fraction distribution was studied by comparing the CFD predictions of gas volume fraction, R_2, for the two different values of current density, i.e. 3.5 kA/m^2 (cases 1 and 2) and 4.2 kA/m^2 (cases 3 and 4). Figures 3 and 4 were obtained for the current density of 4.2 kA/m^2. By comparing Figures 1 to 4 it can be seen that the gas volume fractions increase significantly with the current density. As was observed with the previously described cases, the predicted average gas volume fractions at the cell outlet (last column in Table 2) match well with the experimental values [2] and the estimates based on the homogeneous model (R2=1/(1+k)), assuming the zero slips of phase velocities.

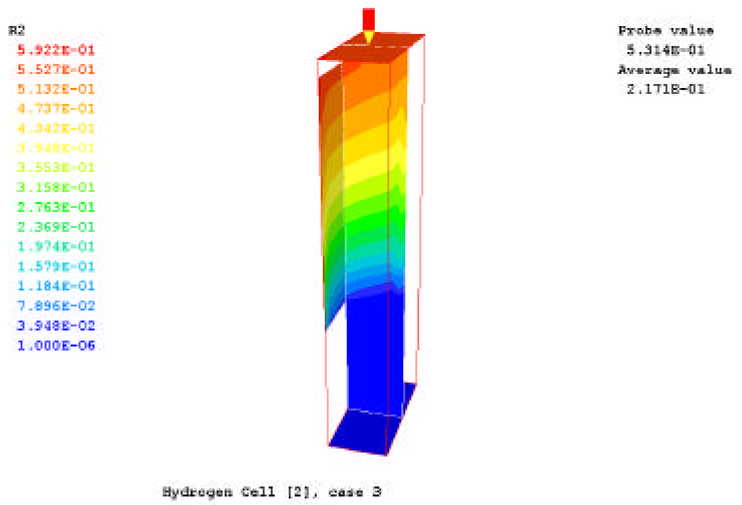

Fig. 3. Gas volume fraction in Case 3: V_L=0.091 m/s, i=4.2 kA/m^2.

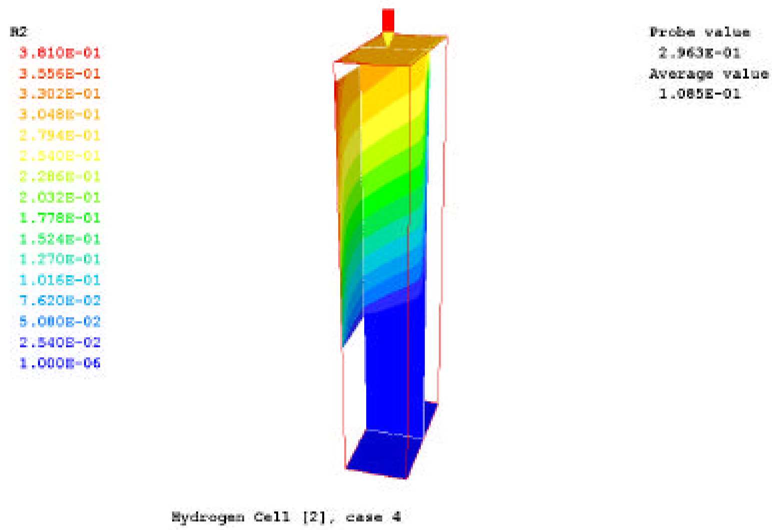

Fig. 4. Gas volume fraction in Case 4: V_L=0.244 m/s, i=4.2 kA/m^2.

5. Model Validation and Development

The simulation results obtained with the basic CFD model have been validated by comparing PHOENICS modeling results to the experimental data of Thorpe et al. [2] available for a low-pressure rectangular electrolysis cell. PHOENICS predictions of the hydrogen volume fraction compare well with the experimental results [2]. To further develop and validate the CFD models, the experimental data are needed under high-pressure input conditions. Liquid flow rate, gas volume fraction, local pressure and average bubble size are the primary parameters, which are needed for the model development and validation.

6. Conclusions

The PHOENICS CFD software has been applied for the modeling of gas-liquid flows within hydrogen cells and separators. The CFD modeling results have been validated using the published data on hydrogen cells. Due to the sensitivity of CFD predictions on the liquid flow rate, the bubble size and the inlet gas volume fraction, it is important to obtain accurate experimental data on these input parameters in order to validate the models. The validated CFD models could then be used as a cost-effective and reliable design tool.

7. References

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