Comparison between Turbulent and Laminar Bubbly-Flow for Modeling H_2/H_2O Separation

E. Amores Vera[1,*] and J. Rodríguez Ruiz[1]
[1] Centro Nacional del Hidrógeno. Prolongación Fernando El Santo s/n, 13500 Puertollano (C. Real). Spain
* Corresponding author: ernesto.amores@cnh2.es, +34 926 420 682

Abstract: Forced convection can increase electrolysis process efficiency. However, using a pump could favor the return of gas to the electrolysis stack, reducing the separation yield, and making possible the generation of explosive mixtures. A suitable design of separator devices could avoid these problems, by introducing gas traps. On the other hand, these separator components could allow turbulent phenomena. The present work reports a comparison between laminar and turbulent bubbly-flow modules for gas-liquid separation process in a separator. The aim is to evaluate the differences between both modules, and validate the adopted simplifications in laminar regime.

Keywords: gas traps, water electrolysis, gas-liquid separation, hydrogen, forced convection.

1. Introduction

Hydrogen production by water electrolysis combined with renewable energies is one of the most environmentally - friendly method, compared to traditional technologies based on fossil fuels since no CO_2 emissions are generated.

One of the most critical aspects on water electrolysis is the gas-liquid separation, especially in systems with an electrolyte being recirculated by a pump (forced convection). The main problem of this kind of circulation is that a gas fraction could return to the electrolysis circuit (Figure 1), which may have undesiderable consequences [1], such as the generation of explosive mixtures and pump damages.

A suitable design of separator devices could be a solution in order to avoid a gas return to the electrolysis circuit. In this sense, the use of gas traps or deflectors might reduce hydrogen suction by pump action. However, introduction of traps or new bodies inside the separator could strongly influence the fluid dynamics of gas and liquid, and turbulence phenomena could be generated (Figure 2).

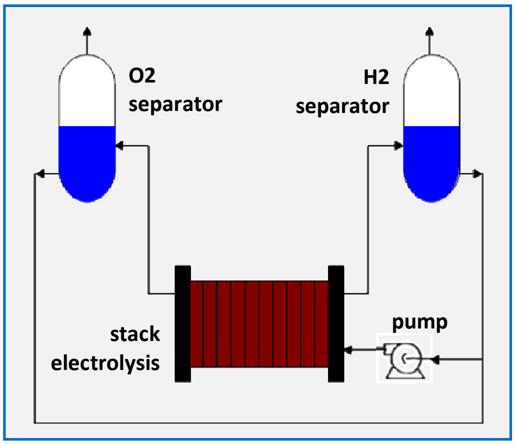

Figure 1. Simplified scheme of a water electrolyzer

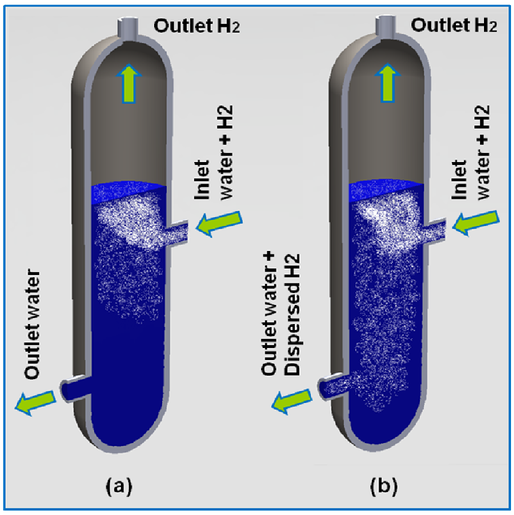

Figure 2. Gas-Liquid separation: (a) without pump; (b) with pump (forced convection)

In the present study, simulations results obtained by laminar and turbulent bubbly-flow modules are compared. The main objectives are to analyze the differences between both modules, and to evaluate whether the adopted simplifications for laminar regime correctly describe the behavior of two-phase flow within the separator.

2. Model Set-Up

2.1 Gas-Liquid separator

During electrolysis, H_2 and O_2 are generated and they leave the stack until reaching the hydrogen and oxygen separators, respectively (Figure 1). In this device, the phases can be separated because the gravity force acts differently on them.

In a typical operation, the two-phase flow enters in the separator by the half-height inlet. The gas leaves the separator through the upper outlet and the liquid return to the electrolyzer through the bottom outlet (Figure 2).

Sometimes, convection is forced by a pump because it improves the process: reduce mass transfer limitations and favor transport of bubbles inside the stack electrolysis. According to Takeuchi and col. [2] velocity of forced convection clearly affects the efficiency of water electrolysis: when flow velocity becomes larger, the efficiency of water electrolysis becomes higher.

However, a gas fraction could return to the electrolysis circuit in forced convection. In order to avoid these problems, introduction of gas traps or deflectors in the separator device could reduce pump action (Figure 3).

On the other hand, introduction of traps or new bodies inside the separator could strongly influence the fluid dynamics of gas and liquid, and turbulence phenomena could be generated.

2.2 Model geometry

The geometry of the model was built in 2D, including the gas traps, and considering only the domain occupied by the two-phase flow (water-hydrogen). In this way, simplifications were made in order to reduce the model complexity (Figure 4).

2.3 Mesh

For the separator model, a triangular mesh was generated (Fig 4). Mesh elements were normal predefined on the fluid domain with a refinement in the walls and deflectors to capture the viscous effects.

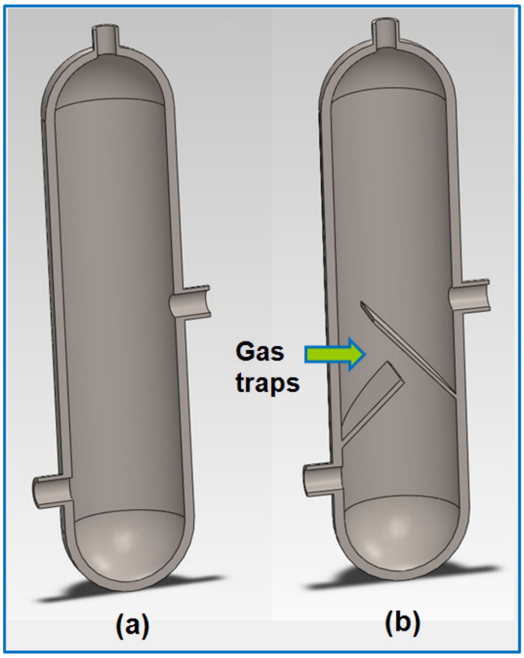

Figure 3. Types of separators: (a) standard separator; (b) separator used in the model

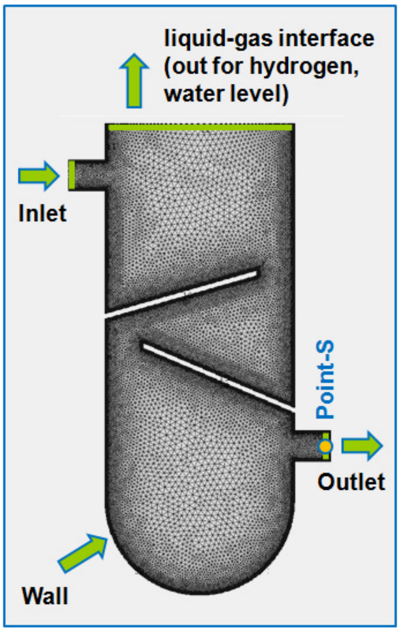

Figure 4. Geometry implemented in COMSOL and boundary conditions

3. Computational Methods: Formulation of the problem in COMSOL Multiphysics

The study of the gas-liquid separation was realized with the following modules of COMSOL® [3]:

- Laminar bubbly-flow
- Turbulent bubbly-flow

In a typical operation, due to buoyancy, the bubbles rise, inducing a circulating motion of the liquid in the separator. Under certain simplifications (boundary settings and initial conditions), this separation process can be described by a laminar regime. This allows a lower computational cost and faster results.

However, the introduction of deflectors increases turbulence phenomena (smaller section, areas where the gas is trapped, increasing speed, etc.), so that the adopted simplifications for laminar regime may not correctly describe the behavior of two-phase flow within the separator with gas-traps.

To compare the obtained results between both modules, the values of the simulation at the point-S (Figure 4) were measured.

Table 1 shows the boundary settings and initial conditions used in the model (see Appendix).

3.1 Laminar bubbly-flow

The movement of gas and liquid was modeled applying *laminar bubbly flow* module of COMSOL®. This application mode describes the two-phase flow using an Euler-Euler model. The module solves for the volume fraction occupied by each of two phases, without defining each bubble in detail. It is a macroscopic model for two-phase fluid flow. It treats the two phases as interpenetrating media, tracking the averaged concentration of the phases.

For *Laminar Bubbly Flow*, sum of the momentum equations for the two phases gives: a momentum equation for liquid (1):

$$\phi_l \cdot \rho_l \cdot \frac{\partial \vec{u}_l}{\partial t} + \phi_l \cdot \rho_l \cdot \vec{u}_l \cdot \nabla \vec{u}_l = -\nabla p + \nabla \cdot \left[\phi_l \cdot (\eta_l + \eta_T) \cdot \left(\nabla \vec{u}_l + \nabla \vec{u}_l^T - \frac{2}{3} \cdot (\nabla \vec{u}_l) \cdot \bar{I} \right) \right] + \phi_l \cdot \rho_l \cdot \vec{g} + \vec{F} \quad (1)$$

A continuity equation (2),

$$\frac{\partial}{\partial t}(\phi_l \cdot \rho_l + \phi_g \cdot \rho_g) + \nabla \cdot (\phi_l \cdot \rho_l \cdot \vec{u}_l + \phi_g \cdot \rho_g \cdot \vec{u}_g) = 0 \quad (2)$$

And a transport equation (3) for the volume fraction of gas,

$$\frac{\partial \phi_g \cdot \rho_g}{\partial t} + \nabla(\phi_g \cdot \rho_g \cdot \vec{u}_g) = -m_{gl} \quad (3)$$

Where (m_{gl}) is the mass transfer rate from gas to liquid.

3.2 Turbulent bubbly-flow

For turbulent flows, the movement of gas and liquid was modeled applying *turbulent bubbly flow* module of COMSOL®. The turbulence model for bubbly-flow is similar to the single-phase k-ε turbulence model. However, there are additional source terms in order to account for the extra production of turbulence due to the relative motion between the gas bubbles and the liquid in the separator [3].

The k-ε model adds a turbulent viscosity to the physical viscosity in the momentum transport equation. The turbulent viscosity is modeled by (4), where (C_μ) is a model constant:

$$\mu_T = \rho_l C_\mu \frac{k^2}{\varepsilon} \quad (4)$$

The transport equation (5) for the turbulence kinetic energy "k" is:

$$\rho_l \frac{\partial k}{\partial t} + \rho_l (\vec{u}_l \cdot \nabla) k = \nabla \cdot \left[\left(\mu + \frac{\mu_T}{\sigma_k} \right) \nabla k \right] + P_k - \rho_l \varepsilon + S_k \quad (5)$$

And the evolution of the turbulent's energy dissipation rate "ε" is governed by (6):

$$\rho_l \frac{\partial \varepsilon}{\partial t} + \rho_l (\vec{u}_l \cdot \nabla)\varepsilon = \nabla \cdot \left[\left(\mu + \frac{\mu_T}{\sigma_\varepsilon} \right) \nabla \varepsilon \right] +$$
$$C_{\varepsilon 1} \frac{\varepsilon}{k} P_k - C_{\varepsilon 2} \rho_l \frac{\varepsilon^2}{k} + C_\varepsilon S_k \frac{\varepsilon}{k} \tag{6}$$

The term (S_k) accounts for the bubble induced turbulence and the term (P_k) is given by:

$$S_k = -C_k \phi_g \nabla p \cdot \vec{u}_{slip} \tag{7}$$

$$P_k = \mu_T \left[\nabla \vec{u}_l : \left(\nabla \vec{u}_l + (\nabla \vec{u}_l)^T \right) \right] \tag{8}$$

4. Results

Figure 5 and Figure 6 show the obtained results for laminar and turbulent bubbly flow fluid dynamics simulations of a gas-liquid separator in the same operation conditions. Evolution of gas distribution and speed profiles are shown. As can be seen, in both cases with increasing time gas goes down into the separator, due to effect of the pump.

However, strong “fluctuations” are observed in the case of laminar bubbly flow results (Figure 5). These "fluctuations" do not appear in the case of turbulent bubbly flow module because the k-ε model can explain these effects and suitably modeling the turbulence phenomena.

The k-ε is a two equation model that includes two extra transport equations to represent the turbulent properties of the flow. This allows a two equation model to account effects like convection and diffusion of turbulent energy.

In Figure 7 the evolution of the gas fraction measured on point-S (Figure 4) with time is presented. Laminar simulations show strong “fluctuations”, while a sweet curve was obtained for turbulent bubbly flow simulation.

These results for different times are explained again, because laminar bubbly flow module cannot adequately analyze turbulent phenomena taking place inside the separators, caused by relative movement between liquid-gas and by the use of gas traps.

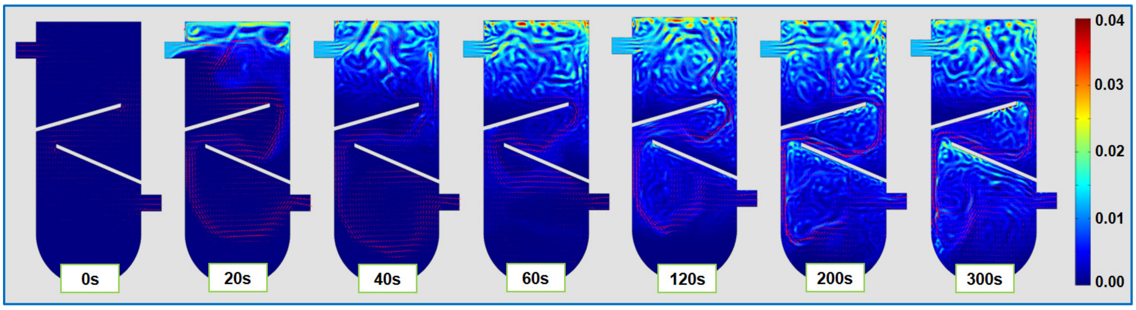

Figure 5. Gas fraction (surface) and velocity profiles (arrows) obtained by laminar bubbly flow.

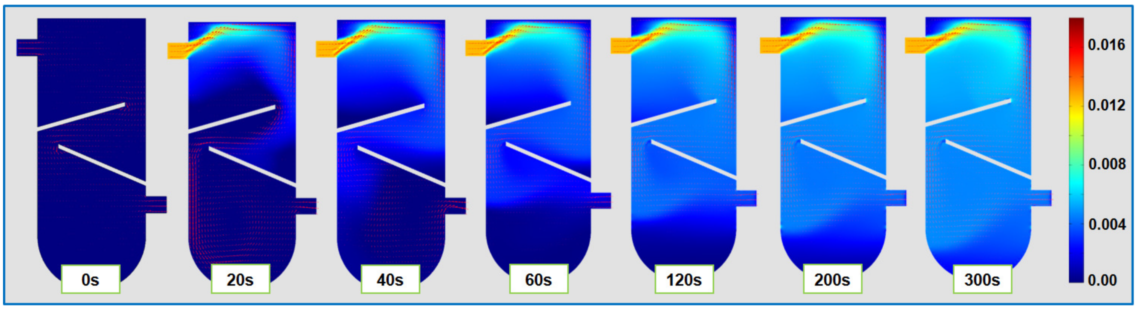

Figure 6. Gas fraction (surface) and velocity profiles (arrows) obtained by turbulent bubbly flow.

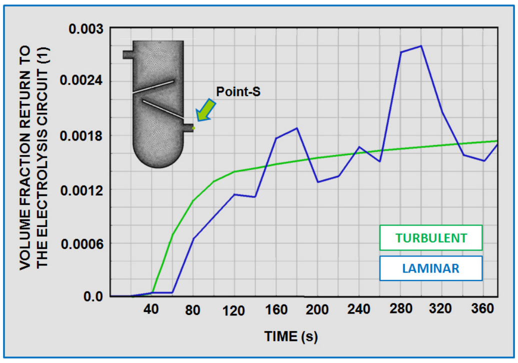

Figure 7. Volume gas fraction measured in point-S

5. Conclusions

- Introduction of deflectors or gas-traps increases turbulence phenomena.
- COMSOL® was used to model the behavior of a separator device for H_2/H_2O separation.
- Turbulence bubbly flow model allows a suitable analysis of turbulence dynamics in multiphase flow.
- Future development will be oriented to the comparison of the present results with other simulation modules which take into account the gas-liquid interface.

6. References

[1] Hug W., Divisek J., Mergel J., Seeger W., Steeb H., *Highly efficient advanced alkaline electrolyzer for solar operation*, 699-705, Int. J. Hydrogen Energy 9 (1992)

[2] Takeuchi M., Furtua T., *Efficiency and two-phase flow of alkaline water electrolysis under forced convection of electrolyte*, Annals of Assembly for Int. Heat Transfer Conference 13, (2006). ISSN: 1-56700-225-0

[3] COMSOL Multiphysics - User's Guide. *Bubbly Flow Model, Chemical Engineering Module*. Burlington, MA: *COMSOL, Inc*; 2007

7. Acknowledgements

The work described in this paper have been developed within the project *Experimentación, Simulación y Validación de Celdas de Electrólisis Alcalina para Producción de Hidrógeno mediante Energías Renovables* (EXSIVA) in the facilities of the *Centro Nacional del Hidrógeno* (CNH2), whose financial support are *Ministerio de Economía y Competitividad* (MINECO, Spain), *Junta de Comunidades Castilla-La Mancha* (JCCM) and *Fondos Europeos de Desarrollo Regional* (FEDER).

8. Appendix

Table 1: Constants, Sub-domain and Boundary Settings

Symbol	Value	Description
v_{in}	0.035 m/s	Inlet velocity (when pump is ON)
T	60°C	Temperature operation
V_{out}	0.035 m/s	Outlet velocity (when pump is ON)
λ	10%	Initial hydrogen fraction
$Ø_{bubble}$	10^{-3} m	Bubble diameter of hydrogen