Simulation Study Of The Gas-liquid System In The GDEx Process For PGMs Recovery

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Abstract

Chemical processes at any level, from laboratory to industrial scale, rely on catalysts due to their ability to reduce energy consumption and increase the yield of the desired products through faster, more effective, and selective reactions. Catalysts such as platinum group metals (PGMs) are included in the Critical Raw Materials Act, identifying them as materials highly vulnerable to supply disruptions. With the expected increase in global demand for catalysts, addressing these challenges involves strategies to reduce extraction dependence by improving circularity and sustainability of raw materials.

As part of the sustainable evolution of the catalyst-based industry, the FIREFLY project proposes developing circular and sustainable technologies to recover value-added metals from industrial waste, spent, and off-specification catalysts available in Europe. This involves integrating physical, chemical, and electrochemical processes to extract the maximum quantity of metals possible, ranging from low to high purity, for end chemical users.

This study focuses on Gas-Diffusion Electrocrystallization (GDEx) technology for recovering PGMs, as part of the FIREFLY project's electrochemical technologies. The primary investigation involves simulating a gas-liquid system where CO2 gas is introduced into an H2O-NaCl liquid mixture through a porous electrode. The simultaneous reduction of H2O and CO2 generates in situ reactants, H2 and CO, which drive the precipitation of ionic platinum, palladium, and rhodium species, as well as control their particle size (Martinez-Mora et al., 2023).

The preliminary mathematical model employs a laminar two-phase flow and level set interface to determine the position and growth of the injected gas bubbles and their buoyant ascend through the liquid, ultimately scaping the electrochemical cell. This initial model is coupled with the transport of diluted species to analyze the influence of the H2 and CO, both in their dissolved form in the liquid on ionic metals precipitation process.

The available experimental data for model validation pertains to the dissolved concentration of H2 (cH2-(ℓ)) in the liquid under different inlet liquid flow rates (20-200 ml min-1), applied current densities (J, 10-30 mA cm-2), and inlet gas flow rate (Q, 5-10 sccm). A good correlation between experimental and simulation results was obtained, as illustrated in Figure 1. The applied current density played a crucial role in H2 generation and consequently its cH2-(ℓ) values, showing that higher J values resulted in higher cH2-(ℓ). Conversely, cH2-(ℓ) decreased with increased liquid flow rate, which is associated with the reduced contact time between the generated gas phase and the liquid phase.

For PGMs precipitation, the concentration of ionic species in solution was monitored over time and is presented in Figures 2-4. These figures suggest a good correlation between experimental and simulated data under different J and Q conditions. The injection, growth, and ascent of the gas bubbles were not matched experimentally during the GDEx system operation due to the inner position of the electrode within the electrochemical cell.

Reference

O., Martinez-Mora, et al., Platinum nanoclusters made by gas-diffusion electrocrystallization (GDEx) as electrocatalysts for methanol oxidation, Materials Advances, 4, 6183-6091(2023).

Figures used in the abstract

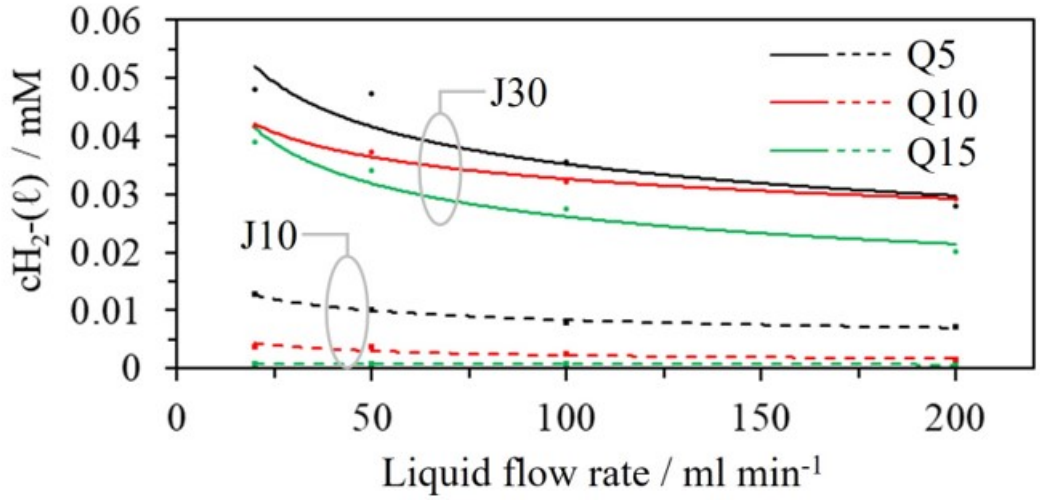

Figure 1 : Figure 1. Dissolved concentration of H2. Dots: experimental results, lines: simulation results.

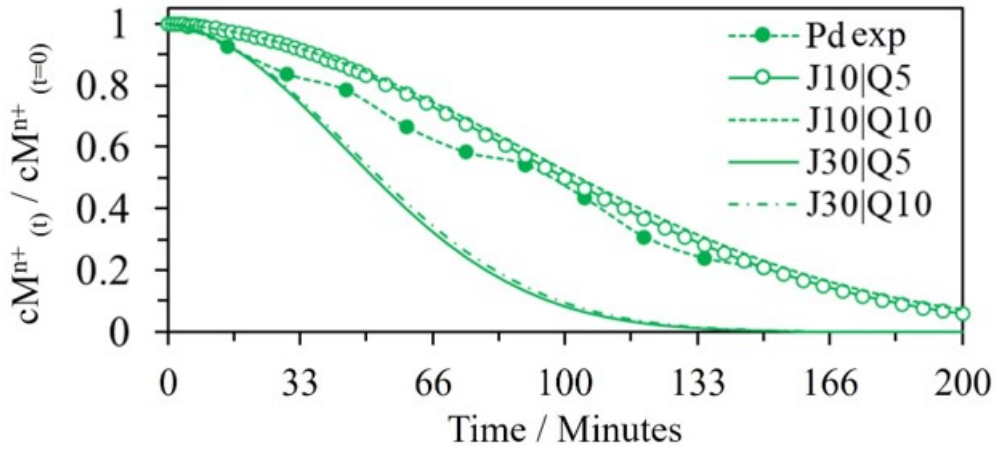

Figure 2 : Figure 2. Palladium ion concentration.

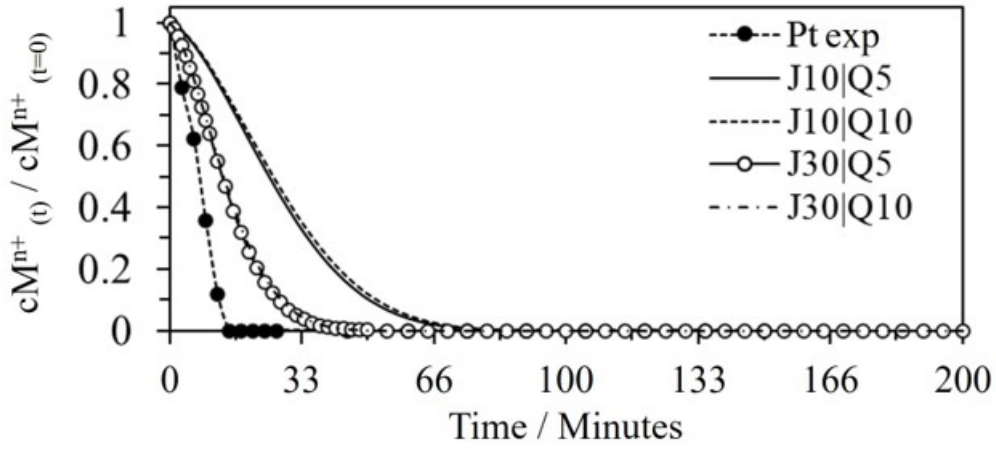

Figure 3 : Figure 3. Platinum ion concentration.

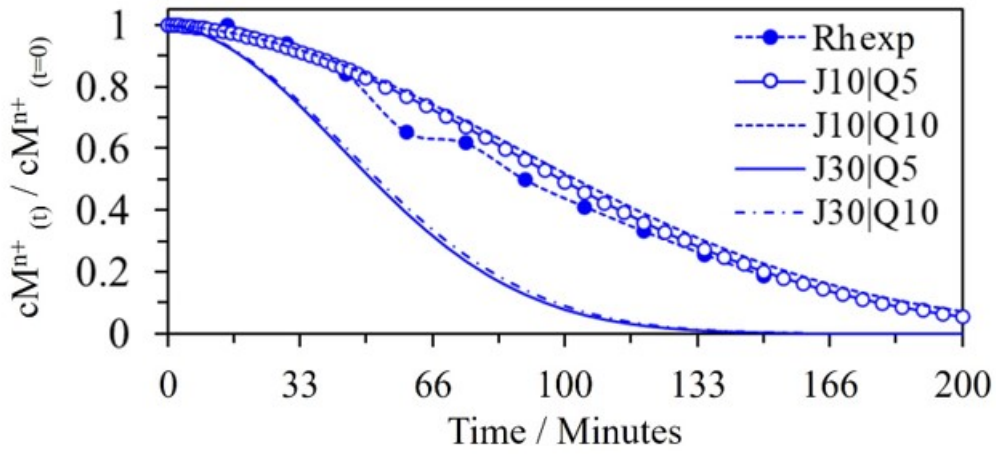

Figure 4 : Figure 4. Rhodium ion concentration.