Formulation and Solution of Gas-Liquid Adsorption Inverse Problems Using a Hybrid Combination of Stochastic and Deterministic Methods

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Introduction

In recent years it has been observed an increasing interest on both theoretical and experimental research on the mechanism of protein adsorption at gas-liquid interfaces because of the potential use of bubble and foam columns as an economically viable means for surface-active compounds fractionation from diluted solutions.

The bubble and foam column for gas-liquid adsorption is schematically represented in Fig. 1. It works basically through the gas injection at the base of the column containing the solution. The gas bubbles formed in the distributor rise and along this path adsorb the solute. In the foam region, formed above the bubble column, it is made the extraction of the material of interest with a higher concentration [1].

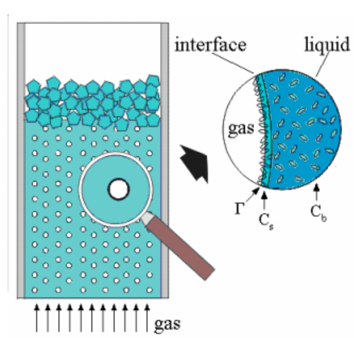

Figure 1. Schematic representation of the gas-liquid adsorption process in a bubble and foam column.

To have a better understanding of the processes involved, as well as to allow the scale up from the laboratory to the industrial size, mathematical and numerical models have been developed. Nonetheless, for their use, physicochemical properties and some correlated operational parameters must be known. For example, the direct determination of adsorption isotherms from experiments is not an easy task [1].

Inverse Problem Formulation

The inverse problem is implicitly formulated as a finite dimensional optimization problem [2,3] where one seeks to minimize the squared residues functional

$$S = \left[\vec{C}_{bcalc}(\vec{P}) - \vec{C}_{bmeas}\right]^T \left[\vec{C}_{bcalc}(\vec{P}) - \vec{C}_{bmeas}\right] \tag{1}$$

where $\vec{C}_{bmeas}$ is the vector of measurements, $\vec{C}_{bcalc}$ is the vector of calculated values, and $\vec{P}$ is the vector of unknowns.

The inverse problem solution $\vec{P}^*$ minimizes the norm given by Eq. (1), that is

$$S(\vec{P}^*) = \min_{\vec{P}} S(\vec{P}) \tag{2}$$

In the present research we consider different vectors of unknowns, $\vec{P}$, which are associated with different adsorption isotherms: (i) K and B (linear isotherm); (ii) $K_1(T)$ and $\hat{a}$ (Langmuir isotherm); (iii) $K_1(T)$, $K_2(T)$, λ and $\hat{a}$ (two-layers isotherm). In this work, studying BSA, the adsorption was modeled as a two-layer isotherm.

Inverse Problem Solution

After training, an Artificial Neural Network (ANN) [4-6] is able to quickly provide an inverse problem solution. This solution is then used as an initial guess for the Levenberg-Marquardt (LM) method [7].

The canonical LM depends on the calculation of the gradient, which is usually approximated by finite differences. It means that the direct problem has to be solved many times. In this work a second ANN was trained to calculate the solute concentration, using the information on K_2, λ, $\hat{a}$ and t. This ANN was used to provide an approximation for the Jacobian matrix used in the first step of LM iterative procedure. In the last steps one uses the FDM gradient approximation.

Results

In this work, it is necessary to design two different experiments, one to estimate $K_2(T)$ and $\hat{a}$, called experiment 1, and another to estimate λ, called experiment 2. In all cases studied the sensitivity to $K_1(T)$ is low, and therefore this parameter was not estimated with the inverse problem solution.

The results obtained using the ANN, LM 1 (gradient approximated by FDM), LM 2 (gradient approximated by ANN), SA and hybrid combinations, for different values of the standard deviation for the measurements errors, σ, are shown in Tables 1 and 2.

Conclusions

The hybrid combination ANN-LM resulted in good estimates for the gas-liquid adsorption isotherm inverse problem.

The use of the ANN to obtain the derivatives in the first steps of the LM method reduced the time necessary to solve the problem.

Table 1 – Results obtained using ANN, LM 1, LM 2, SA and hybrid combinations for experiment 1.

Case	Method	σ	Time (s)	K_2	$\hat{a}$	S [mg²/l²] Eq. (1)
1	LM 1 (grad. FDM)	0	169	0.0104	0.322	0
2	LM 2 (grad. ANN)	0	80	0.0104	0.322	0
3	LM 1 (grad. FDM)	10	170	0.0079	0.158	8.39
4	LM 2 (grad. ANN)	10	78	0.0081	0.157	8.64
5	ANN	10	1	0.0110	0.377	6.81
6	LM 1 (grad. FDM)	10	172	0.0108	0.335	6.27
7	LM 2 (grad. ANN)	10	79	0.0106	0.314	5.68
8	ANN-LM	10	80	0.0110 0.0106	0.377 0.335	5.68

The exact values used are: $K_2 = 0.0104\, mg/(m^2\, wt\%)$ and $\hat{a} = 0.322\, m^2/mg$.

$\sigma = 10$ corresponds to errors up to 5% in the experimental data.

Table 2 – Results obtained using ANN, LM 1, LM 2, SA and hybrid combinations for experiment 2.

Case	Method	σ	λ	Time (s)	S [mg²/l²] Eq. (1)
1	LM 1 (grad. FDM)	0	1.117	40	0
2	LM 2 (grad. ANN)	0	1.117	29	0
3	LM 1 (grad. FDM)	0.1	1.159	45	7.96
4	LM 2 (grad. ANN)	0.1	1.159	30	7.96
5	ANN	0.1	1.432	1	202.9
6	LM 1 (grad. FDM)	0.1	1.159	6	7.96
7	LM 2 (grad. ANN)	0.1	1.159	4	7.96
8	ANN-LM	0.1	1.432 1.159	5	7.96

The exact value used is: $\lambda = 1.117\, m^2/mg$.

$\sigma = 0.1$ corresponds to errors up to 5% in the experimental data.

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