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A Novel AI-Driven Approach for Parameter Estimation in Gas-Phase Fixed-Bed Experiments

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ABSTRACT

The transition to renewable energy sources, such as biogas, requires purification processes to separate methane from carbon dioxide, with adsorption-based methods being widely employed. Accurate simulations of these systems, governed by coupled PDEs, ODEs, and algebraic equations, critically depend on precise parameter determination. While traditional approaches often result in significant errors or complex procedures, optimization algorithms provide a more efficient and reliable means of parameter estimation, simplifying the process, improving simulation accuracy, and enhancing the understanding of these systems. This work introduces an Artificial Intelligence-based methodology for estimating the isotherm parameters of a mathematical phenomenological model for fixed-bed experiments. The separation of CO_2 and CH_4 is used as case study. This work develops an algorithm for parameter estimation for the system's mathematical model. The results show that the validated model has a close fit with experimental results.

Keywords: Adsorption, Optimization, Artificial Intelligence, Parameter Estimation

INTRODUCTION

The need to reduce greenhouse gas emissions has driven the shift toward renewable energy sources such as biogas. However, to use biogas as a substitute for natural gas, it must undergo a purification process to separate methane from carbon dioxide. Adsorption-based separation processes are standard methods for biogas separation. Fixed-bed systems form the fundamental step for many separation processes in this context [1].

Parameter estimation is a usual step in developing mathematical models which affects not only the model prediction in itself, but also the future use of the model in process control and optimization.

By solving a system of coupled Partial Differential Equations, Ordinary Differential Equations, and Algebraic Equations, it is possible to accurately simulate fixed-bed units used in these processes [1, 2]. However, a rigorous simulation and, consequently, a better understanding of the intrinsic phenomena governing these systems, such as adsorption isotherms, film and particle mass transfer, energy transfer phenomena, among others, heavily depends on the parameter values [3]. These parameters can be estimated using well-known mathematical correlations or trial and error. However, these methods often introduce significant errors [4]. For a more accurate determination, an optimization algorithm can be employed to find the best set of parameters that minimize the difference between the simulation and experimental data, thereby providing a better representation and understanding of the real process.

Different optimization methodologies can be employed for this purpose. For example, deterministic methods are known for ensuring convergence to an optimal solution, but the starting point selection significantly impacts their performance [5]. In contrast, meta-heuristic techniques are often preferred for their adaptability and efficiency since they do not rely on predefined initial

conditions [6]. However, these approaches may not always guarantee finding the optimal solution for every problem.

Within the field of Artificial intelligence, Reinforcement Learning (RL) emerges as self-supervised technique. RL uses a trial-and-error algorithm, guided by rewards, to help agents learn optimal behaviors, mapping situations to actions to maximize long-term rewards [7]. RL excels at handling delayed feedback, where actions impact both immediate and future outcomes, enabling effective long-term planning. However, RL faces challenges in balancing exploration (seeking new optimal actions) and exploitation (using current knowledge to maximize rewards). Striking this balance is critical, as premature exploitation can lead to suboptimal solutions, while excessive exploration delays progress [8].

Recent advancements, including algorithms like Deep Deterministic Policy Gradient (DDPG), have expanded RL's reach by using deep neural networks for high-dimensional action spaces. This has driven success in multiple fields, including robotics, games, and industrial optimization by a more efficient management of delayed rewards and refining exploration-exploitation [9, 10].

This work introduces an AI-based approach for estimating adsorption isotherm parameters in the mathematical model of fixed-bed experiments for CH_4/CO_2 separation. Using a DDPG agent in a Reinforcement Learning algorithm, this methodology addresses the common limitations of deterministic methods by leveraging a deep neural network capable of balancing exploitation and exploration, aiming to optimize the fit between simulated results and experimental data by minimizing the error between the two datasets, thereby enhancing the accuracy and predictive capability of the model.

MATERIALS AND METHODS

Objective

Adsorption in a fixed bed unit can be described through a mathematical model that includes the mass, energy, and momentum balances that govern the process. Proper modeling of the equilibrium data is critical for effective process design. Using three different approaches, the main objective of this work is to determine the parameter set, θ, of the Extended Langmuir isotherm (Equation 1) that, when incorporated into the mathematical model (available in [1]) for simulating the gas composition in fixed-bed experiments, enables accurate reproduction of experimental data, and achieves a close-to-optimal fit between simulated and experimental results.

$$q_i = q_{sat,i}\frac{b_i P_i}{1 + \Sigma_{1=1}^{n}(b_i P_i)} \quad (1)$$

Experimental Dataset

This work used experimental data collected by Ferreira and colleagues [1] , using MIL-53(Al) as the adsorbent for the CH_4/CO_2 separation in fixed-bed experiments. The dataset comprises 17 breakthrough experiments conducted under varying feed composition and pressure (from 0.1 to 4 bar) conditions, all at constant temperature (303 K). The conditions can be consulted in Tabel SI.1. At the start of each breakthrough experiment, the column, initially filled with He, was fed with either pure gas or with a gas mixture of CO_2 and CH_4. Once the column reached saturation under the specified feed conditions the inlet stream was switched to helium at the same total flow rate to initiate the regeneration step. The dataset includes 7 experiments with pure CO_2, 7 with pure CH_4, and 3 with varying mixtures of CO_2/CH_4.

Since all experiments were conducted at the same temperature, the estimated parameters were $q_{sat,CO2}$, $q_{sat,CH4}$, $b_{\infty,CO2}$ and $b_{\infty,CH4}$. The parameters b_{CO2} and b_{CH4} can be calculated using Equation 2, based on a constant value of $(-\Delta H_i)$ obtained from the literature: 26000 J·mol^{-1} for CO_2 and 18300 J·mol^{-1} for CH_4 [11].

$$b_i = b_{\infty,i}\, exp\left(\frac{-\Delta H_i}{R_g T}\right) \quad (2)$$

Ferreira et al. [1] obtained the adsorption isotherms parameters through breakthrough experiments. The adsorbed amount of gas was calculated using breakthrough curve data from adsorption and desorption experiments. For adsorption, the area under the breakthrough curve was integrated and subtracted from the total gas fed into the column. For desorption, the area under the curve was directly integrated. Comparing both adsorbed amounts (adsorption and desorption), one can verify whether the mass balance closes. These values were normalized by dividing by the dry adsorbent mass, yielding the adsorbed amount per mass unit of adsorbent.

Subsequently, the Extended Langmuir Isotherm parameters were determined using the Generalized Reduced Gradient Nonlinear Solver by fitting the experimental data for adsorbed amounts to the Extended Langmuir Equation, using the partial pressures from each experiment. The parameters obtained can be consulted in Table 1 and were used as reference values for this work.

Reinforcement Learning Algorithm

The RL setup requires defining: (1) the Environment, representing the system where actions are applied; (2) the Reward, which guides the algorithm's learning process; (3) the State, reflecting the environment's response to an action; (4) the Agent, the decision-making component of the RL algorithm; and (5) the Actions, indicating how the algorithm interacts with the environment.

The action represents how the RL agent affects the environment to maximize the reward. In this work, the action is the set of parameters, θ, that needs to be

estimated. The action must be constrained between a lower (Act_{min}) and an upper bound (Act_{max}) and an initial guess must be given (Act_0).

The agent is the core of the RL algorithm, responsible for learning from past trials (exploitation) and exploring new possibilities (exploration) to maximize long-term rewards by deciding the next action to take. The selection of the best agent depends on the desired policy, observation space, action space, and learning process. For this project, since a deterministic policy is preferred over a stochastic one, both the observation and action spaces are continuous, and the objective function is too complex for a simpler Q-learning process so a deep neural network-based agent was chosen, a Deep Deterministic Policy Gradient agent was selected.

The tuning of the neural networks responsible for the agent is crucial, as their hyperparameters play a key role in balancing exploration and exploitation.

Parameter Estimation

All the work was done on a computer with a processor 13th Gen Intel(R) Core (TM) i7-13700F 2.10 GHz, 32 GB of RAM and a graphic card NVIDIA GeForce RTX 4070.

The first approach tried replicating the method described in [1], replacing the used solver with the RL algorithm. This enabled the direct adjustment of the Extended Langmuir model for each experiment with the experimental values of q_{CO2} and q_{CH4}, obtained after mass balance, as previously described.

In this approach, the Environment is defined as the calculation of the predicted q_{CO2} and q_{CH4} values for all experiments using Equation 1. The Action corresponds to the set of parameters to be applied in Equation 1, while the State represents the Mean Squared Error (MSE) between the calculated and experimental q_{CO2} and q_{CH4} values. In RL, the reward is typically designed to be maximized. However, since the objective is to minimize the error between experimental and simulated data, the Reward is defined as the negative of the MSE between the simulated and experimental results.

This entire approach was implemented in MATLAB. After the training, the parameter set that best minimized the MSE was used to simulate the 17 breakthrough experiments and the error between the experimental and simulated dataset was compared with the one obtained with the reference parameters.

The second and third approaches involved the direct adjustment of parameters based on the breakthrough curves simulations. The Environment is the simulation of the breakthrough experiments used for training, utilizing the parameter set provided by the agent in each trial. The simulations were conducted in the gPPROMS environment (Process Systems Enterprise, London, UK) and numerically solved using the orthogonal collocation on finite elements method, with second-order polynomials and 115 intervals, using the phenomenological model available at [1, 2]. The RL Algorithm was implemented in MATLAB.

As mentioned, RL algorithms typically aim to optimize a problem by maximizing the reward. Since the goal is to minimize the difference between experimental and simulated data, the reward is the negative of the error between the two datasets. The number of comparison points per experiment is denoted as N_{points}. Since this value varies across experiments, a weighting factor, ω, is applied to normalize the MSE between experiments.

Equation 3 shows the objective function (f_{obj}) to be minimized and Equation 4 the Long-Term Reward (Rew_{LT}) that the agent aims to maximize. In these equations, y corresponds to the molar composition of a determined component, j represents the experiment number, N_{exp} is the total number of experiments, k is the time corresponding to the simulated and experimental points, T is the total duration of the experiment, and i represents 1 and/or 2 (depending on the type of experiment) corresponding to CO_2 and CH_4, respectively.

$$f_{obj} = \sum_{j=1}^{N_{exp}} \omega_j \left[\frac{1}{N_{points,j}} \sum_{k=1}^{T} \left(\sum_{i=1}^{2} (y_{k,exp,i} - y_{k,sim,i})^2 \right) \right] \quad (3)$$

$$\text{Rew}_{\text{LT}} = \sum_{\text{trial}=1}^{\text{N}_{\text{trials}}} \text{Rew}_{\text{trial}} = \sum_{\text{trial}=1}^{\text{N}_{\text{trials}}} - f_{obj_{trial}} \quad (4)$$

To ensure consistency in the rate of change for each parameter across trials, the action generated by the agent is normalized in a range between -1 and 1. Before being sent to the environment, the action is re-normalized, converting it into a set of parameters suitable for simulating the experiments. This helps nullify the high difference in the order of magnitude between the parameters to be estimated.

To reduce computational effort, 6 experiments were selected from the dataset of 17. These included 2 experiments with pure CO_2, 2 with pure CH_4, and 2 binary experiments. The RL algorithm focused on maximizing the long-term reward for these 6 breakthrough curves during training by maximizing the reward function in each trial. Once the optimal θ was identified for these experiments, it was used to simulate the remaining experiments, and the objective function was evaluated across all experiments to assess the methodology's results.

The primary difference between approaches two and three lies in the range of the search for the optimal set of parameters, specifically in the range of the action. The first and second approaches aimed to improve the results obtained by the authors of the base article. To achieve this, a range of ±20% around the reference

values was used as the upper and lower limits for the action to be taken in each trial. The reference values served as the initial guess. The third methodology was implemented to assess the RL algorithm's ability to find the optimal set of parameters without prior knowledge of the system. In this case, a broader range of exploration was allowed for each parameter. The initial guess was set as the mean value of the action limits. The action limits for each approach can be consulted in Table SI.4.

RESULTS

Agent

A DDPG agent is an actor-critic RL agent that, using neural-networks, searches for an optimal policy that maximizes the expected cumulative long-term reward. The actor takes observations and returns the corresponding action that maximizes the long-term reward. The critic takes observations and actions as inputs and returns the corresponding expectation of the long-term reward.

The architecture and structure used are based on the one presented in [1], with some adaptations. The actor is a feedforward neural network with three fully connected layers. The first two dense layers have 256 neurons each, followed by ReLU activations. The final dense layer has 4 neurons, and its output is transformed using the Tanh activation function. The critic is a multi-input architecture with two neural network branches. Both input features through a fully connected layer with 256 neurons. The outputs of these branches are concatenated and passed through a ReLU activation, followed by a fully connected layer with 256 neurons and a subsequent ReLU activation. The agent uses an Ornstein–Uhlenbeck noise function to develop an exploration policy.

The hyperparameters were manually tuned following a sensitivity analysis, in which each of the main hyperparameters was varied within a specified search range. Although relevant, it was observed that hyperparameter manipulation within the selected tuning range had little impact on the algorithm's performance. Therefore, the agent was kept as small as possible without compromising its predictive capabilities. A more detailed description of the agent, as well as the process of hyperparameter tuning and selection, is provided in the SI.

Parameters Estimation

On the first approach, 500,000 trials were used to estimate θ. Despite the extensive number of iterations, the best parameter set only managed to reduce the error by 8% on the breakthrough curves compared to the reference parameters. Thus, while this methodology is more straightforward than the next two, it does not offer significant advantages to the standard approach, as it requires the same previous work, is more time-consuming and provides no meaningful improvements in accuracy.

For the second approach, the search for the optimal set of parameters was conducted over 350 trials, with the best result achieved at trial number 276. The obtained θ reduced the objective function by 26% for the training experiments and by 28% across all experiments. However, to achieve this result, all the manual work done in [1] to find the initial guess and a small margin of search must still be performed. This approach proved to be a valid methodology for achieving high accuracy, allowing for fine-tuning of the parameters, although exhaustive work is still required.

For the third approach, the search was done for 350 trials, with the best result achieved at trial number 119. The obtained θ resulted in a 15% reduction in the objective function for the training experiments and a 31% reduction in the objective function across the entire set of experiments, indicating a substantial improvement in the alignment between the simulated and experimental data. More significantly, this result demonstrates that the RL algorithm can map the surface area of the objective function and identify a function minimum, surpassing the derivative-based solver used in the reference work.

Table 1 summarizes the parameter sets obtained from each approach, the reference values used for process simulation, and the objective function obtained with each methodology. Table S.I.5 provides a more detailed analysis of the results. These results highlight the effectiveness of approach number 3. It resulted in the set of parameters that most significantly reduced the global error between the experimental and simulated datasets and was the only approach that improved the fit for the pure CH_4 experiments when compared to the reference work. Additionally, this methodology does not rely on all the previous work already done by the authors, like approach one and two, allowing a broad exploration of each parameter without prior knowledge of the system and, so, can be applied directly after experimental work.

Table 1: Reference and Estimated Parameters and objective function value obtained via Approach (Ap.) 1, 2 and 3

$\boldsymbol{\theta}$	Units	Ref.	Ap.1	Ap.2	Ap.3
$q_{sat,CO2}$	[mmol g^{-1}]	6.38	6.76	7.65	6.46
$q_{sat,CH4}$	[mmol g^{-1}]	7.38	6.87	6.48	6.86
$b_{\infty,\mathrm{CO2}}$	[Pa^{-1}]	1.55	1.40	1.24	1.67
$b_{\infty,\mathrm{CH4}}$	[Pa^{-1}]	8.07	8.87	9.68	8.74
$\boldsymbol{f_{obj}}$ $(\times 10^3)$		3.06	2.82	2.19	2.11

To evaluate the exploration behavior over trials, Figure SI.1 displays the action values assigned per trial in this approach. It demonstrates that the algorithm initially explores the entire parameter space. However, as iterations progress, it begins to focus more on a specific region,

prioritizing exploration in that area to identify a minimum. This underscores the algorithm's ability to explore the parameter space effectively while simultaneously learning to refine its search for optimal solutions.

When analyzing the evolution of the objective function over the trials (Figure 1), two main conclusions can be taken that coincide with the two main concepts of Reinforcement Learning. Firstly, a clear trend of reduction in the objective function emerges as the RL agent begins to learn. This demonstrates the agent's ability to leverage past experiences to maximize long-term rewards (exploitation). This learning process is further corroborated by the convergence observed in Figure SI.1 for all actions. Secondly, significant fluctuations in the objective function are still evident, even after numerous trials. These fluctuations can be attributed to the algorithm's continued exploration of the parameter space and the high sensitivity of the simulation to small parameter changes.

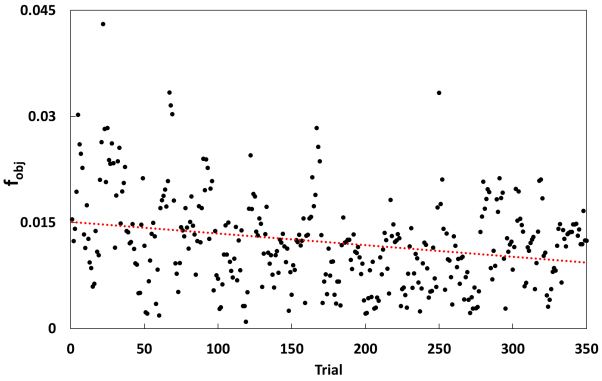

Figure 1: Evolution of the Objective Function Across Iterations: Objective function per iteration (•) and Trendline of the objective function (┈┈)

To assess the impact of these small fluctuations of the parameters set on the objective function, a sensitivity analysis was conducted. The 17 breakthrough experiments were simulated using the parameter set obtained on the third approach, adjusted by multiplication factors of ± 0.01, 0.1, 1, 5, and 10%. The objective function values for the full set of experiments, corresponding to each parameter set, are presented in Table SI.6.

This analysis is particularly relevant as it leads to several conclusions. Firstly, as mentioned previously, even small changes in the parameter set can result in significant variations in the objective function. For instance, decreasing the parameters by just 1% can increase the objective function by 38%. However, increasing all the parameters by the same 1% can reduce the objective function, demonstrating no straightforward correlation. This conclusion is supported by the results in Table SI.7, which presents the outcomes of a sensitivity analysis similar to the one described earlier. However, in this case, only a 1% variation was applied to each parameter individually. Even such a small change of 1% can lead to a 10% increase in the objective function.

This underscores the challenges faced by the RL algorithm in mapping the objective function surface, given its high sensitivity to minor parameter changes. Nonetheless, it also highlights the effectiveness of the algorithm in learning from past trials and converging toward an optimal region, as evidenced by Figure 1. These results also indicate that the best parameter set achieved with approach 3 does not correspond to the global minimum, as evidenced by better outcomes obtained after incrementing all parameters by 1%, 0.1%, and 0.01%. This was somewhat expected after analyzing Figure 1. While there is a clear trend of reducing the objective function across trials, the best result occurred at trial 119 out of 350. This suggests that the result was achieved more due to exploration than exploitation. Furthermore, since the RL algorithm did not immediately converge to the region of this trial, that area was not thoroughly explored, preventing further refinement of the result. This explains the presence of better outcomes near the identified optimum that were not found by the algorithm.

Finally, to evaluate the capability of the new set of parameters on predicting the adsorbed amount on every experiment, the Extended Langmuir Isotherms were plotted and the MSE values between the experimental (obtained in [1] after mass balance) and calculated (using both the reference parameters and those obtained from approach 3) q_{CO2} and q_{CH4} were determined (Table SI.8 ,Figures SI.2 and SI.3) . Although the new parameter set improves the fit between predicted and experimental adsorbed amounts for some experiments (especially for pure CH_4 experiments), it globally increases the MSE from 3.97×10^{-3} to 5.87×10^{-3}. This leads to the conclusion that this methodology does not improve the precision of the model in predicting the adsorbed amount. However, the adjustment of the simulated breakthrough curves to the experimental data is still enhanced by the new parameter set (Figure SI.4), as previously discussed. This improvement can be attributed to the ability of the new parameters to compensate for inaccuracies in other parameters of the mathematical model. Thus, while the prediction of the adsorbed amount is negatively affected, the overall adjustment benefits from this compensation. This is another advantage of using a broad range of search.

To assess the algorithm's reproducibility, approach 3 was repeated. After 207 trials, the objective function was reduced by 7%. Although this result did not match the previous outcome (likely due to earlier success driven by exploration), it confirms that the RL algorithm reliably identifies a set of parameters for the Extended Langmuir Equation that accurately simulates fixed-bed experiments for CH_4/CO_2 separation. Additionally, the same trends observed in Figures 1 and SI.1 were visualized when repeating the methodology, highlighting the

capability to replicate the behavior of the training.

CONCLUSIONS

This work introduces an AI-based methodology using Reinforcement Learning to estimate parameters in the mathematical model of gas-phase fixed-bed experiments for CO_2 and CH_4 separation and minimize the error between simulated and experimental breakthrough data.

Using the same DDPG agent, three approaches were tested. In the first, the RL algorithm replaced the traditional solver to determine Extended Langmuir isotherm parameters that best fit the experimental adsorbed amounts obtained from breakthrough curves. In the second and third approaches, the RL agent directly provided parameters for breakthrough curve simulations. The key difference lies in parameter exploration: the second approach used literature values as an initial guess with a limited search range, while the third treated it as a zero-knowledge problem, allowing wide parameter exploration without prior system knowledge.

While RL, like other meta-heuristic approaches, does not guarantee global optimality, it offers a flexible framework that adaptively explores and exploits the search space. By incorporating learning into the exploration process, RL can reduce the number of iterations typically required by standard meta-heuristic methods. Despite its simplicity and lack of manual work required after the experimental phase, the third approach delivered the best results. It reduced the global error between experimental and simulated data by 31% after just 119 iterations, when compared with the parameters obtained using the Generalized Reduced Gradient. The new set of parameters can compensate for misadjustments in other system parameters, which was not possible when obtaining the parameters by adjusting the Extended Langmuir Equation to only the adsorbed amount. Using RL as an optimization algorithm proved to be an efficient, reproducible, and highly effective method for parameter estimation. It exhibited strong iterative learning and thorough exploration of the objective function surface, successfully identifying a set of parameters that align the mathematical model with the experimental data.

DIGITAL SUPPLEMENTARY MATERIAL

For a more detailed explanation and analysis of the methodology and results, the Digital Supplementary Materials referenced throughout the work can be consulted here.

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