Evolutionary Dynamic Optimization of Control Trajectories for the Catalytic Transformation of the Bioethanol-To-Olefins Process using Neural Networks

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ABSTRACT

This paper presents a study on dynamic optimization of the catalytic transformation of Bioethanol-To-Olefins process. The main objective is to maximize the total production of Olefins by calculating simultaneously the optimal control trajectories for the main operating variables of the process. Using Neural Networks trained with two different types of Evolutionary Algorithms, the optimal trajectories have been automatically achieved, defining both an adequate shape and their corresponding parameters. The results suggest that, comparing with constant setpoints, the maximum production is increased up to 37.31% when using Neural Networks. The optimization procedure has become totally automatic and therefore very useful for real implementation.

CCS Concepts

•Mathematics of computing → Evolutionary algorithms; •Computing methodologies → Neural networks;

Keywords

Evolutionary dynamic Optimization; BTO process

1. INTRODUCTION

The Bioethanol-To-Olefins process (BTO) consists of the catalytic transformation of bioethanol into olefins over an acid catalyst. This is a key process in the concept of sustainable refinery, incorporating biomass or derivatives as an alternative feedstock to petroleum [1, 2].

The key point for the implementation of this process is to perform an advanced control strategy by adjusting the operating variables in a dynamic manner so that the product quality can be maintained while extending the lifespan of the catalyst. Due to the influence of multiple variables simultaneously over the reaction kinetics and the catalyst deactivation, it is necessary to develop advanced optimization strategies of the operational conditions that guarantees specific production objectives without exceeding the operation limits to avoid an irreversible deactivation of the catalyst.

The present work has the objective of performing a multivariable dynamic optimization of the Bioethanol-To-Olefins (BTO) process in order to maximize the total production of olefins while extending the catalyst lifespan. An Artificial Neural Network (NN) is trained using two different types of Evolutionary Algorithms: the genetic algorithm available in Matlab (GA) and the covariance matrix adaptation evolution strategy (CMA-ES) [3] to optimize the operational conditions of the process.

2. MATERIAL AND METHODS

The olefins production, given by the Equation (1), is the objective function to be maximized.

$$\max_{T, X_w, WF_{EO}^{-1}} \frac{\int_0^\tau R_O\left(T, X_w, WF_{EO}^{-1}\right) dt}{WF_{EO}^{-1}} \tag{1}$$

The NN receives as inputs the main operating variable of the process (reaction temperature (T), mass fraction of water in the feed (X_W) and space-time WF_{EO}^{-1}) for the previous time step and the current catalyst activity level (a). The output of the model are the current (at each time step) operational set points of each variable. Please note that the

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Table 1: NN training results for the implemented structures.

	Best Production ($g_o g_{catalyst}^{-1}$)		Mean Production ($g_o g_{catalyst}^{-1} \pm \sigma$)		Optimisation performance	
#	CMA-ES	GA	CMA-ES	GA	CMA-ES	GA
-	72.75	72.14	70.53 ± 0.78	70.22 ± 0.63	0.5729	0.0059
4	**99.91**	92.89	90.56 ± 7.37	81.73 ± 6.63	0.1546	0.0357
5	98.97	98.32	93.53 ± 5.01	88.36 ± 7.62	0.1132	0.0194
6	99.83	98.54	90.93 ± 4.80	91.76 ± 6.73	0.0955	0.0323
7	99.61	**99.35**	93.04 ± 4.13	90.58 ± 8.06	0.0962	0.0296
8	97.99	96.26	91.81 ± 4.63	90.19 ± 4.04	0.1027	0.0356

upper bound of the integral (τ parameter) will attend two early stopping criteria: catalyst activity (a) below 0.1; and olefins conversion rate (X_O) below 0.1. Whenever any of the above criteria is violated, we consider that the production has reached its maximum and should be stopped to proceed with the catalyst regeneration phase.

In order to define the trajectories for each control variable, it is necessary to define both the type of curve and the shape, defining the parameters for each of them. In this work, an NN has been used to directly generate the dynamic control trajectories for each operating variable that maximize the production of olefins (see Equation (1)).

The weights and biases of the NN have been trained directly using an EA that aims at maximizing the final total production of olefins when simulating the process behaviour under the control trajectories generated by the NN defined by each individual of the EA.

Two different types of EA have been used. The GA available in Matlab and the CMA evolution strategy developed by N. Hansen [3] using the default parameters. In both cases, the individuals consist of vectors of real numbers with the weights and biases defining the mapping computed by the NN. During the optimization procedure, these weights matrices and bias vectors are updated in order to define the NN that is able to generate the dynamical control trajectories that maximize the objective function.

The obtained results have been compared with previous ones where constant set points were optimized for the main operating variables using evolutionary algorithms [4].

3. EXPERIMENTATION

The first row in Table 1 shows the results using constant operational conditions (without any NN); the following rows present the number of hidden neurons tested. The second and third columns show the production of olefins for the best operational conditions (out of 10 repetitions) generated by each of the implemented NNs optimized by the two evolutionary algorithms. The next two columns show the mean production and standard deviation. Finally, the last two columns contain the `Optimisation performance` (ratio of the maximum production divided by the number of function evaluations).

The best solution obtained by the CMA-ES algorithm corresponds to the feed-forward NN with 4-4-3 topology. Figure 1 shows an example of the control trajectories generated with this topology. It should be emphasized that CMA-ES has obtained similar results regardless of the neural topology. On the other hand, the best solution found by the GA corresponds to higher number of hidden neurons (feed-forward NN with 4-7-3 topology). Moreover, the best solution for this topology found by the GA is slightly worse than both the overall best solution and the best solution for this

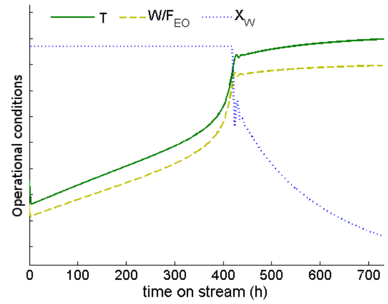

Figure 1: An example control policy generated by the NN.

topology found by the CMA-ES. Finally, solutions provided by the GA show differences up to 9 % depending on the type of neural topology used.

When analysing the performance of both evolutionary algorithms, it seems clear that CMA-ES produces better solutions requiring fewer fitness evaluations, and therefore obtaining better optimization performance indexes. Finally, it should be noted that trajectories optimized by the CMA-ES procedure produce between 34.68 % to 37.31 % higher production of olefins than when using constants trajectories.

The results are very promising. The trained neural networks have been able to find different trajectory types that maximize the production objective. They have been able to detect simultaneous regimen changes in all the operational variables definitely determining an increase of the production. This necessary regimen changes in the trajectories of the control variables are very difficult to detect using standard techniques with no previous knowledge about the process. The conclusion is that a NN succeeded in generating the main control trajectories of the BTO process by defining their most convenient curve form and shape defining parameters.

4. ACKNOWLEDGMENTS

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