Process Systems Engineering

(Process) Optimization

KEYWORDS: Particle Swarm Optimization, Fisher-Snedecor Test, Deep Neural Networks, Simulated Moving Bed, Pressure Swing Adsorption, Adsorption Heat Pumps

In the period of this report, various studies were performed in the area of optimization, including chemical process optimization. The research group has contributed to new algorithms for metaheuristic techniques, as well as the statistical treatment of the data obtained by such algorithms. The novel optimization techniques were applied to chemical industry study cases, namely to Simulated Moving Bed (SMB), Pressure Swing Adsorption (PSA), or Adsorption Heat Pumps (AHPs).

Introduction

Optimization in chemical engineering is always evolving thanks to cutting-edge techniques. Enhancements in reactor systems, SMB, PSA, and AHPs are driven by metaheuristic techniques, such as Particle Swarm Optimization (PSO), which effectively maximize performance and minimize the costs associated with production. Deep Neural Networks transform complex system models with higher computational times into models with lower fidelity but faster running times, allowing for faster optimization.

Feasible operational zones play important roles in strategies that address complicated decision-making scenarios and provide insights into system capabilities. Together, these approaches advance chemical engineering by effectively addressing problems such as multiple local minima, uncertainty, and multi-objective optimization, as well as by greatly improving process knowledge and efficiency.

Current Development

Part 1- Development of new Particle Swarm Optimization Strategies and Statistical Expansion of the obtained results

In this line of research, multiple algorithms for PSO were developed to mitigate different obstacles.

Parallel PSO was used for multi-objective optimization and relies on the differentiated update of the particles' position throughout the iterative process. The particles are divided into the same number of sets as the objective functions and prioritize the evolution and optimization of the attributed objective during their evolution. This algorithm was compared to the two-steps and traditional PSOs and has come back at the top as the one that led to the best compromise between the different objectives proposed.

Sliding Particle Swarm Optimization (SPSO) was created to promote the progressive exploration of the problem landscape, limiting the original area explored by the swarm and expanding it throughout the optimization. This procedure aimed to reduce the entrapment of the particles on local minima by enforcing the full exploration of the problem's landscape. SPSO was later expanded to CSPSO, where the problem constraints were considered in the landscape limitation.

A statistical expansion of the results obtained during the optimization procedure was also developed. The Fisher-Snedecor test was used as the filtering condition between the global swarm of particles produced. This tool was applied to single and multi-optimization problems, leading from the Most Probable Value (MPV) to the Feasible Operating Region (FOR) and from the Pareto Front to the Pareto Region, respectively.

Part 2- Optimization of adsorption processes with Particle Swarm Optimization

The separation of Bi-naphthol enantiomers through SMB operation was optimized using the Parallel PSO. In this process, the TMB model was used to provide the first approximation of the problem. With this approach, one aimed to minimize eluent consumption while maximizing productivity. The final results for TMB showed an improvement of 30% in average productivity when compared with other PSO approaches and 44% when considering the triangle theory. The employment of Parallel PSO allowed for the reduction of the computational time, since the algorithm promoted the evolution of all the variables simultaneously, which was not the case for two-steps and traditional PSOs. This process was also thought with the Varicol design and again optimized with the Parallel PSO algorithm, resulting in a further improvement of 30% in TMB productivity and 15% in SMB productivity compared to the latter design. Still concerning the separation of Bi-naphthol enantiomers, SPSO was used to design the Feasible Operating regions in three different scenarios: (i) standard one, where the eluent consumption was reduced by 30% compared to the equilibrium theory, (ii) high-purity production, associated with the fine chemicals and pharmaceutical industries, where the SPSO successfully contributed to the FOR construction and a knowledgeable operation of the SMB above the minimum purities required, and (iii) where limitations to the pumping capacity were considered and SPSO was able to overcome the limitation and still optimize the unit operation and provide insightful information on the operating conditions for the minimum requirements of the operation.

Another line of research invested in Deep Neural Networks (DNNs) for model acceleration and reduction of computational time in the PSO application. A clear example of the advantages of this methodology was given with its employment in SMBR (Simulated Moving Bed Reactor) synthesis of n-propyl propionate. The use of the surrogate model allowed for a reduction in the computational time of 448x when compared to the high-fidelity model previously employed, with no drawback for the optimal results achieved, as the scatter plot presented in Figure 1 accentuates.

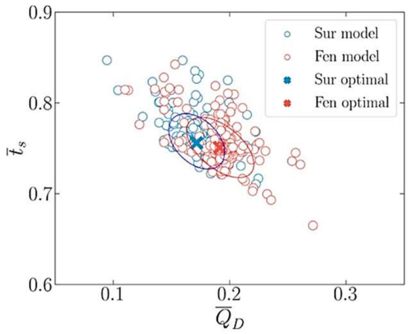

Fig. 1. Scatter plot of points for 99.5% confidence level for rigorous (Fen) and surrogate (Sur) model (DRNN) for desorbent flow rate vs switching time.

DNN models were further employed in material screening for PSA applications. One of the case studies evaluated the performance of a downstream PSA cycle for the separation of a CO_2 and CH_4 stream with origin in the extract product of a gas-phase SMB process for CH_4/N_2 separation using CO_2 as the eluent species. During the optimization, it was perceived that the evaluation of the materials solely based on metrics such as the maximum capacity of adsorption was deficient when compared to a full evaluation of the materials' performance in the process. Furthermore, the optimal materials to be used did not belong to a single family of materials. They were able to achieve the optimal operation within a differentiated set of operating conditions, further demonstrating that the comparison of different materials under the same values for the operation variables is biased.

Material screening was also performed in an Adsorption Heat Pump system. This study represented a broadening of the previously employed strategies that relied on parametric evaluation or fixed conditions to compare different materials. Through the application of CSPSO and the Fisher-Snedecor test, it was possible to obtain a novel design and control tool. The advantage of the statistical test is demonstrated in the expansion of the materials fitted to provide a suitable operation according to the more prominent objective, as can be seen in Figure 2.

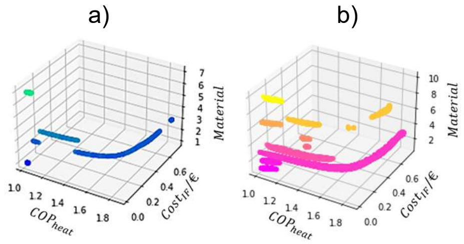

Fig. 2. Pareto Front (a) and Pareto Region (b) as a function of the adsorbent material.

<u>Part 3- Chemical Processes Scheduling</u>

Biased Random Key Genetic Algorithm was proven effective in solving job-shop scheduling problems (JSP) with deterioration effects. By considering instances from the literature and comparing the results with those obtained by other algorithms, it is evident that the BRKGA performs well in these instances. Implementing the multi-population approach further enhances the algorithm's performance, providing better solutions with smaller optimality gaps and standard deviations. Moreover, considering deterioration effects in the scheduling process has proven crucial for achieving realistic and efficient solutions. The optimization approach, which accounts for job and machine deterioration, outperforms the approach that considers deterioration after solving the problem. For linear, exponential, and sigmoid job deterioration cases, the optimization approach significantly improves the makespan, reducing it by an average of 4.7%, 38.1%, and 17.7%, respectively. Similarly, the optimization approach effectively reduces the makespan by an average of 22.9% for linear machine deterioration. By incorporating deterioration into the scheduling algorithm, jobs can be assigned more efficiently, resulting in shorter makespans compared to scenarios where deterioration is not considered. Furthermore, maintenance should also be considered in the scheduling optimization process for machines subject to deterioration. Its inclusion resulted in an improvement of approximately 746% in the makespan for a specific instance, highlighting the importance of scheduling periodic maintenance instead of random or end-of-production maintenance without optimization (see Figure 3). These findings contribute to the body of knowledge in the field of JSP and provide valuable insights for industrial applications.

Future Perspectives

The potentialities of this research line within the investigation group are vast since all the processes developed in the other lines can benefit from optimization and the side-by-side evolution allows for a better understanding of the potential improvements and algorithm gaps that can be solved.

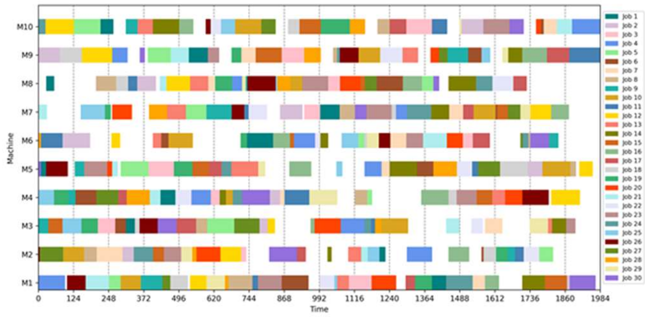

Fig. 3. Instance la31 schedule considering linear machine deterioration with optimization and maintenance.

A plausible development lies in the Real-Time Optimization of the dynamic cyclic processes that are SMB and PSA, where parameter estimation and modeling simplification will be key features for achieving optimization of the current conditions of operation with reasonable precision and speed.

With metaheuristic techniques, one might also look towards the scheduling of the operation of the different separation steps or tasks, for resource optimality.

Related Sustainable Development Goals

Outputs

Master Dissertations

[1] Beatriz Cambão da Silva, Modelling and optimization of adsorption-based heat pumps, MEQ, FEUP, 2022

[2] Diana G. Campinho, Scheduling of a multi-product batch process in the chemical industry with deteriorating effects, MEQ, FEUP, 2023

Selected Publications

[1] Matos. *et al.*, Comput Chem Eng. 123, 344–356 (2019).

[2]I. B. R. Nogueira. *et al.*, Chemical Engineering Research and Design. 180, 243–253 (2022)

[3]C. M. Rebello *et al.*, Chemical Engineering Research and Design. 178, 590–601 (2022)

[4]I. B. R. Nogueira *et al.*, Chemical Engineering and Processing - Process Intensification. 148, 107821 (2020)

[5] I. B. R. Nogueira *et al.*, Comput Ind Eng. 135, 368–381 (2019)

[6] B. C. Silva *et al.*, ACS Omega. 8, 19874–19891 (2023)

[7]V. V. Santana *et al.*, ACS Omega. 8, 6463–6475 (2023)

[8] I. B. R. Nogueira *et al.*, A.M. IFAC-PapersOnLine. 55, 211–216 (2022)

[9]I. B. R. Nogueira *et al.*, Ind Eng Chem Res. 59, 14037–14047 (2020)

[10] J. Matos *et al.*, IFAC-PapersOnLine. 54, 542–547 (2021)

[11] M. J. Regufe, *et al.*, IFAC-PapersOnLine. 54, 43–48 (2021)

[12]J. Matos, *et al.*, IFAC-PapersOnLine. 54, 548–553 (2021)

[13] R. V. A. Santos *et al.*, Ind Eng Chem Res. 60, 7904–7916 (2021)

Team

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