Efficient Evaluation of Vacuum Pressure-swing Cycle Performance using Surrogate-based, Multi-objective Optimization Algorithm

Héctor Octavio Rubiera Landa, a Yoshiaki Kawajiri, b,a Matthew J. Realff a,*

a School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, 311 Ferst Drive N. W., Atlanta, GA 30332-0100, U.S.A.
b Department of Materials Process Engineering, Nagoya University, Furo-cho 1, Engineering Building 1, Nagoya, 464-8603, Japan
matthew.realff@chbe.gatech.edu

Abstract
The performance evaluation of vacuum pressure-swing adsorption (VPSA) cycles with detailed, full-order models (FOMs) is typically a time-consuming and resource-intensive task. Popular state-of-the-art approaches include e.g., dynamic optimization approaches—see e.g., Swartz and Kawajiri (2019); and application of evolutionary algorithms, i.e., genetic algorithms, see e.g., Fiandaca et al. (2009). In this work, we present a strategy that combines two techniques in order to improve the computational efficiency of VPSA process modeling. Firstly, we improve the convergence in the calculation of cyclic steady state (CSS), using the FOM, by treating the calculation task as a fixed-point iteration (FPI) problem. We apply the FPI acceleration method by Anderson (1965) to improve FPI computations. Secondly, we embed the accelerated CSS computation into algorithm ‘Surrogate Optimization of Computationally Expensive Multiobjective Problems’ (SOCEMO) created by Müller (2017), which specifically addresses multi-objective optimization of expensive-to-evaluate black-box functions. This combination of approaches improves computational performance for Pareto frontier estimation that requires evaluation of process metrics at CSS, without sacrificing high-fidelity of the full-order VPSA model, and thus constitutes an attractive alternative to evaluate cyclic adsorption processes.

Keywords: surrogate-based multi-objective optimization, periodic processes

1. Introduction
The dynamic character of periodic adsorption operations, as well as their required spatiotemporal description, continues to represent a challenge from the computational point of view. The lack of closed-form solutions to the mathematical models applied to represent these processes is traditionally addressed by numerical approximations, which oftentimes can become challenging to solve. Moreover, if the end goal is to conduct parametric investigations or optimization for conceptual process design using these models, we are confronted with a computationally-intensive task. The process optimization of periodic adsorption processes may become even more expensive if we include competitive adsorption equilibria principles with non-trivial adsorption isotherm courses, see e.g., Rubiera Landa et al. (2013), or more-detailed mass-transfer mechanisms meant to describe particle-level adsorption phenomena dynamically. Another potential source of complexity—not addressed herein—is related to multi-
column processes with column-interacting steps, e.g., pressure equalization. Therefore, there is an inherent need to develop computational tools & strategies to surmount these challenges.

**Investigated vacuum pressure-swing adsorption cycle:** The process that we consider in this work is a 4-step VPSA cycle with light-product pressurization (LPP) that targets heavy-product recovery at high purity. Figure 1 illustrates graphically this cycle and its operational steps. We have developed a full-order model (FOM) to describe the dynamic operation of this process applying a thermally-modulated structured fiber contactor in Rubiera Landa et al. (2020b).

Interest in these types of adsorbents has grown in the last years driven by process intensification, as well as addressing difficult gas separations such as CO$_2$ capture by economically-viable routes—see e.g., Bui et al. (2018) and references therein. The applied mathematical model consists of a set of one-dimensional, time-dependent PDEs that represent the coupled, nonisothermal, non-isobaric, mass, energy & momentum balances, characterizing the dynamic behavior of a packed-bed adsorber. These equations describe the periodic features of the 4-step VPSA cycle by adscribing appropriate BCs and ICs. The model implementation includes competitive adsorption equilibria as expressed by the Ideal Adsorbed Solution Theory (IAST) developed by Myers and Prausnitz (1965), as well as other well-known explicit competitive equilibria equations. In order to represent thermal modulation, we consider microencapsulated PCM embedded in the fibers as demonstrated by DeWitt et al. (2019). A smooth-interface model, see e.g., Surana et al. (2015), is included in the energy balance equation to account for the phase-transition enthalpy and temperature-dependent physical properties of the PCM. Model details may be consulted in Rubiera Landa et al. (2020b).

2. Methods & algorithms

**Numerical solution of model equations:** We transform the PDEs that describe adsorber dynamics into a time-dependent ODE system by applying the method of lines with a cell-centered finite-volume spatial discretization (FVM). Cell averages of the state variables, $x = \left[ \bar{y}_1, \bar{q}_i, \bar{y}_2, \bar{q}_j, \bar{p}_j, \bar{T}_j \right]^T$, $j = 1, \ldots, J$, are integrated in time by adaptive step, multi-stepping, backward differentiation formulæ (BDF). This discretization warrants the necessary robustness to treat the adsorber model as a black-box function as required by the applied MOO algorithms.

**Genetic algorithms for MOO of VPSA cycle:** Several approaches exist to perform MOO of cyclic adsorption processes. If the process simulation is sufficiently robust,
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then we can apply evolutionary optimization techniques—e.g., a genetic algorithm (GA). The FOM is hereby treated as a black-box function, without requiring its gradient information, which in turn may be difficult to generate for some adsorption process models. On the other hand, this aspect of evolutionary algorithms can be a drawback, because identifying non-dominated points that constitute the sought-after Pareto frontiers usually requires many function evaluations. Clearly, if these functions are expensive to evaluate, this becomes a computationally-intensive procedure. For the purpose of benchmarking our results, we applied a variant of the well-established NSGA-II algorithm by Deb et al. (2002) to our FOM.

**Applied black-box function formulation:** The function calls executed by the optimization algorithms entail the CSS simulation of the 4-step VPSA cycle for given values of the design variables and evaluating subsequently process performance metrics that define the objective space of the MOO tasks to solve. The selected design variables, \( u \), include process conditions of the cycle or design parameters of the FOM; these are: 1.) high-pressure level, \( p_{\text{high}} \); 2.) feed gas velocity, \( v_{\text{feed}} \); 3.) adsorption step time, \( t_{\text{Ad}} \); 4.) evacuation pressure level, \( p_{\text{Ev}} \); & 5.) weight fraction of adsorbent in fiber composites, \( \omega_{\text{MOF}} \). The objective variables considered for the VPSA cycle are: 1.) product purity, \( \Phi_{\text{Pu}}(u) \); 2.) product recovery, \( \Phi_{\text{Re}}(u) \); 3.) productivity, \( \Phi_{\text{Prod}}(u) \); & 4.) specific energy consumption, \( \Phi_{\text{En}}(u) \).

**Fixed-point iteration formulation of CSS calculation:** Traditionally, calculation of CSS entails the dynamic simulation that the process would follow during transient operation, e.g., start-up. In essence, we simulate for a cycle \( \ell \), store the vector of state variables, \( x_{\ell} \), at a specified time of the cycle, e.g., at the end of the evacuation step, \( t = t_{\text{Ev.,end}} \), and then apply it as IC to obtain the next iterate, \( x_{\ell+1} \). This is equivalent to the procedure expressed by Picard Iteration (PI)

\[
x_{\ell+1} = g(x_{\ell}), \quad \ell = 0, 1, 2, \cdots, \text{(until convergence)}
\]

where we simply substitute successively \( x_{\ell} \) in map \( g \) to obtain \( x_{\ell+1} \). In practice, we verify if CSS is attained by applying e.g., the \( \ell_2 \)-norm, \( \| e \|_2 \leq \delta_{\text{tol}} \), with \( e := g(x_{\ell}) - x_{\ell+1} \), for a small, specified threshold, \( \delta_{\text{tol}} \). The simulation of the process is therefore formulated as a fixed-point iteration (FPI) task, which can be solved efficiently by applying methods for the acceleration of sequences, such as the vector extrapolation methods published by Sidi (2017).

**Anderson Acceleration (AA):** An interesting alternative that we investigate in Rubiera Landa et al. (2020a) consists of applying the algorithm developed by Anderson (1965) to accelerate the FPI calculation, Eq. (1), therefore reducing its computational cost. We implement AA as described by Walker and Ni (2011), employing their code. Application of this FPI acceleration technique helps to reduce the cost in terms of number of iterations required to fulfill the CSS condition by factors ranging from 1.3x
to 2x w.r.t. PI, with superlinear convergence rate, as documented in Rubiera Landa et al. (2020a).

**Initialization of the fixed-point iteration:** The CSS calculation may be initialized in two ways, depending on the IC applied at the start of the dynamic simulations: a) cold-start mode: the adsorber is either free of the more-adsorbed component or has been fully-regenerated; & b) warm-start mode: the adsorber has been partially loaded with adsorbates. Typically, a stored vector of state variables, \( x = x(t,z) \), from a previous CSS calculation may be applied to perform warm-start initialization with the purpose of attaining CSS with a smaller number of iterations—this is the mode applied below.

**Surrogate-based multi-objective optimization using accelerated black-box function evaluation:** We apply the SOCEMO algorithm, a bound-constraint surrogate-based multi-objective optimization strategy created by Müller (2017) that has been designed to address expensive black-box problems with relatively large numbers of decision variables and objectives. In brief, this optimizer generates a radial-basis function (RBF) approximation for each objective constituting the specified multi-objective problem. A careful, well-thought-out algorithm that applies a GA plus adaptive sampling using the RBF surrogates’ information aims at reducing the expensive black-box function evaluations—i.e., the accelerated FPI calculations—to a minimum, whilst simultaneously refining the quality of the RBF surrogates as the algorithm continues to identify the Pareto frontiers. This yields a powerful general-purpose MOO solver that can be applied easily to the periodic adsorption process at hand. We denominate the proposed combined solution strategy as ‘SOCIMO+AA’.

**Investigated MOO task:** In order to assess the computational performance of this combination of techniques, we formulate a two-objective (bi-objective, BOO) task and solve it first with NSGA-II, applying the conventional PI and name this strategy ‘NSGA-II+PI’. Afterwards, we solve identical tasks applying the ’SOCIMO+AA’ strategy.

**Table 1:** Applied bounds for design variables of BOO Task.

<table>
<thead>
<tr>
<th>Variable</th>
<th>( p_{\text{high}} )</th>
<th>( v_{\text{feed}} )</th>
<th>( t_{\text{Ad}} )</th>
<th>( p_{\text{Ev}} )</th>
<th>( \omega_{\text{MOF}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Units</td>
<td>atm</td>
<td>m / s</td>
<td>s</td>
<td>atm</td>
<td></td>
</tr>
<tr>
<td>Lower bound</td>
<td>3.0</td>
<td>0.1</td>
<td>15</td>
<td>0.10</td>
<td>0.15</td>
</tr>
<tr>
<td>Upper bound</td>
<td>7.5</td>
<td>1.0</td>
<td>120</td>
<td>0.35</td>
<td>0.35</td>
</tr>
</tbody>
</table>

The optimization tasks explore the process performance of the aforementioned 4-step VPSA cycle w/ LPP for a typical dry flue gas stream, employing a thermally modulated fiber composite loaded with a metal-organic framework (MOF) and decision variables’ bounds listed in Table 1:

- **BOO Task.** Identify the Pareto frontier for recovery vs. purity formulated as:

\[
\text{maximize } \{ \Phi_{\text{Pu,CO}_2}(u), \Phi_{\text{Re,CO}_2}(u) \}, \text{ s.t. } -\infty \leq u^{lb} \leq u \leq u^{ub} \leq \infty.
\]

For ‘NSGA-II+PI’ we allow a maximum of 30 generations with a population size of 80 function evaluations. In the case of ‘SOCIMO+AA’ we set a total budget of 150 function evaluations.
3. Results & discussion

Figure 2 illustrates the Pareto frontiers obtained by applying ‘NSGA-II+PI’ as well as ‘SOCEMO+AA’ for cold-start and warm-start initialization modes. Table 2 summarizes the computational performance results of all runs. Both strategies allow us to identify non-dominated points accurately at the prescribed tolerances. A slightly worse result was obtained for the particular ‘NSGA-II+PI’ run executed with cold-start initialization mode. The two runs performed with ‘SOCEMO+AA’ yielded almost identical Pareto frontiers with good spread, while outperforming slightly the warm-start ‘NSGA-II+PI’ run in terms of the identified non-dominated points.

The two results obtained with ‘NSGA-II+PI’ would likely improve with tighter tolerances and increased function evaluations’ budget, at the expense of an even higher computational cost, in order to match the obtained ‘SOCEMO+AA’ Pareto frontiers. The ‘SOCEMO+AA’ strategy applying warm-start initialization mode gave the most efficient result, requiring approximately 6% of the time needed by ‘NSGA-II+PI’ with cold-start initialization mode. In other words, for this particular example, we achieved roughly a 17-fold reduction in computational cost. The effect of the initialization mode can be observed from the mean times required for computing a single CSS. Both warm-start runs required less time than their cold-start counterparts.

<table>
<thead>
<tr>
<th></th>
<th>NSGA-II+PI cold-start</th>
<th>NSGA-II+PI warm-start</th>
<th>SOCEMO+AA cold-start</th>
<th>SOCEMO+AA warm-start</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. generations (max. 30)</td>
<td>25</td>
<td>30</td>
<td>n/a</td>
<td>n/a</td>
</tr>
<tr>
<td>No. function evaluations</td>
<td>2000</td>
<td>2400</td>
<td>160</td>
<td>152</td>
</tr>
<tr>
<td>No. non-dominated points</td>
<td>80</td>
<td>80</td>
<td>47</td>
<td>47</td>
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<tr>
<td>Mean calculation time per CSS, s</td>
<td>46</td>
<td>37</td>
<td>84</td>
<td>36</td>
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<tr>
<td>Total calculation time, s</td>
<td>92815</td>
<td>88326</td>
<td>13440</td>
<td>5467</td>
</tr>
</tbody>
</table>

4. Conclusion

We have introduced a powerful and easy-to-implement strategy to perform multi-objective optimization of cyclic adsorption processes, exemplified by a 4-step VPSA
cycle designed for CO$_2$ capture. The strategy consists of applying AA to improve the convergence efficiency to CSS when evaluating expensive black-box function evaluations of FOMs for periodic adsorption processes. In combination with the MOO solver SOCEMO, we estimated the Pareto frontier of a typical VPSA process optimization task in a computationally efficient manner. An important feature of the proposed ‘SOCEMO+AA’ strategy is that no offline or a priori sampling phase needs to be carried out, as it is often required by other meta-modeling techniques, since SOCEMO constructs surrogates of objective functions and identifies non-dominated points ‘on the fly’, i.e., their calculation is embedded in the execution of the algorithm. We demonstrated that a reduction in computational cost of one order of magnitude, with only a fraction of the number of black-box function evaluations needed by a GA, can be achieved with the proposed strategy, preserving high-fidelity of the optimization results.

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**References**


