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A Study on Accelerated Convergence of Cyclic Steady State in Adsorption Process Simulations

Sai Gokul Subraveti[a]*, Kian Karimi[b], Matteo Gazzani[b], and Rahul Anantharaman[a]

[a] SINTEF Energy Research, Trondheim, Norway
[b] Utrecht University, Copernicus Institute of Sustainable Development, Princetonlaan 8a, 3584 CB Utrecht, the Netherlands
* Corresponding Author: sai.gokul.subraveti@sintef.no.

ABSTRACT

Cyclic adsorption processes attain a cyclic-steady state (CSS) condition by undergoing repeated cycles in time, owing to their transient and modular nature. Mathematically, solving a set of underlying nonlinear partial differential equations iteratively for different steps in a cycle until the CSS condition is attained presents a computational challenge, making the simulation and optimization of cyclic adsorption processes time-consuming. This paper focuses on expediting the CSS convergence in adsorption process simulations by implementing two vector-based acceleration methods that offer quadratic convergence akin to Newton's methods. These methods are straightforward to implement, requiring no prior knowledge of the first derivatives (or Jacobian). The study demonstrates the efficacy of accelerated convergence by considering two adsorption processes that exhibit complex dynamics, namely, a four-step vacuum swing adsorption and a six-step temperature swing adsorption cycles for post-combustion CO_2 capture. The case studies showcase the potential for improved computational efficiency in adsorption process simulations.

Keywords: cyclic adsorption processes, modeling, optimization, process design, acceleration methods

INTRODUCTION

Cyclic adsorption processes are widely employed for industrial gas separations [1, 2]. The underlying separation mechanism involves the solid adsorbent to selectively adsorb one or more gases from a gaseous mixture. Depending on the choice of regeneration, i.e., by either varying temperature or pressure or both, the adsorbed gases are recovered or removed. Accordingly, different process operational modes such as pressure swing adsorption (PSA), vacuum swing adsorption (VSA), temperature swing adsorption (TSA), etc. are implemented [3].

Unlike distillation and absorption, which typically operate at steady-state conditions, cyclic adsorption processes are transient in nature and are operated cyclically in a sequence of constituent steps, thus attaining a cyclic steady-state condition (CSS), instead of a true steady state [2]. From a process design perspective, these processes are dictated by the set of nonlinear partial differential equations (PDEs) resulting from mass, momentum, and energy balances. Further, the modular nature allows these processes to undergo several constituent steps in each cycle. The choice and the sequence of steps, as well as the direction of flows, can give rise to several process configurations [4], which need to be optimized [5]. Another critical design parameter is the choice of the solid adsorbent and the contactor structure. Therefore, designing cyclic adsorption processes for a given adsorbent requires solving the nonlinear PDEs for each step repeatedly until CSS and then calculating the key process performance indicators based on the transient profiles of state variables obtained at the CSS. The CSS ensures that these profiles no longer vary as the numerical iterations are continued.

Despite such flexibility in adsorption process design, the main bottleneck for designing optimal process configurations lies in very high computational costs associated with repeated solving of nonlinear PDEs in process simulations to attain the CSS condition from an arbitrary initial condition. Although simulating one process configuration for a given adsorbent takes a few minutes of computational time [5], process models are often coupled with optimizers where thousands of operating conditions are probed, which makes the process design and

optimization computationally demanding. Given the flexibility of synthesizing different process configurations and the recent advent of a multitude of adsorbents for gas separations [6], the problem of finding the optimal design for a given separation further exacerbates as evaluating different process configurations and adsorbents will be a computationally daunting task.

To speed up adsorption process simulations, there have been some previous efforts to accelerate the determination of CSS [7-13]. For instance, Croft and LeVan in their first paper [7] incorporated Newton's method to speed up the iterations to attain CSS. Newton's method provided quadratic convergence near the CSS solution and converged faster than the cycle iterative procedure. However, the extra computation time for the calculation of the Jacobian matrix in each Newton iteration impaired the convergence acceleration [7, 8]. In the third paper of the series [9], Ding and LeVan developed several acceleration algorithms for the convergence of adsorption process simulations, which include a hybrid Newton-Broyden method, an iterative secant method, a sensitivity interpolation method, and a dynamic error tolerance method. These methods achieved better accelerations compared to the Newton's method [9]. Despite this, some of the methods rely on the prior knowledge of the Jacobian matrix. On the other hand, Nilchan and Pantelides [11] completely discretized the PDEs into algebraic equations and imposed the CSS condition as a constraint. Perturbation techniques have also been explored for accelerated convergence of CSS [12]. Moreover, Pai et al. [13] recently developed machine learning models to predict approximate CSS condition which is then fed as an initial condition to the PDE-based process model for rapid determination of CSS condition. The machine learning model for initial condition prediction was developed for a four-step VSA cycle based on the CSS profiles from hundreds of different operating conditions. In the context of other related separations, methods such as the single shooting method were considered for the convergence of semicontinuous distillation process simulations [14].

This study focuses on implementing two acceleration methods for the convergence of the CSS condition in adsorption process simulations, with an overall goal of significantly reducing the computational times of current adsorption process design and optimization tools. These acceleration methods require no prior knowledge of the

Table 1: Governing partial differential equations of the adsorption process model.

Gas-phase component mass balance

$$\frac{\partial y_i}{\partial t}+\frac{y_i}{P}\frac{\partial P}{\partial t}-\frac{y_i}{P}\frac{\partial T}{\partial t}=\frac{T}{P}D_{\mathrm{L}}\frac{\partial}{\partial z}\left(\frac{P}{T}\frac{\partial y_i}{\partial z}\right)-\frac{T}{P}\frac{\partial}{\partial z}\left(\frac{y_i P}{T}v\right)-\frac{RT}{P}\frac{1-\varepsilon}{\varepsilon}\frac{\partial q_i}{\partial t}$$

Gas-phase total mass balance

$$\frac{1}{P}\frac{\partial P}{\partial t}-\frac{1}{T}\frac{\partial T}{\partial t}=-\frac{T}{P}\frac{\partial}{\partial z}\left(\frac{P}{T}v\right)-\frac{RT}{P}\frac{1-\varepsilon}{\varepsilon}\sum_{i}^{m}\frac{\partial q_i}{\partial t}$$

Column energy balance

$$\left[\frac{1-\varepsilon}{\varepsilon}\left(\rho_s C_{p,s}+C_{p,a}\sum_{i=1}^{m}q_i\right)\right]\frac{\partial T}{\partial t}$$
$$=\frac{K_z}{\varepsilon}\frac{\partial^2 T}{\partial z^2}-\frac{C_{p,g}}{R}\frac{\partial(vP)}{\partial z}-\frac{C_{p,g}}{R}\frac{\partial P}{\partial t}-\frac{1-\varepsilon}{\varepsilon}C_{p,a}T\sum_{i=1}^{m}\frac{\partial q_i}{\partial t}+\frac{1-\varepsilon}{\varepsilon}\sum_{i=1}^{m}(-\Delta H_i)\frac{\partial q_i}{\partial t}-\frac{2h_{in}(T-T_w)}{\varepsilon r_{in}}$$

Wall energy balance

$$\rho_w C_{p,w}\frac{\partial T_w}{\partial t}=K_w\frac{\partial^2 T_w}{\partial z^2}+\frac{2r_{in}h_{in}(T-T_w)}{r_{out}^2-r_{in}^2}-\frac{2r_{out}h_{out}(T_w-T_a)}{r_{out}^2-r_{in}^2}$$

Darcy's pressure drop

$$v=\frac{4}{150\mu}\left(\frac{\varepsilon}{1-\varepsilon}\right)^2 r_p^2\left(-\frac{\partial P}{\partial z}\right)$$

Linear driving force model

$$\frac{\partial q_i}{\partial t}=k_i(q_i^{*}-q_i)$$

Jacobian matrix and are easier to implement for any cyclic process. Simulation of two different adsorption processes is chosen to test the two acceleration methods. As a first case, a four-step VSA cycle designed for post-combustion CO_2 capture [5] was used for the process simulation. The second case explores the simulation of a six-step TSA cycle designed again for post-combustion CO_2 capture [15]. Despite both processes exhibiting complex dynamics and taking several cycles to achieve CSS, they differ in their process dynamics and how they converge to CSS. This makes them an ideal case study for testing the vector-based acceleration methods.

METHODOLOGY

Adsorption Process Model

The mathematical model for simulating adsorption column dynamics consists of a system of nonlinear PDEs obtained by solving mass, momentum, and energy balances [5]. The model assumptions include (1) ideal gas, (2) axially dispersed plug flow representing the bulk flow, (3) linear driving force model describes the bulk-to-surface mass transfer, (4) there exist no radial gradients for state variables, i.e., composition, pressure, and temperature, (5) Darcy law used for pressure drop calculations, (6) thermal equilibrium between the gas and the solid phases, and (7) uniform column properties. The resulting governing equations based on these assumptions are provided in **Table 1**.

The model is numerically solved by discretizing the spatial terms in PDEs into 30 finite volumes with a total variation diminishing (TVD) scheme involving the van-Leer flux limiter [5]. The resulting ordinary differential equations (ODEs) are then integrated based on standard ODE solvers in Python [16]. The process simulations are carried out using a uni-bed approach where a single column undergoes all constituent steps sequentially. The column is initialized with feed composition at low pressure and the cycle is simulated until the CSS condition. At CSS, state variables such as composition, pressure, and temperature profiles are obtained.

Cyclic-steady state (CSS) condition

Several mathematical criteria can be employed for the attainment of CSS from a pre-defined initial condition in adsorption process simulations [5, 17-19]. For instance, few studies assumed that the process reaches CSS after a very large number of cycle iterations [16]. Most of the other studies, however, assume that the CSS criterion is met when absolute integral differences in axial profiles of state variables [5] or absolute overall mass balance errors [5, 18] fall below a tolerance limit. Effendy et al. recently proposed a rigorous CSS criterion, reducing the differences between the current and CSS states of axial profiles to a set tolerance limit without needing prior knowledge of the CSS [19].

This study uses the same definition for the CSS condition as that of the case study [5], which assumes that the CSS criterion is met when the overall mass balance error for the process is less than 0.5%.

Methods for Accelerated Convergence of CSS condition in process simulations

An important basis for implementing the acceleration methods in the present study is that the process simulation of cyclic adsorption processes is a fixed point (or Picart) iteration problem [19]. Schematically shown in **Figure 1**, a number of cycles are simulated (cycle iterations) from an arbitrary initial condition to a fixed-point CSS condition. If f is a function representing the adsorption process simulator, then the fixed-point iteration problem can be written as

$$\Delta_{n+1} = f(\Delta_n) \tag{1}$$

In the above equation, the adsorption process simulator, f, takes the previous state of the adsorption column (Δ_n) as an input and returns the subsequent state of the adsorption column (Δ_{n+1}). Note that Δ represents a vector of state variables such as gas-phase composition, solid-phase concentrations, pressure, and column and wall temperatures across the adsorption columns. After

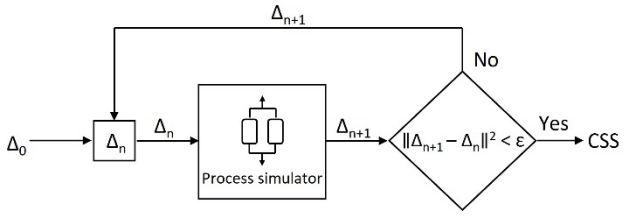

Figure 1. Schematic of a cyclic adsorption process simulator. Adapted from [19].

several iterations, the CSS condition is achieved. Although fixed point iterations are the simplest way to obtain nonlinear solutions without any prior knowledge of f and its derivative [20], linear convergence to CSS makes it computationally slow [19].

Alternatively, Eq. 1 can be reformulated as a root-finding problem:

$$\varphi(\Delta) := f(\Delta) - \Delta = 0 \tag{2}$$

A common approach for solving Eq. 2 is Newton's method,

$$\Delta_{n+1} = \Delta_n - \frac{\varphi(\Delta_n)}{\varphi'(\Delta_n)} \tag{3}$$

which provides a quadratic and faster convergence to solutions, compared to fixed-point iterations. The main drawback of Newton's method as a convergence

accelerator is the prior knowledge of first derivatives or Jacobian, i.e., $\varphi'(\Delta)$, which is not straightforward to calculate for many realistic systems.

Without affecting the order of convergence, Newton's method can be modified into "derivative-free" algorithms such as Steffensen's methods or its equivalents [19, 20]. Steffensen's convergence acceleration for a scalar nonlinear fixed-point equation, $x = g(x)$, can be represented as:

$$x_{n+3} = x_n - \frac{(x_{n+1}-x_n)^2}{(x_{n+2}-2x_{n+1}+x_n)} \quad (4)$$

Practical problems such as adsorption process simulations often deal with many unknown variables and systems of nonlinear PDEs. Obtaining the solutions typically requires the spatial discretization of PDEs which introduces a vector of state variables (Δ) across the column. Several vector-based acceleration methods are available in the literature to deal with vector nonlinear fixed-point problems [20].

In this study, two vector-based acceleration methods proposed in the literature are considered for the accelerated convergence of the CSS condition in adsorption process simulations. Particularly, the acceleration algorithms proposed by Irons and Tuck [22] and Graves-Morris [23] are evaluated for CSS convergence acceleration. It is worth noting that both methods are the vector extensions of Steffensen's scalar method (Eq. 4).

Irons and Tuck Acceleration Method

The vector acceleration method proposed by Iron and Tuck [22] can be expressed as:

$$\Delta_{n+3} = \Delta_{n+2} - \frac{(\Delta_{n+2}-\Delta_{n+1})\cdot(\Delta_{n+2}-2\Delta_{n+1}+\Delta_n)}{\|\Delta_{n+2}-2\Delta_{n+1}+\Delta_n\|^2}(\Delta_{n+2}-\Delta_{n+1}) \quad (5)$$

Note that this acceleration method is invoked alternately with a basic fixed-point cycle iteration.

Graves-Morris Acceleration Method

The approach of Graves-Morris [23] is given by:

$$\Delta_{n+3} = \Delta_{n+1} - \frac{\|\Delta_{n+2}-2\Delta_{n+1}+\Delta_n\|^2}{(\Delta_{n+1}-\Delta_n)\cdot(\Delta_{n+2}-2\Delta_{n+1}+\Delta_n)}(\Delta_{n+2}-\Delta_{n+1}) \quad (6)$$

This accelerator is also applied alternately with a basic fixed-point iteration in adsorption process simulations.

RESULTS AND DISCUSSION

Two case studies involving different adsorption processes are considered to test the convergence accelerator methods. The first examines a VSA cycle, where the process dynamics are heavily influenced by the pressure swing between the adsorption and desorption steps. The second explores a TSA cycle, where the dynamics are driven by the temperature swing during the process. Thus, the two cases differ in terms of their process dynamics and their convergence to CSS.

Case 1: Four-step VSA cycle

Here, the vector acceleration methods are incorporated into the process simulation of a four-step VSA cycle separating the binary mixture of CO_2/N_2 for postcombustion CO_2 capture [5]. The VSA process was designed to recover CO_2 from a binary mixture of 15% CO_2 and 85% N_2 at ambient pressure, which represents dry flue gas from coal-fired power plants.

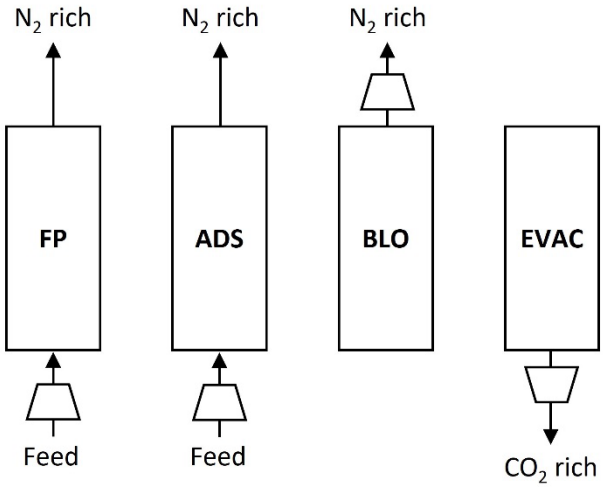

Figure 2. Four-step vacuum swing adsorption cycle designed for post-combustion CO_2 capture [5].

Figure 2 illustrates the schematic of the four-step VSA cycle. The cycle consists of feed pressurization (FP), adsorption (ADS), co-current blowdown (BLO), and counter-current evacuation (EVAC) steps. Each step can be implemented using appropriate boundary conditions and isotherm parameters provided by Haghpanah et al. [5]. Commercial zeolite 13X was used as the adsorbent. The example considered represents the complex dynamics of adsorption processes, and several cycles are needed to reach CSS. Similar to reference work, CO_2 and N_2 isotherms on zeolite 13X were described using the competitive dual-site Langmuir isotherm model. Finally, the cycle operating conditions used for the simulation are as follows: P_H = 1 bar, P_I = 0.2 bar, P_L = 0.1 bar, v_0 = 1.0 m s^{-1}, t_{FP}= 15 s, t_{ADS} = 15 s, t_{BLO} = 30 s, t_{EVAC} = 40 s. Note that P_H, P_I, and P_L are the feed, intermediate, and low pressures in adsorption, blowdown, and evacuation steps, respectively. The feed is introduced into the column in the adsorption step with an interstitial velocity v_0. t_{FP}, t_{ADS}, t_{BLO}, and t_{EVAC} are the step durations of feed pressurization, adsorption, blowdown, and evacuation steps, respectively. The column was first initialized with feed composition, and the simulation was conducted until CSS.

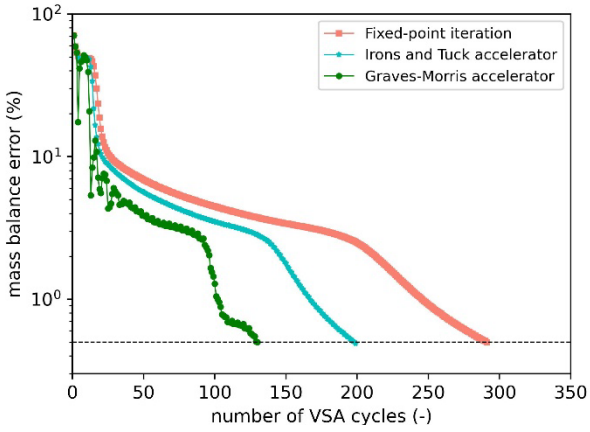

Figure 3. Convergence of overall mass balance error for the four-step VSA process simulation using the fixed-point iteration, Irons and Tuck [22] algorithm, and Graves-Morris method [23].

Figure 3 shows the convergence of the overall mass balance error for the simulation. Without any accelerator, the fixed-point iteration took 291 cycles to reach the CSS. The four-step VSA process simulations are repeated for the same operating conditions with the two acceleration methods. The convergence of the overall mass balance for the simulation with the accelerators can also be seen in **Figure 3**. Using the acceleration algorithm by Irons and Tuck, the CSS convergence was achieved after 199 cycles. The computations were reduced by approximately one-third. On the other hand, Graves-Morri's acceleration method almost reduced the number of iterations to CSS by less than half, i.e., 130 cycles, outperforming the Irons and Tuck algorithm. The CO_2 purity and recovery obtained at CSS using all the three methods are reported in **Table 2**. The acceleration methods offered faster convergence to CSS while achieving the same performance as that of the conventional fixed-point iteration with rather straightforward implementation.

Table 2: Performance of the VSA process using three different approaches for the convergence of CSS.

Method	CO_2 purity (%)	CO_2 recovery (%)
Fixed-point iteration	79.64	37.36
Irons & Tuck [21]	79.65	37.36
Graves-Moris [22]	79.64	37.36

Case 2: Six-step TSA cycle

In this case study, the vector acceleration methods are employed in the process simulation of a six-step TSA cycle proposed by Joss et al. [15] to separate the binary feed mixture of 12% CO_2 and 88% N_2 using commercial zeolite 13X. **Figure 4** shows the six-step TSA cycle consisting of the adsorption (ADS), recovery (REC), two heating (HEAT), purge (PUR), and cooling (COOL) steps. For simulating this process, the cycle operating conditions and the simulation parameters have been retrieved from Joss et al. [15]. The adsorption step occurs under a constant pressure of 1.3 bar and at an ambient temperature of 300 K. In the heating steps, the column is externally heated to 420 K to desorb CO_2. The cycle is simulated for the following operating conditions: T_{COOL} = 300 K, T_{HEAT} = 420 K, v_0 = 1.4 m s^{-1}, t_{ADS} = 150 s, t_{REC} = t_{PUR} = 25 s, t_{HEAT1} = 150 s, t_{HEAT2} = 600 s, t_{COOL} = 600 s. It is worth noting that the durations of TSA cycles are much longer compared to VSA cycles due to heat transfer limitations. Here, a column that is completely saturated with N_2 is used as an initial condition to simulate the cycle until CSS.

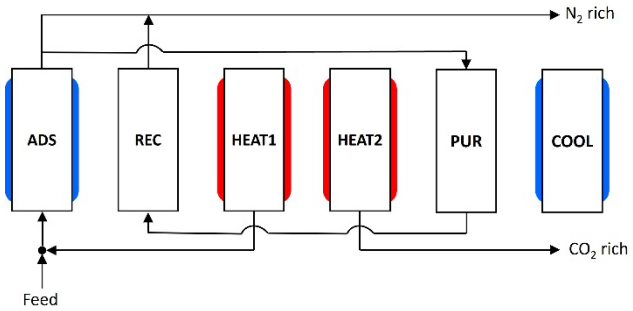

Figure 4. Six-step temperature swing adsorption cycle proposed by Joss et al. [15] for post-combustion CO_2 capture.

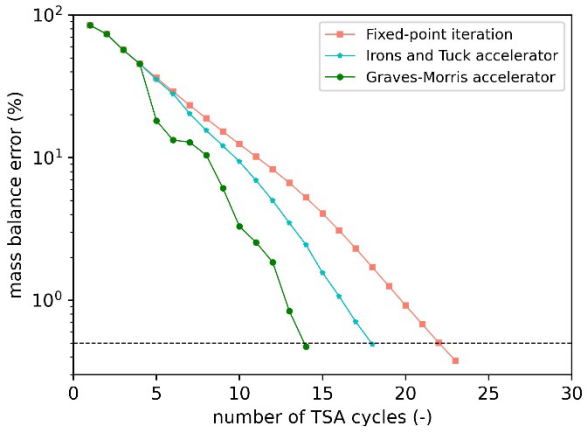

Figure 5. Convergence of overall mass balance error for the six-step TSA process simulation using the fixed-point iteration, Irons and Tuck [22] algorithm, and Graves-Morris method [23].

Figure 5 and **Table 3** present the comparative performances of the vector acceleration methods for this

simulation. As can be seen from **Figure 5**, the fixed-point iteration needed 23 cycles to reach CSS, where the overall mass balance convergence is less than 0.5%. When the accelerators are incorporated into the process simulations, the cycle converges to CSS in 18 and 14 cycles using Irons and Tuck and Graves-Morri's methods, respectively. While the TSA cycle reached CSS in fewer cycles compared to the VSA cycle, each TSA cycle requires a significantly longer computational time. Hence, utilizing accelerator methods facilitated almost 1.25 – 1.67 times faster CSS convergence compared to the fixed-point iteration. The true impact of accelerators on computational speeds up will further be realized in process optimizations. It is worth reiterating that the implementation of the considered acceleration methods is straightforward. Table 3 reports the comparable CO_2 purity and recovery obtained at CSS using all the methods.

Table 3: Performance of the TSA process using three different approaches for the convergence of CSS.

Method	CO_2 purity (%)	CO_2 recovery (%)
Fixed-point iteration	93.08	99.02
Irons & Tuck [21]	93.06	98.92
Graves-Moris [22]	93.06	98.94

CONCLUSIONS

The computational complexity in cyclic adsorption process simulations mainly arises from solving a set of nonlinear partial differential equations iteratively for every cycle until the cyclic-steady state (CSS) is achieved making the simulation and optimization routines of these processes exceedingly time-consuming. Despite prior efforts to expedite CSS convergence, the computational burden of CSS still persists in adsorption process simulations.

This study contributes to overcoming the computational challenges of CSS determination in adsorption process simulations by implementing two vector-based acceleration methods proposed previously in the literature. The acceleration methods of Irons and Tuck and Gravis-Morris can offer quadratic convergence near the CSS solutions, like Newton's method without requiring the prior information of the first derivatives or Jacobian. These methods are straightforward to implement in adsorption process simulations. The acceleration capabilities of these methods are demonstrated by considering two different adsorption processes, namely, a four-step VSA cycle and a six-step TSA cycle, which undergo complex dynamics and take multiple cycles to reach CSS. The results showed that the Graves-Morris accelerator provided expedited convergence by speeding the convergence of VSA simulations more than double. For the same case, Irons and Tuck's method reduced the cycle iterations to CSS by one-third. When the accelerator methods are incorporated into the process simulations of a six-step TSA cycle, the Graves-Morris accelerator marginally provides better convergence than Irons and Tuck's method by reducing the number of iterations to 14 from the original 23 fixed-point cycle iterations. In the context of process optimization, where thousands of operating conditions must be probed, these acceleration methods can significantly reduce the overall computational times with no extra effort. This work is a first step in addressing the computational challenges associated with adsorption process simulations. In the future, these methods will be extended to different adsorption processes and efforts will be directed to further improve the convergence of CSS. For instance, incorporating machine learning principles into the acceleration framework can further boost CSS convergence speeds.

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