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PREDICTIVE CONTROL OF PRESSURE SWING ADSORPTION

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Abstract: Pressure swing adsorption requires a repeated cycle of four steps. The periods of these steps, or other defined terminal conditions, determine the rate and quality of the product, and its cost. In transient situations such as upsets or grade changes, it is not intuitively obvious how the steps should be progressively altered to bring the plant to the desired operating point in an optimal fashion. The present work considers the problem of real-time maximization of the production of a single adsorber, and maintaining a set-point concentration in its product receiving vessel. In a modelling exercise, these objectives have been met using predictive control based on completion of the present step, plus two full future cycles to reduce the end-effect. The approach sought to be fast and robust by suitable linearisation of the system. This allowed MILP solution in the mixed logical dynamical (MLD) framework as a mixed integer dynamic optimisation (MIDO). However, this problem was ultimately solved faster and more reliably by testing all combinations for constraint violations and the objective value.

Keywords: PSA, hybrid systems, dynamic optimisation, predictive control.

1 INTRODUCTION

An increasing range of adsorbent materials is extending the use of pressure swing adsorption (PSA) in the separation of gas mixtures. These materials are designed to selectively adsorb one component from a mixture. As in vapour-liquid equilibrium, the equilibrium quantity of this adsorbed component in the solid phase increases with its partial pressure in the gas phase. Thus the solid can be used to adsorb the component at high pressure, and it can be “regenerated” by expelling the adsorbed species at low pressure. In air separation, N_2 is selectively adsorbed, leaving an O_2 -rich product stream. A number of adsorbers can be arranged to work in complementary cycles so as to smooth out production flow and the use of common resources. However, the present analysis will focus on a single adsorber with a product storage vessel as in figure 1.

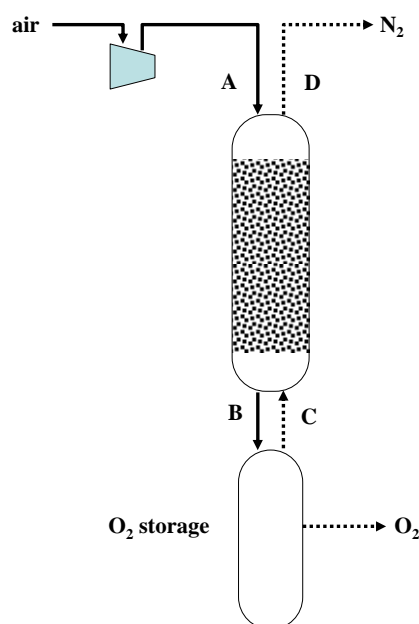


Fig. 1 A basic pressure swing adsorption configuration for air separation

Four distinct steps, comprising the Skarstrom cycle, are required:

(1) **pressurisation:**

A open; B,C & D closed

(2) **adsorption at high pressure:**

A & B open; C & D closed

(3) **depressurisation:**

D open; A,B & C closed

(4) **purge at low pressure:**

C & D open; A & B closed

During step 2, a high purity product can be obtained, particularly if some of the product itself is used in step 4 for purging, as is shown here.

The mechanism by which a high-purity product is obtained is not entirely self-evident. It is in fact achieved by developing a suitable composition profile in the solid phase which acts to “screen” the down-ward moving air in step 2. That profile will of course oscillate through each full cycle of four steps, but the so-called “cyclic steady state” (CSS) is achieved once a fixed associated profile arises at the end of each step. Even with fixed sequencing of the valves A,B,C and D (ie. fixed periods for each step), the approach to CSS may take many cycles.

In figure 2 an adsorber is represented as discretised into N compartments in series. If thermal effects are neglected, this system is defined by $2 \times N + 1$ states. These are the moles of the adsorbed species in the gas phase (m_i) and the solid phase (w_i) in each compartment i , as well as the total number of moles (M) in the gas phase of a compartment. For a uniformly packed bed with no frictional losses one notes that M is the same in all compartments, and the total number of gas moles in the system is $N \times M$ which is clearly proportional to the pressure. To re-iterate the comment above regarding the CSS, the repeated cycles needed to achieve CSS are required to achieve the supporting profiles of m_i and w_i , with the latter determining longer settling times as the adsorbent capacity increases. If one imagines the control problem associated with the unsteady process, one thus foresees several major hurdles:

- (a) high number of states
- (b) few measureable states
- (c) hybrid (switched and continuous)
- (d) long time-constants

To date, most of the work aimed at optimising PSA operation has focused on the optimal “positioning” on the CSS cycle. The cycle can be positioned by choosing a particular set of four times, one for each of the Skarstrom steps. Alternatively, it can be posi-

tioned by choice of a particular set of heuristic rules, eg.

- [1] pressurise until pressure reaches P_{max}
- [2] adsorb until a total of M_{FEED} moles of feed have been introduced in this step
- [3] depressurise until pressure reaches P_{min}
- [4] purge until a total of M_{PURGE} moles of product have been returned in this step

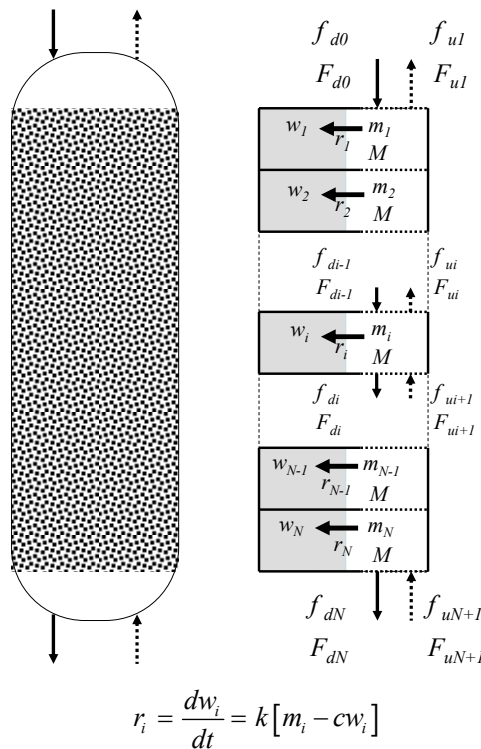


Fig. 2 Discrete representation of states in a pressure-swing adsorber

Models have been quite detailed, accounting for thermal effects, pressure losses, nonlinear adsorption isotherms, energy, etc, and optimisations have aimed at overall economic operation. These are large non-linear optimisation problems, such as tackled by Latifi *et al.* (2008), Jiang *et al.* (2005) and Kvamsdal and Hertzberg (1995). Indeed, Latifi *et al.* do not look for a convergence in time, but rather formulate the optimisation problem around a single cycle, including in the objective function a minimisation of the deviation between the states at the beginning and end of the four steps of the cycle.

The relatively small amount of work on the unsteady-state quite likely arises from the difficulties (a),(b),(c) and (d) mentioned above. Bitzer and Zeitz (2002a) developed a nonlinear distributed parameter observer for PSA based on a Luenberger arrangement for error feedback. In Bitzer and Zeitz (2002b)

these authors present a control scheme which has two parts: A feed-forward section sets the time-periods for each step of the cycle, based on the sensitivity of production and purity predicted offline at CSS. A degree of adjustment of the time-periods is superimposed for correction of measured quality by PID feedback. This type of approach is extended by Bitzer (2005), with the feedforward based on the inversion of a reduced-order model, for example a Hammerstein representation.

One can reflect for a moment on what advantages might accrue from dynamic feedback control of PSA. A distributed process with long time-constants is inherently difficult to adjust, so manual operations are likely to be determined by heuristic criteria such as above. In start-up, shut-down or recovery from an upset, these are likely to be conservative and inefficient. What one seeks is an optimal strategy to bring the process from its current point to one which ensures product quality and rate, at minimum cost, possibly in coordination with other adsorbers. With this aim, the work below investigates the possibility of using robust linear tools in an optimal predictive control format, initially applied to a single adsorber and product tank.

2 MODEL

The adsorber is modelled as a series of N mixed compartments as in figure 2. Typical values are used for air separation, using a linear equilibrium relationship for the N_2 ($m^* = cw$) and ignoring the small amount of O_2 adsorbed. Pressure losses through the bed and thermal effects are likewise neglected. In the equations, M and F respectively represent the total gas inventory of a compartment, and the total gas flow, whereas m and f refer only to the species which is being adsorbed (N_2). Flows are divided into “downward” (d) and “upward” (u), of which one or the other will be zero depending on the step of the cycle.

$$\frac{dM}{dt} = \frac{1}{N} \left\{ \begin{array}{l} F_{d,0} + F_{u,N+1} - F_{d,N} - F_{u,1} \\ - \sum_{i=1}^N k [m_i - cw_i] \end{array} \right\}$$

$$\frac{dm_i}{dt} = f_{d,i-1} + f_{u,i+1} - f_{d,i} - f_{u,i} - k [m_i - cw_i] \quad (1)$$

$$\frac{dw_i}{dt} = k [m_i - cw_i]$$

The only nonlinearity arises as the requirement that the effluent composition from a compartment obeys the following equations for downward or upward flow respectively.

$$\frac{f_{d,i}}{F_{d,i}} = \frac{m_i}{M} \quad \text{or} \quad \frac{f_{u,i}}{F_{u,i}} = \frac{m_i}{M} \quad (2)$$

This was linearised using deviations (Δ) from an estimated operating point ($'$)

$$\frac{f' + \Delta f}{F' + \Delta F} = \frac{m' + \Delta m}{M' + \Delta M} \quad (3)$$

and neglect of the deviation products. The total flow profile F_i in either direction (ie. F'_i , $i = 1, \dots, N$) can be estimated relatively closely, as can the total number of moles in a compartment M . Estimates of the flow and inventory profiles of the adsorbed species, f_i' and m_i' , were obtained by multiplying F'_i and M by a composition y_{av} appropriate to each Skarstrom step. The linearisation conditions are thus summarised as follows:

[1] **pressurisation:** M' at P_{max} ; F' reducing linearly from F_{feed} at top to 0 at bottom; y_{av} at 0

[2] **adsorption at high pressure:** M' at P_{max} ; F' reducing linearly from F_{feed} at top to $F_{feed} - f_{feed}$ at bottom; y_{av} at 0

[3] **depressurisation:** M' at $75\% P_{max} + 25\% P_{min}$; F' increasing linearly from 0 at bottom to a flow $F_{depress}$ at top; y_{av} at $(1+y_{feed})/2$

[4] **purge at low pressure:** M' at P_{min} ; F' profile constant at the purge gas flow rate F_{purge} ; y_{av} at y_{purge}

In this way, a discrete linear model for the $2N+1$ states is constructed for a unique Δt_j suited to each of the Skarstrom steps:

[1] **pressurisation:**

$$\mathbf{x}(t + \Delta t_1) = \mathbf{A}_1 \mathbf{x}(t) + \mathbf{b}_1 \quad \text{with} \quad \Delta t_1 = 8s \quad (4)$$

[2] **adsorption at high pressure:**

$$\mathbf{x}(t + \Delta t_2) = \mathbf{A}_2 \mathbf{x}(t) + \mathbf{b}_2 \quad \text{with} \quad \Delta t_2 = 16s \quad (5)$$

[3] **depressurisation:**

$$\mathbf{x}(t + \Delta t_3) = \mathbf{A}_3 \mathbf{x}(t) + \mathbf{b}_3 \quad \text{with} \quad \Delta t_3 = 16s \quad (6)$$

[4] **purge at low pressure:**

$$\mathbf{x}(t + \Delta t_4) = \mathbf{A}_4 \mathbf{x}(t) + \mathbf{b}_4 \quad \text{with} \quad \Delta t_4 = 8s \quad (7)$$

Should the flow settings F_{feed} , F_{purge} , $F_{depress}$ (or feed or purge stream compositions) change, the corresponding matrix \mathbf{A}_j (new linearisation point) and vector \mathbf{b}_j (new process input) are updated. Exit flows are determined automatically in the solutions for the constant-pressure steps 2 and 4.

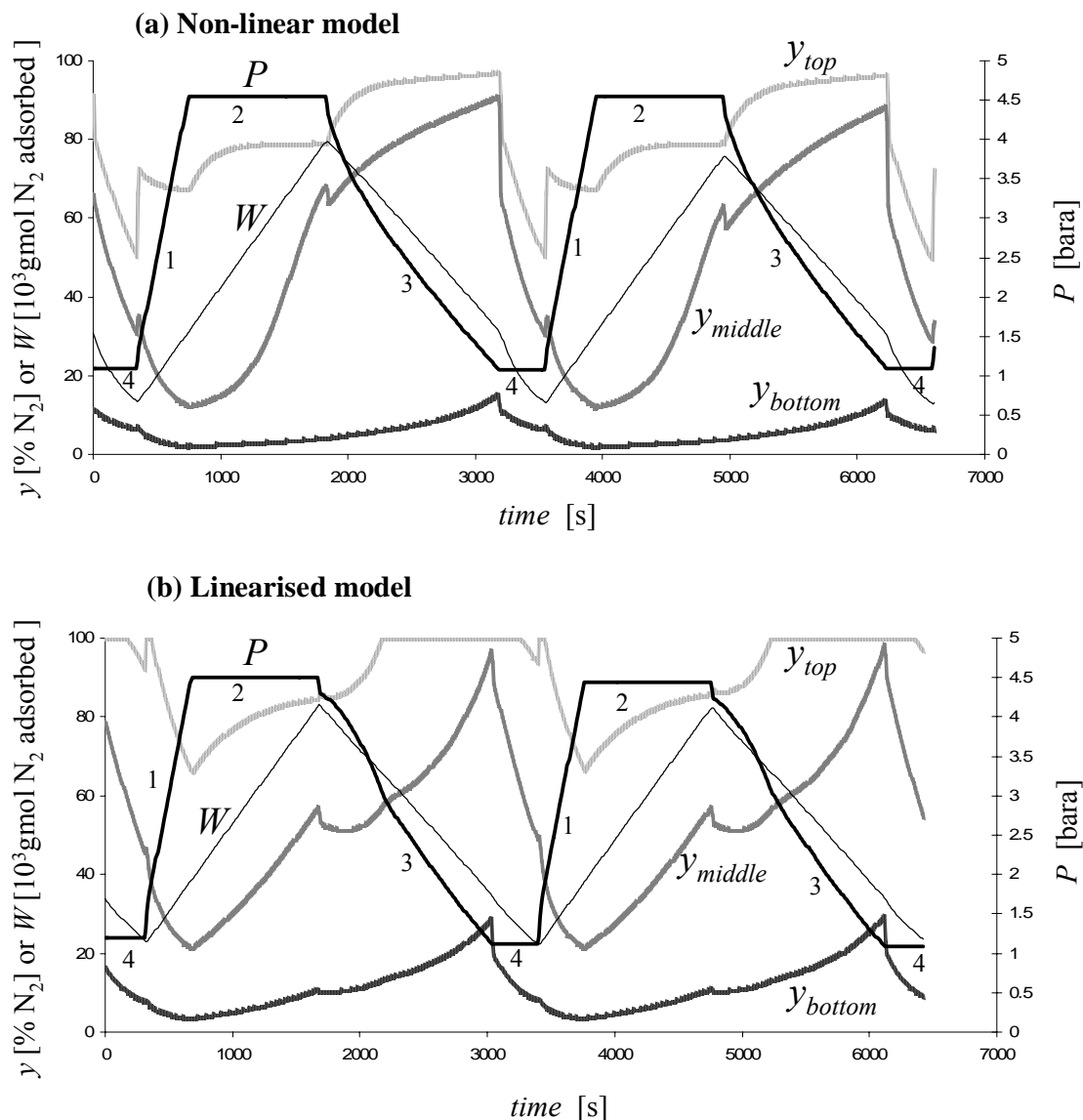


Fig. 3 Comparison of (a) *Nonlinear Model* and (b) *Linearised Model* predictions for Skarstrom cycles using the same switching criteria (Section 1)

In figure 3 the non-linear and linearised model predictions, both using 9 compartments, are compared for Skarstrom cycles determined by the heuristic switching rules in section 1 ($P_{min} = 1$ bara; $P_{max} = 4.5$ bara; Total Air used in step 2 = 6×10^4 gmol; Total product used for Purge in step 4 = 1×10^4 gmol). For this analysis the composition of the “Product” used for purging was fixed at 5% N₂. Actual cumulative product compositions were in fact 2.8% N₂ for the non-linear model, and 5.2% N₂ for the linear model, with about 1.5×10^4 gmol of product being made on each cycle (ie. reflux ratio = 2).

3 PREDICTIVE CONTROL

A single PSA unit does not appear to offer a lot of scope for dynamic optimisation. The compositions

and achievable flows of the *feed air*, and the *product used for purging*, are likely to be fixed. The only control freedom left thereafter is the length of each step of the Skarstrom cycle, which could equivalently be set by heuristic rules (eg. varying the target “breakthrough” composition of the product stream in step 4). Even if the flow rates of the feed and purge streams could be varied, equation (1) shows that this is equivalent to varying the time intervals if the adsorption is not rate-controlling (k large enough).

Thus a single PSA unit offers just these four adjustments. In section 1 it was mentioned how these are manipulated for optimisation of the CSS. In contrast, the motive for *unsteady-state* optimisation lies in dealing with extraneous disturbances or objectives. Thus, if the system state finds itself away from its optimal value (after a disturbance, or during start-up/Shut-down), it needs to be guided back in an op-

timal fashion. Additionally, there will be requirements to maintain a set-point inventory within the product storage vessel, and to keep it close to a set-point composition. Even for a single PSA unit, this offers interesting scope for strategic manipulation of its Skarstrom step lengths. With multiple PSA units feeding and drawing from the same product storage vessel, the problem becomes much more complex, and it may be anticipated that an *integer programming* (IP) approach for unit coordination will truly be advantageous here.

Bearing the above unsteady-state optimisation objectives in mind, the present work thus seeks to use robust linear system tools for constrained optimisation of one or more complete future Skarstrom cycles, by correct choice of the first and subsequent switching points for the steps. Only the first switch is implemented, once it is shown to be “due” (immediate). Of course, the remaining switches are only evaluated as part of the overall optimisation, and not for use. Though the step lengths could be treated as continuous variables for optimisation, a “modulated” approach is rather used, entailing a *choice* of one of several distinct periods for each step. Apart from facilitating an IP solution, this will in due course also allow coordination with other PSA units.

3.1 Optimal predictive control with constraints

In predictive control, one is generally aiming to make the best choice of a series of control decisions which affect the system output up to a defined future time-horizon. Only the first choice is actually imple-

mented, before the entire optimisation is repeated on the next controller time-step. If some of the choices are discrete (eg. gears of a car), or indeed, as seen above, if there are system behavioural changes, integer variables enter the problem, and one has a *mixed integer dynamic optimisation* (MIDO) problem.

Consider the problem of a single PSA column supplying a purified gas to a storage vessel, from which users draw their requirements at arbitrary rates (figure 1). Removal of N_2 from air to provide an O_2 supply will be the example. The objective will be to maintain a desired O_2 -rich inventory in the storage vessel, and to control its composition at a given set-point. Discretionary situations arise, for example, if demand is low, and composition is poor - in which case production can be reduced and a greater proportion of the N_2 removed, to raise the O_2 concentration in the storage vessel.

In the real-time situation, the controller is cycling asynchronously at its own time-interval. In the present case this is 10s. It does not need to match the Δt_j of any of the Skarstrom steps j because the entire optimisation calculation is repeated *a priori* on each controller time-step. What is important to the control algorithm is to know the system *state* at this time. A first step was thus to develop a *state observer*. A Kalman filter based on the linearised models in equations (4) to (7), changing in sequence, was able to provide good estimates of the $2 \times N + 1$ state values using just three “measurement” outputs of the original *non-linear* model [(i) pressure P ; (ii) product outflow composition during step 2; and (iii) purge outflow composition during steps 3 and 4].

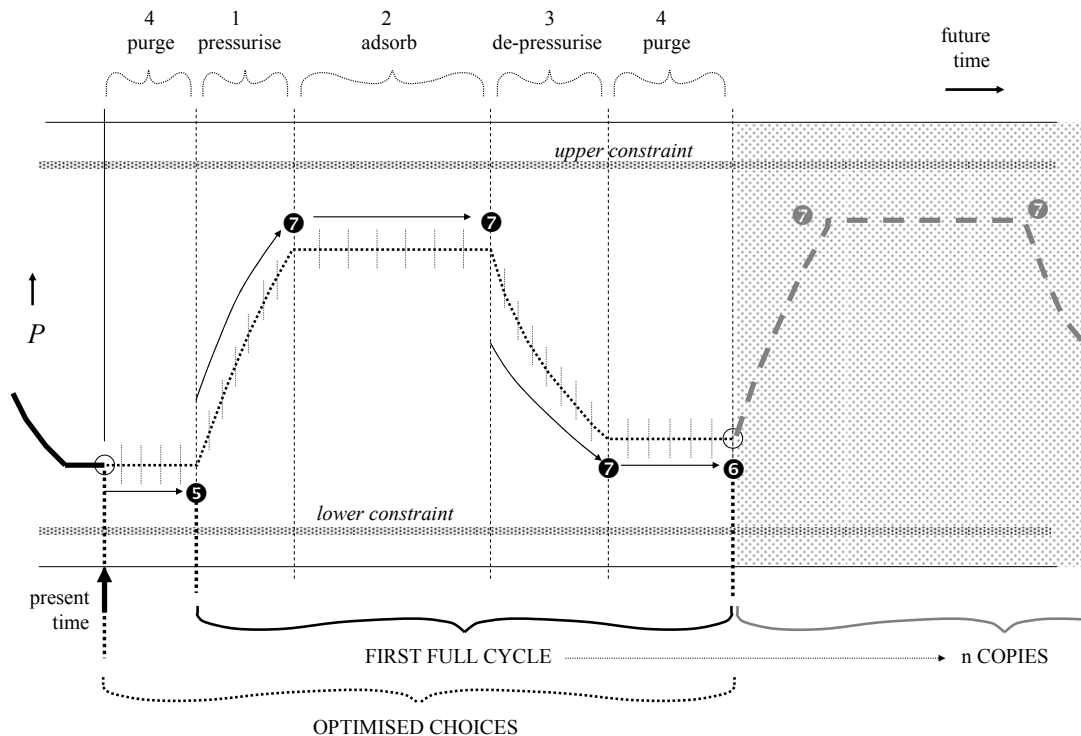


Fig. 4 Concept of future Skarstrom step length optimisation for a system found (for example) to be in a purge mode on the controller time-step

Apart from these state values, the predictive control algorithm of course needs to know which of the four possible steps of the Skarstrom cycle is presently being conducted. (Historical information - eg. how long it has been in this step - is not required). A look-up table indicates the required future sequence for completion of an entire Skarstrom cycle (constrained), followed by a repeat full cycle with the same step lengths (unconstrained):

[1] **pressurisation:**

complete 1 then do 2→3→4→1 , 2→3→4→1

[2] **adsorption at high pressure:**

complete 2 then do 3→4→1→2 , 3→4→1→2

[3] **depressurisation:**

complete 3 then do 4→1→2→3 , 4→1→2→3

[4] **purge at low pressure:**

complete 4 then do 1→2→3→4 , 1→2→3→4

The identified future sequence is then the basis of the optimisation. It amounts to a choice of the number of intervals Δt_j to spend in each of the Skarstrom steps j (figure 4). The result is five separate interval counts. Steps occurring *after* the production step 4 would appear to play a neutral or negative role (eg. use of Product for purging). Thus the objective function used here is based on one further repetition of the cycle ($n=1$) to reduce such “end-effects”. The computational load is reduced by forcing the “copies” to use the Skarstrom step lengths of the first full cycle.

The main interest is in whether the intervals left in the first (partial) step add up to less than the controller time-step. In that case the controller must take action *now* by switching to the next Skarstrom step.

The easiest way to structure the optimisation is to constrain the operation between liberal bounds such as determined by the heuristic rules in section 1 - viz, maximum and minimum pressure, and maximum total amounts of Feed and Product to be used in the adsorption and purge steps respectively. These bounds on their own determine a default Skarstrom cycle. The purpose of the optimisation then is to bring the terminal points of the cycle inwards in order to maximise the objective function.

The optimisation scheme is represented schematically in figure 4 in terms of pressure. The variable constraints are only considered at the *end* of each step - ie. at the switching point. This will however not be problematic, since the variables associated with the specified constraints all vary monotonically in each step (figure 3). An important motivation for this scheme is that if necessary, computation can be reduced by narrowing the range of choice in each step, eg. close to the number of intervals determined for that mode in the preceding optimisation. Using a centred search range, migration will still occur at successive controller steps. However, the first partial step must always extend down to 1 owing to its function in determining the switching time. Figure 5 illustrates how a selection is made on each step from a limited number of “models” for that step, each representing a different number of intervals – ie. a different time-span.

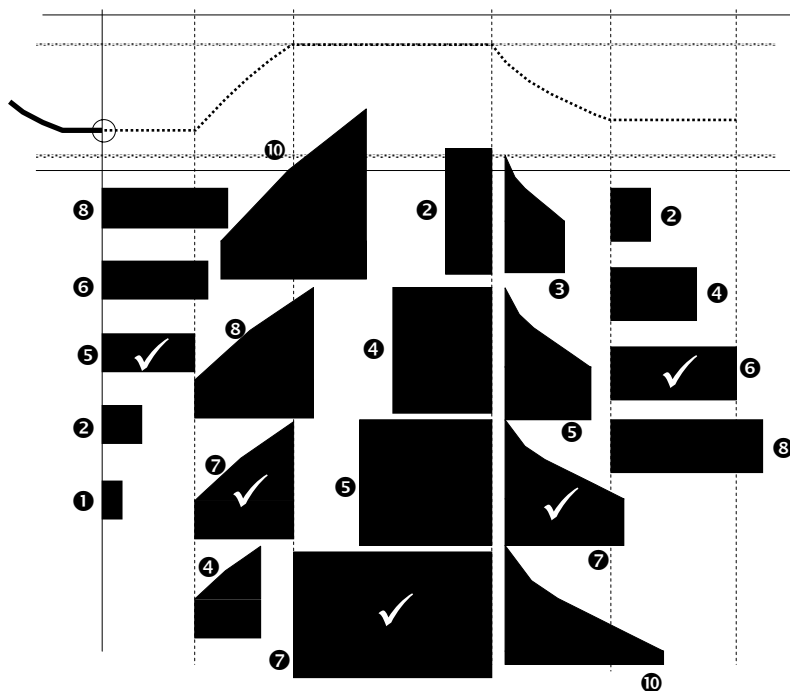


Fig. 5 Choice of transfer functions of different numbers of intervals for each Skarstrom step

3.2 Solution method

For each of the Skarstrom steps $j=1, \dots, 4$ a range of transition models is pre-prepared, one for each of the possible number of intervals $1 \leq i \leq n_{\max}$ that could be used for that step:

$$\mathbf{x}(t+i\Delta t_j) = \mathbf{A}_j^{(i)} \mathbf{x}(t) + \mathbf{b}_j^{(i)} \quad (8)$$

The new arrays $\mathbf{A}_j^{(i)}$ and $\mathbf{b}_j^{(i)}$ are obtained by individually recursing equations (4) to (7). Now if the particular choices of i made to complete the present step j and the next 4 complete steps are

$$i[j], i[j+1], i[j+2], i[j+3], i[j+4],$$

where it is understood that the index values will “wrap” around in the range 1,2,3,4, then it is these choices that must be made optimally in determining the future state sequence. Representing $\mathbf{x}(t+i[j]\Delta t_j)$ by \mathbf{x}_j one has

$$\mathbf{x}_j = \mathbf{A}_j^{(i[j])} \mathbf{x}_{j-1} + \mathbf{b}_j^{(i[j])} \quad (\text{partial step}) \quad (9)$$

$$\left. \begin{aligned} \mathbf{x}_{j+k} &= \mathbf{A}_{j+k}^{(i[j+k])} \mathbf{x}_{j+k-1} + \mathbf{b}_{j+k}^{(i[j+k])} \\ \mathbf{x}_{j+k+4} &= \mathbf{A}_{j+k+4}^{(i[j+k])} \mathbf{x}_{j+k+3} + \mathbf{b}_{j+k+4}^{(i[j+k])} \end{aligned} \right\} k = 1, \dots, 4 \quad (10)$$

After completion of the present partial step, two whole cycles are executed, with the second cycle re-using the same number of intervals in each step as in the first cycle.

In this form, the problem lends itself to solution in the *mixed logical dynamical* (MLD) framework of Morari and co-workers (Bemporad and Morari, 1999; Morari *et al.*, 2000; Morari, 2002). Furthermore, the use of linear dynamic models allows solution by *mixed integer linear programming* (MILP). The selection of the optimal number of steps is facilitated by binary variables δ_i , eg. for equation (9) one requires the constraints

$$\begin{aligned} \mathbf{x}_j + \delta_{ij} \mathbf{e}_{\max} &\leq \mathbf{A}_j^{(i)} \mathbf{x}_{j-1} + \mathbf{b}_j^{(i)} + \mathbf{e}_{\max} \\ \mathbf{x}_j + \delta_{ij} \mathbf{e}_{\min} &\geq \mathbf{A}_j^{(i)} \mathbf{x}_{j-1} + \mathbf{b}_j^{(i)} + \mathbf{e}_{\min} \end{aligned} \quad (11)$$

$$\sum_{i=1}^{n_{\max}} \delta_{ij} = 1$$

Here the vectors \mathbf{e} contain the maximum and minimum deviation values when (all but one of) the i -models are not obeyed (large positive and negative numbers).

Whereas the task required was quite simple - *viz.* choose the best combination of interval numbers in the first five Skarstrom steps - it became clear that the linear program was an inefficient means of solving the problem. The numerous additional constraints required for model choice as in equation (11), and to deal with variable saturation, slowed down *LPsolve* (Michel Berkelaar), and caused failures. Even if con-

tinuous variables were included in the search, it would be quicker to evaluate *every apex* of the system for its objective value and compliance with constraints. Indeed, this was the procedure used to produce the results below.

3.3 Example

A physical description of the system is provided in figure 6. The bed is represented as $N=9$ compartments, and is considered to behave close to plug flow. Four constraints are set on the operation: $P_{\max}=4.5$ bara, $P_{\min}=1.0$ bara, maximum feed air during the adsorption step 2 $M_{\text{FEED}}=60000$ gmol; maximum product reflux during the purge step 4 $M_{\text{PURGE}}=10000$ gmol.

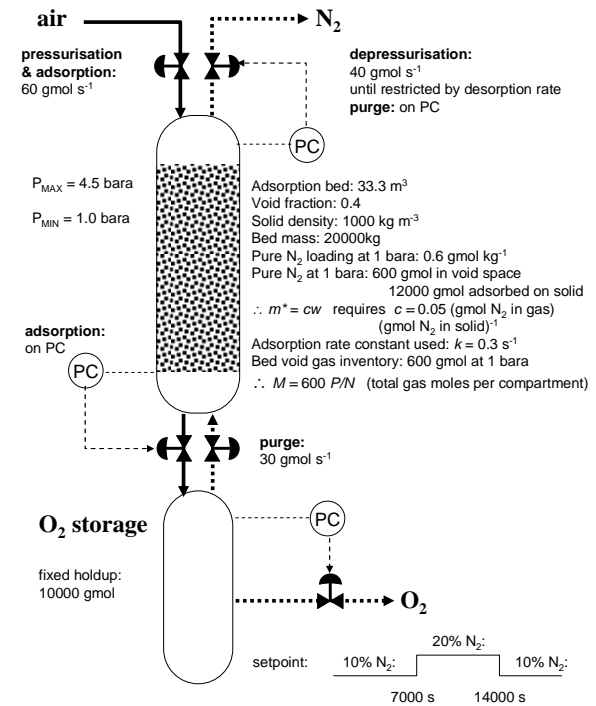


Fig. 6 Configuration for predictive control of product concentration in O₂ storage vessel

The storage vessel is modelled simply using the balances

$$\begin{aligned} \frac{dM_S}{dt} &= F_{d,N} - F_S \\ \frac{dm_S}{dt} &= f_{d,N} - f_S \\ \frac{f_S}{F_S} &= \frac{m_S}{M_S} \end{aligned} \quad (12)$$

where F_S and f_S are the total and adsorbed species outflows from the storage vessel. In this example, a constant molar inventory is maintained in the vessel (“overflow” mode), so that $F_S = F_{d,N}$.

The maximisation objective weightings for the 9 Skarstrom steps to the prediction horizon have been set as follows:

$$\begin{aligned}
 \text{objective} = & \\
 & -100 \times \sum_{k=j}^{j+8} \left| \begin{array}{l} \text{deviation from setpoint concentration} \\ \text{in storage vessel at end of step } k [\% \text{N}_2] \end{array} \right| \\
 & + 1 \times \sum_{k=j}^{j+8} \left\{ \begin{array}{l} (\text{product to storage in step } k [\text{gmol}]) - \\ (\text{purge from storage in step } k [\text{gmol}]) \end{array} \right\}
 \end{aligned} \tag{13}$$

The second term represents the net production of the oxygen-rich product up to the end of the present Skarstrom step, plus the following two full Skarstrom cycles. The optimisation considers all constraints up to the end of the first cycle, but the second cycle, using the same step-lengths as the first cycle, only contributes to the objective function. It is reasoned that such constraint transgressions as may be implied in the second cycle should be small.

At the start-up the contents of the storage vessel are at 20% N₂. The setpoint is initially at 10% N₂, stepping up to 20% N₂ at time= 7000 s, and back to 10% N₂ at time = 14000 s. Figure 7 shows how the Skarstrom cycles are manipulated in order to achieve the desired concentration in the storage vessel. In this example, the storage vessel has a constant molar inventory and the objective function encourages a high production rate. The objective function is easily altered for the case of “level control” in the storage vessel, where users are drawing the product at arbitrary rates. Viewing figure 7 one recalls that the bottom material in the adsorber only proceeds to the

storage vessel during the adsorption phase - ie where downflow occurs through the adsorber at a steady high pressure. Clearly the algorithm is manipulating the bottom concentration during this phase in order to progressively bring the storage vessel contents towards the setpoint.

4 CONCLUSION

In order to make use of fast and robust observation and optimisation algorithms, a lot of effort went into finding an adequate linear representation of the pressure swing adsorption process. This required careful choice of typical flow and composition profiles for each of the four steps of the Skarstrom cycle, to act as operating points about which the linearisation could be conducted.

The distinct steps of the Skarstrom cycle presented an unusual predictive control problem. At any point in time, the optimal control must be based on completion of the present step, followed by a continuation of the Skarstrom sequence up to a defined horizon. The four steps of one cycle have different positive, negative or zero cost implications for the objective function. Possible “end-effect” bias was reduced by continuing with *whole* Skarstrom cycles up to the horizon. Two whole cycles proved adequate, of which only the first was subjected to the constraints.

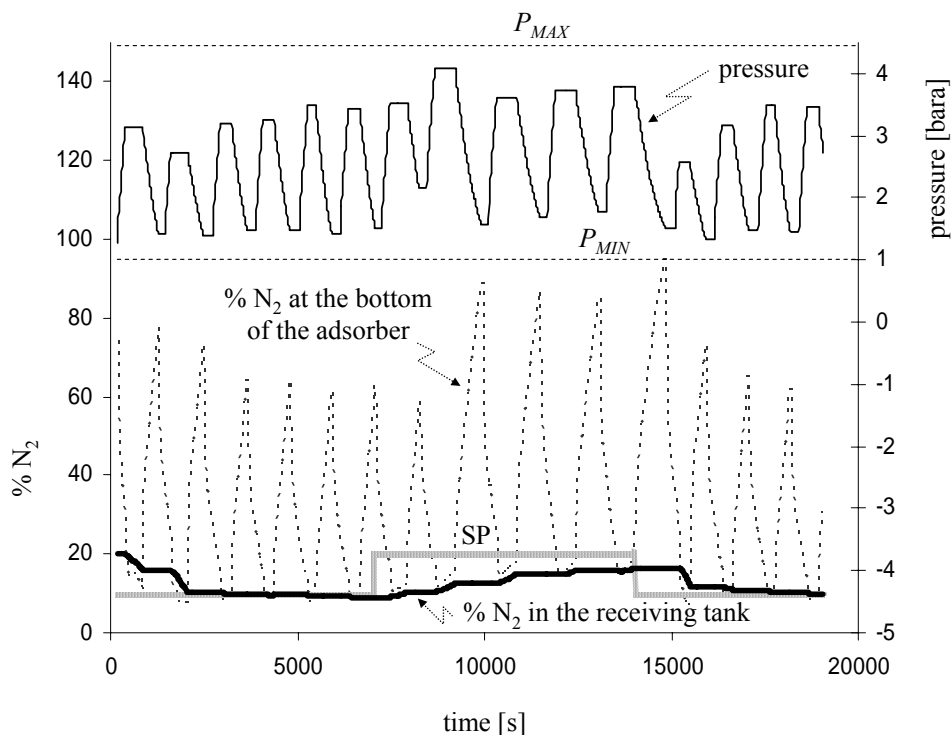


Fig. 7 Predictive control of the N₂ concentration in the storage vessel

The optimisation problem was perceived to be hybrid in nature, so the initial approach was to formulate it entirely in the *mixed logical dynamical* (MLD) framework as a *mixed integer dynamic optimisation* (MIDO) problem. To handle the choice of the dynamic equations, however, this required the introduction of many constraints which slowed the solution down and made it unreliable. Far better performance was achieved by solving the combinatorial problem (residual step length, plus next four step lengths) directly by exhaustive interrogation of all combinations for constraint compliance and objective value.

Example applications so far have focused on production maximisation and product composition control in an overflow-type receiving vessel. Good potential was found for predictive control of the composition by manipulation of the Skarstrom cycles. Indeed, this type of automatic control promises significant benefits, as the necessary control moves are not intuitively obvious for manual control. In future work the problem of combined composition and level control will be considered, so that users can draw product from the storage vessel at arbitrary rates.

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