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Numerical Simulation and Optimal Control of Air Separation Plants

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Abstract. Numerical simulation has already become an indispensable tool in the chemical engineering industry. In this paper, the extension of an already existing simulation package to the efficient and reliable solution of optimal control problems for optimal plant operation is discussed.

1 Introduction

Industrial gases such as Oxygen, Nitrogen and Argon are needed for many modern industrial processes, e. g., for the production and refinement of steel, for the production of mineral oil, or for the production of fertilizers. Usually, the required amount of gases has to be produced in the guaranteed purity on the spot by air separation plants. The Linde AG designs, constructs and operates air separation plants worldwide.

The optimization of design and operation of air separation plants is a must for increasing efficiency and productivity. Here, the importance of numerical simulation as a key technology in the design and operation of chemical engineering plants is increasing. The Linde AG has developed the state-of-the-art process simulation tool OPTISIM® [5] which is used both for the steady-state simulation and optimization, and for the dynamical simulation of plants [7,8]. The newly addressed optimization of operation of air separation plants results in optimal control problems. Numerical optimal control methods have originally been developed for trajectory optimization of aircrafts and space vehicles from the late sixties on [2,23].

In this paper, we discuss how the optimal control problems for chemical production plants can be solved efficiently.

2 Numerical Simulation of Air Separation Plants

The key tool for modeling a chemical production plant is the flowsheet [7,25], an abstract, graph-oriented scheme of a planned or existing chemical plant (Fig. 1). It contains in its nodes the relevant single process steps which are

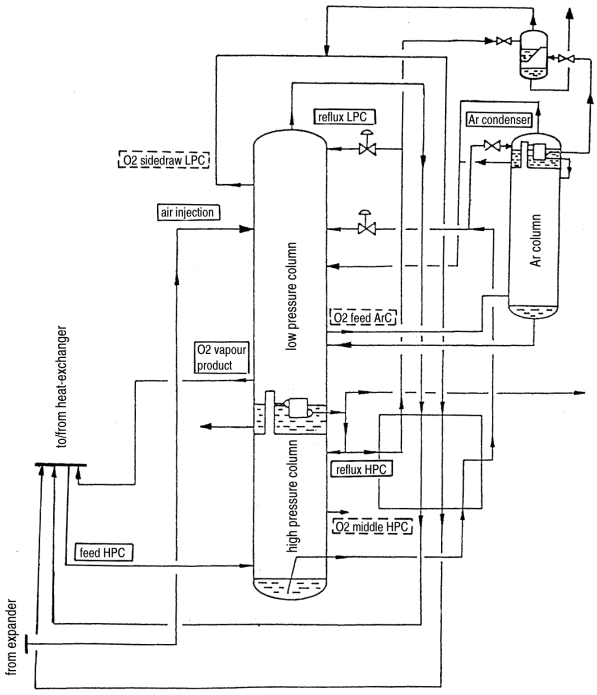

Fig. 1. Flow diagram for the Linde air separation process [30].

modeled independently. In a node, the incoming streams of material and data are transformed into new output streams. Practical experience in this field during the last decade has proven modern equation oriented simulation techniques used in the process simulation tools OPTISIM® [5], DIVA [16], gPROMS [1], and SpeedUp [22] superior to the classical, sequential modular approach [7,25]. Here, a large-scale system of equations describing all process units must be solved simultaneously, e. g., from 10 000 up to 100 000 equations for a petrochemical plant.

Dynamical modeling of a chemical engineering process results in a large-scale set of linearly implicit differential-algebraic equations (DAEs) of the form $(\dot{(.)} = \mathrm{d}(.)/\mathrm{d}t)$

$$\begin{pmatrix} A_1(y,z,p,u,\operatorname{sign} q) & A_2(y,z,p,u,\operatorname{sign} q) \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \dot{y} \\ \dot{z} \end{pmatrix} = \begin{pmatrix} f(y,z,p,u,\operatorname{sign} q) \\ g(y,z,p,u,\operatorname{sign} q) \end{pmatrix}. \tag{1}$$

Here, the state variable $x = (y,z)$ consists of the variable $y : \mathbb{R} \to \mathbb{R}^{n_y}$ and the variable $z : \mathbb{R} \to \mathbb{R}^{n_z}$, hence $n_x = n_y + n_z$. The functions $f : \mathbb{R}^{n_x+n_p+n_u+n_q} \to \mathbb{R}^{n_y}$, $g : \mathbb{R}^{n_x+n_p+n_u+n_q} \to \mathbb{R}^{n_z}$, $A_1 : \mathbb{R}^{n_x+n_p+n_u+n_q} \to \mathbb{R}^{n_y \times n_y}$, $A_2 : \mathbb{R}^{n_x+n_p+n_u+n_q} \to \mathbb{R}^{n_y \times n_z}$ are piecewise continuously differentiable. The matrix A_1 is regular. For numerical simulation, the design parame-

ters $p \in \mathbb{R}^{n_p}$ are given constants, the control variables $u : \mathbb{R} \to \mathbb{R}^{n_u}$ are given functions of time t, and the state variable must satisfy consistent initial conditions $x(t_0) = x_0 \in \mathbb{R}^{n_x}$. Discontinuities in the model equations are described as zeros of the switching functions $q = q(y, z, p, u) : \mathbb{R}^{n_x+n_p+n_u} \to \mathbb{R}^{n_q}$ [7].

The *index* of the DAE is important for the numerical solution [4]. Currently, there are no numerical integration methods for solving general systems of index greater than two directly and reliably. In chemical engineering, the resulting DAEs can be of arbitrary index in general. For the case of air separation plants, we will only consider index-2 systems.

Further problems in the numerical solution of the DAEs result from *discontinuities* in the model equations. These are due to tabular data, piecewise constant control variables, an operation dependent change of model equations or delays due to dead times of transport in pipelines. A *consistent initialization* is needed at the initial time of integration t_0 and after each discontinuity [7,17].

3 Optimization and Optimal Control

Typical objectives for plant optimization are maximization of profit, maximization of production, minimization of energy consumption, or minimization of feed consumption. In the dynamical case, the objective function

$$J[u, p] = \phi(x(t_f), p, t_f) + \int_{t_0}^{t_f} L(x(t), u(t), p)\,\mathrm{d}t, \quad \phi,\ L \in \mathbb{R}, \tag{2}$$

has to be minimized (or maximized) over the time of operation $[t_0, t_f]$ subject to the system of DAEs (1) with given consistent initial conditions $x(t_0) = x_0$, and subject to further linear and nonlinear inequality constraints

$$h(x(t), p, u(t)) \ \leq\ 0, \quad t_0 \leq t \leq t_f, \quad h \in \mathbb{R}^{n_h}. \tag{3}$$

Equations (1) – (3) define an optimal control problem. Its solution must satisfy the Maximum Principle [20]. As the adjoint (costate) differential equations cannot be computed without enormous efforts in our case, a direct transcription method [2,28] is investigated for computing an approximation of the optimal (open-loop) control $u^* : [t_0, t_f] \to \mathbb{R}^{n_u}$ and $p^* \in \mathbb{R}^{n_p}$ numerically.

By a parameterization of the control variable $\tilde{u}(\tilde{p})$, $\tilde{p} \in \mathbb{R}^{n_{\tilde{p}}}$, the optimal control problem becomes a nonlinear programming problem (NLP) for the parameters $\hat{p} = (\tilde{p}, p)$. Two different transcription strategies are possible:

(i) *the iterative simulation and optimization (direct shooting) (e.g., [13]):* In every iteration step of the optimization method, the dynamic equations (1) are solved by a numerical integration method (variable order, variable stepsize) such as backward difference formulas (BDF), Runge-Kutta or extrapolation methods for the current guess of parameters $\hat{p}$.

(ii) *the simultaneous simulation and optimization (direct collocation):* The dynamic equations (1) are only fulfilled at a priori selected points. Using collocation as an implicit integration scheme, the pointwise to be fulfilled DAEs lead to a system of nonlinear equality constraints for the resulting NLP for the parameters, e. g., [27].

While (i) satisfies the DAEs in each iteration step, (ii) only satisfies them at a successful termination of the optimization procedure if a sequential quadratic programming (SQP) method is used [9,10]. If the approach (ii) is applied, then the number of variables of the resulting NLP is of the order of $(n_x + n_u)$ times the number of collocation points. For the chemical production plant models of interest, this number can easily be larger than hundreds of thousand which is beyond the capabilities of current SQP methods [2]. Therefore, we will investigate approach (i) in more detail.

4 Direct Shooting Approach

Without loss of generality, the objective is assumed to be of Mayer form in the sequel, i. e., $L \equiv 0$ in Equation (2).

By a parameterization $\tilde{u}(\tilde{p})$, the optimal control problem is transcribed into a NLP for the parameters $\hat{p} = (\tilde{p}, p) \in \mathbb{R}^{n_{\hat{p}}}$. Due to the modeling approach in OPTISIM® [5], the DAE system (1) is of the form: $A_1 \equiv I$, $A_2 \equiv 0$. Thus the parameterized dynamic optimization problem is to

$$\begin{aligned}
\text{minimize} \quad & \tilde{\phi}(\hat{p}) := J[\tilde{u}, p] = \phi(y(t_f), z(t_f), p, t_f) && (4)\\
\text{subject to} \quad & \dot{y}(t) = f(y(t), z(t), p, \tilde{u}(\tilde{p}, t)),\ y(t_0) = y_0 \in \mathbb{R}^{n_y}, && (5)\\
& 0 = g(y(t), z(t), p, \tilde{u}(\tilde{p}, t)),\ z(t_0) = z_0 \in \mathbb{R}^{n_z}, && (6)\\
& 0 \geq h(y(t), z(t), p, \tilde{u}(\tilde{p}, t)),\ t_0 \leq t \leq t_f. && (7)
\end{aligned}$$

For the sake of simplicity of notation, the switching functions q are not explicitly written here but considered in the implemented algorithm. Using a time grid $t_0 < t_1^h < \ldots < t_{n_t}^h = t_f$, the infinite dimensional path inequality constraints (7) are transcribed into $n_t \cdot n_h$ inequality constraints (cf. [29])

$$0 \geq h\left(y(t_i^h), z(t_i^h), p, \tilde{u}(\tilde{p}, t_i^h)\right) \quad i = 1, \ldots, n_t. \tag{8}$$

The NLP for the parameters $\hat{p} = (\tilde{p}, p)$ given by Eqs. (4), (5), (6), and (8) is defined by piecewise continuously differentiable functions. Therefore, mathematical optimization methods exploiting gradient information will computationally perform much better than any direct search method [9].

An analysis of the gradients of $\tilde{\phi}$ and of the discretized constraints h yields

$$\begin{aligned}
\frac{\partial \tilde{\phi}}{\partial \hat{p}}(\hat{p}) &= \frac{\partial \phi}{\partial y}\frac{\partial y(t_f)}{\partial \hat{p}} + \frac{\partial \phi}{\partial z}\frac{\partial z(t_f)}{\partial \hat{p}} + \frac{\partial \phi}{\partial p} I_p + \frac{\partial \phi}{\partial u}\frac{\partial \tilde{u}(\tilde{p}, t_f)}{\partial \tilde{p}} I_{\tilde{p}},\\
\frac{\partial h}{\partial \hat{p}}\Big|_{t_i^h} &= \frac{\partial h}{\partial y}\frac{\partial y(t_i^h)}{\partial \hat{p}} + \frac{\partial h}{\partial z}\frac{\partial z(t_i^h)}{\partial \hat{p}} + \frac{\partial h}{\partial p} I_p + \frac{\partial h}{\partial u}\frac{\partial \tilde{u}(\tilde{p}, t_i^h)}{\partial \tilde{p}} I_{\tilde{p}}.
\end{aligned}$$

The last n_p diagonal elements of $I_p \in \mathbb{R}^{n_{\hat{p}} \times n_{\hat{p}}}$ are one, all other elements are zero. The matrix $I_{\tilde{p}}$ equals $I - I_p$. Here, I denotes the unit matrix in $\mathbb{R}^{n_{\hat{p}} \times n_{\hat{p}}}$.

For a current guess of $\hat{p}$ the initial value problem (IVP) (5), (6) can be solved numerically. Then y and z denote the *numerical* solution of the DAE-IVP. Several methods for approximating the Jacobians $\partial y(t_i^h)/\partial \hat{p}$ and $\partial z(t_i^h)/\partial \hat{p}$ have been developed: *finite difference methods* (e. g., [12]), solution of the *adjoint equations* (e. g., [11]), or solution of the *sensitivity equations* (e. g., [3,15,19]). Here, the latter results in the linear matrix DAE system

$$\dot{r} = f_y \cdot r + f_z \cdot s + f_p I_p + f_u \tilde{u}_{\tilde{p}} I_{\tilde{p}}, \quad (9)$$

$$0 = g_y \cdot r + g_z \cdot s + g_p I_p + g_u \tilde{u}_{\tilde{p}} I_{\tilde{p}}, \quad (10)$$

$$\text{where } r(t) = \frac{\partial y(t)}{\partial \hat{p}} \in \mathbb{R}^{n_y \times (n_p + n_{\tilde{p}})} \ , \ s(t) = \frac{\partial z(t)}{\partial \hat{p}} \in \mathbb{R}^{n_z \times (n_p + n_{\tilde{p}})} \quad (11)$$

denote the sensitivity matrices ($f_y := \partial f/\partial y,\ f_z := \partial f/\partial z,\ \ldots$).

Finite difference approximations of r and s are not only computationally expensive for large systems of index-2 DAEs but also troublesome because of the discontinuities. Adjoint equations are not available for the model equations here. Therefore, a *simultaneous* numerical integration of the model equations (5), (6) *and* of the sensitivity equations (9), (10) is investigated. An analogous approach has been used in [13,26] for the efficient computation of reliable gradients of optimization problems in systems of index-1 DAEs.

5 Sensitivity Equations

Given a fixed set of parameters $\hat{p}$, the model equations in OPTISIM® are integrated using a BDF method [5]. BDF are fully implicit linear multi-step methods suitable for solving index-1 DAEs numerically [4]. With small modifications they can also be applied to the direct integration of semi-explicit index-2 DAEs.

In the n^{th} integration step of a BDF method, the interpolating polynomial of the $k-1$ previously computed points $(y_{n-k+1}, z_{n-k+1}), \ldots, (y_n, z_n)$ and the next point (y_{n+1}, z_{n+1}) is formally constructed. The new point (y_{n+1}, z_{n+1}) is determined by the condition, that the interpolating polynomial has to fulfil the DAE at t_{n+1}. By extrapolation of the interpolating polynomial of $(y_{n-k}, z_{n-k}), \ldots, (y_n, z_n)$ for t_{n+1}, estimates $\tilde{y}_{n+1}$, $\tilde{z}_{n+1}$, $\tilde{\dot{y}}_{n+1}$ are obtained. A fixed leading coefficient BDF leads to the system of nonlinear equations

$$0 = f(y_{n+1}, z_{n+1}, p, \tilde{u}(\tilde{p}, t_{n+1})) - \tilde{\dot{y}}_{n+1} + \frac{\alpha_k}{\eta_{n+1}}(y_{n+1} - \tilde{y}_{n+1}), \quad (12)$$

$$0 = g(y_{n+1}, z_{n+1}, p, \tilde{u}(\tilde{p}, t_{n+1})). \quad (13)$$

The coefficient $\alpha_k \in \mathbb{R}$ depends on the order k of the method. The step-size is $\eta_{n+1} = t_{n+1} - t_n$. The nonlinear equations (12) and (13) are solved using

a modified Newton algorithm

$$
\begin{aligned}
y_{n+1}^{[0]} &:= \tilde{y}_{n+1} \ , \ z_{n+1}^{[0]} := \tilde{z}_{n+1} \ , \\
\begin{pmatrix} \frac{\alpha_k}{\eta_{n+1}} I + f_y & f_z \\ g_y & g_z \end{pmatrix} \begin{pmatrix} \Delta y^{[m]} \\ \Delta z^{[m]} \end{pmatrix} &= - \begin{pmatrix} f - \tilde{\dot{y}}_{n+1} + \frac{\alpha_k}{\eta_{n+1}} (y_{n+1}^{[m]} - \tilde{y}_{n+1}) \\ g \end{pmatrix} \qquad (14) \\
y_{n+1}^{[m+1]} &:= y_{n+1}^{[m]} + c \Delta y^{[m]} \ , \ z_{n+1}^{[m+1]} := z_{n+1}^{[m]} + c \Delta y^{[m]}, \ 0 < c \leq 1.
\end{aligned}
$$

In each step of the Newton iteration, the linear system (14) is solved by an iterative method using sparse matrix techniques for the large, sparse and unstructured system matrix [7]

$$
D = \begin{pmatrix} \frac{\alpha_k}{\eta_{n+1}} I + f_y & f_z \\ g_y & g_z \end{pmatrix}.
$$

Total differentiation of (12) and (13) with respect to the parameters $\hat{p} = (\tilde{p}, p)$ yields the linear system

$$
\begin{aligned}
0 &= f_y r_{n+1} + f_z s_{n+1} + f_p I_p + f_u \tilde{u}_{\tilde{p}} I_{\tilde{p}} - \tilde{\dot{r}} + \frac{\alpha_k}{\eta_{n+1}} (r_{n+1} - \tilde{r}_{n+1}) \\
0 &= g_y r_{n+1} + g_z s_{n+1} + g_p I_p + g_u \tilde{u}_{\tilde{p}} I_{\tilde{p}} \\
\text{or} \quad 0 &= D \begin{pmatrix} r_{n+1} \\ s_{n+1} \end{pmatrix} + \begin{pmatrix} -(\tilde{\dot{r}} + \frac{\alpha_k}{\eta_{n+1}} \tilde{r}_{n+1}) + f_p I_p + f_u \tilde{u}_{\tilde{p}} I_{\tilde{p}} \\ g_p I_p + g_u \tilde{u}_{\tilde{p}} I_{\tilde{p}} \end{pmatrix}. \qquad (15)
\end{aligned}
$$

If the sensitivity matrices are computed after each integration step for the state variable trajectories, the numerical solution of Equation (15) is computationally cheap, since the matrix D (resp., an approximation of it) is already available in decomposed form in the modified Newton iteration.

Direct application of the BDF scheme to the sensitivity equations (9) and (10) results in the same linear system (15). Thus the method described above is equivalent to the integration of the sensitivity equations with the same sequence of step-sizes and orders as used for the original DAE.

6 Consistent Initial Values

From the theory of DAEs it is known that, in general, arbitrary initial values $y(t_0)$, $z(t_0)$ will not lead to continuous solutions. Therefore, this problem has to be addressed each time a DAE-IVP is integrated numerically. Also, the (differential) index of the DAE has to be taken into account.

Under certain restrictions, *steady-state conditions* can be used [17], as implemented in OPTISIM®. For practical reasons, a slightly modified system

$$
0 = \hat{f}(y(t_0), z(t_0), p, \tilde{u}(\tilde{p}, t_0)) \qquad (16)
$$

$$
0 = \hat{g}(y(t_0), z(t_0), p, \tilde{u}(\tilde{p}, t_0)) \qquad (17)
$$

of nonlinear equations is solved, which originates from Eqs. (5) and (6). Then steady-state state variables have to be assumed in $[t_0 - \epsilon, t_0 + \epsilon]$, $\epsilon > 0$.

Differentiation of Eqs. (16) and (17) yields a linear system of equations for the sensitivities of the initial values

$$0 = \begin{pmatrix} \hat{f}_y & \hat{f}_z \\ \hat{g}_y & \hat{g}_z \end{pmatrix} \begin{pmatrix} r(t_0) \\ s(t_0) \end{pmatrix} + \begin{pmatrix} \hat{f}_p I_p + \hat{f}_u \tilde{u}_{\tilde{p}} I_{\tilde{p}} \\ \hat{g}_p I_p + \hat{g}_u \tilde{u}_{\tilde{p}} I_{\tilde{p}} \end{pmatrix}$$

where all functions are evaluated at $t = t_0$.

Consistent initialization must also be performed when discontinuities are detected during the integration. Discontinuities in the model equations, which are indicated by the sign change of one of the switching functions q, are treated by an efficient switching function algorithm in OPTISIM® [7].

7 Results

The algorithm has been implemented in OPTISIM® and checked for several index-1 and index-2 test problems [18]. Here, we investigate a load-change process of an existing air separation plant.

Air separation plants mainly consist of three parts: Feed air preparation, cooling and rectification. Rectification is done in several distillation columns. A standard configuration as considered here is a high pressure column, where the feed air is crudely separated into two fractions containing more (or less) oxygen, a low pressure column, where highly pure nitrogen and oxygen are produced, and an argon column, where crude argon is obtained (Fig. 1). All process steps are tightly coupled through material and energy streams.

The task is to decrease the load of the plant from 100 % air input to 60 %. The load change takes about one hour, the time of operation is from $t_0 = 0$ [s] to $t_f = 6000$ [s]. It is of outmost importance for stable operation and product quality that several purity restrictions are not violated during the load change. The air separation plant is modeled by a semi-explicit index-2 DAE system consisting of about $n_y = 900$ differential and $n_z = 2600$ algebraic equations. The purity restrictions result in lower and upper bounds $x_{i,\min} \leq x_i(t) \leq x_{i,\max}$ for six state variables, i. e., $n_h = 12$ in Equation (3). They are listed in Table 1. Five constraints refer to product quality. The sixth constraint is a stable operation constraint: Nitrogen must not enter the argon column in concentrations greater than about 0.0001 [mol/mol], otherwise the rectification process will break down. The measurement of the nitrogen content is very expensive in practice, therefore the oxygen fraction is controlled. Due to the construction of the plant the constraint on nitrogen is satisfied, if the oxygen content is larger than 90 %.

The $n_u = 5$ control variables describe opening or closing of valves of the air separation plant. Instead of a full parameterization of the control history, e. g., by piecewise polynomial functions, we investigate a parameterization and optimization of some currently used control schemes. Four of the controls

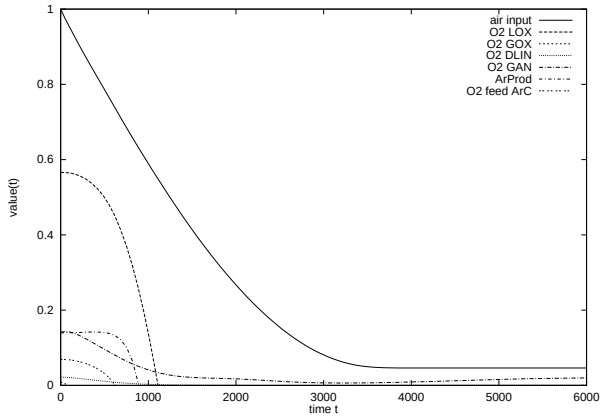

Fig. 2. Purities for starting values of parameter set before optimization.

name	min	max	description
O2 LOX	0.997	1.0	oxygen fraction in liquid oxygen product
O2 GOX	0.997	1.0	oxygen fraction in gaseous oxygen product
O2 DLIN	0.0	$5.0 \cdot 10^{-6}$	oxygen fraction in liquid nitrogen product
O2 GAN	0.0	$5.0 \cdot 10^{-6}$	oxygen fraction in gaseous nitrogen product
Ar Prod	0.965	1.0	argon fraction in argon product
O2 feed ArC	0.90	1.0	oxygen fraction in feed of argon column

Table 1. Lower and upper bounds of purity constraints.

are parameterized by two parameters each, one control is parameterized by one parameter, i. e., $n_{\tilde{p}} = 9$. The state variable inequality constraints are discretized with a time grid of $n_t = 10$ equidistant points yielding $n_t \cdot n_h = 120$ nonlinear inequality constraints of the NLP. The objective is to maximize an integral term describing product gain. However, the operators are in the first place interested in finding a feasible control for this highly complex plant.

For an initial set of parameters $\tilde{p}$, the time histories of the relevant purities are displayed in Fig. 2 before optimization. They lead to a breakdown of the air separation process, as several variables violate their (lower) bounds. These parameters are used as starting values for the optimization.

The NLP of the discretized optimal control problem is solved using a commercially available SQP method. The tolerance for integration of the index-2 DAE system and the corresponding sensitivity equations is 10^{-3}. Optimization tolerance and feasibility tolerance are 10^{-2}. The state histories of the purities of Table 1 for the optimized parameterized controls are displayed in Fig. 3. They are now feasible within their lower and upper bounds which is most important. (Please note that the graphs in Figs. 2 and 3 are in normalized scale between the lower and upper bounds given in Table 1.)

Hence, the developed and implemented optimization method enables the computation of parameterized controls for realistic, large-scale dynamical air separation plant models. The optimized, parameterized controls satisfy

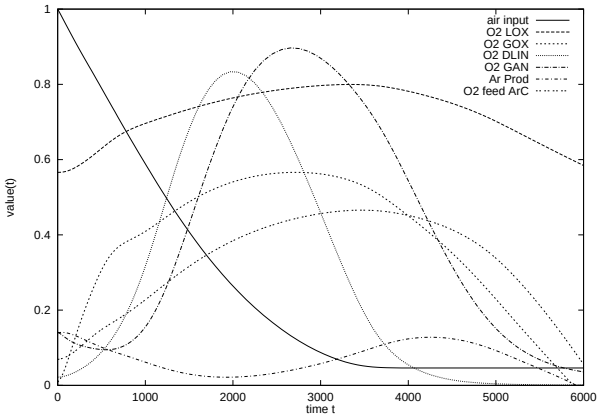

Fig. 3. Purities for the computed optimal parameterized control.

very important, highly nonlinear constraints for stable operation and product quality, and improve the choosen performance index.

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