

PASSIVITY BASED CONTROL AND OPTIMIZATION OF A SILICON PROCESS

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Abstract:

In this paper we develop a Real Time Optimization (RTO) strategy for a silicon reactor. The reactor dynamics are described using parabolic partial differential equations with countercurrent liquid, gas and solid flow with chemical reaction. The model equations are converted to a system of differential algebraic equations using the method of lines and up-winding approximation for the spatial derivatives. The model parameters are matched to industrial data by minimizing a quadratic objective function using a novel interior point SQP method. The dynamic response has been verified and we have shown that passivity based inventory control can be used to stabilize the process at its optimal operating point. *Copyright*©2005 *IFAC*

1. INTRODUCTION

In this paper, we develop a Real Time Optimization (RTO) scheme for making high grade metallurgical silicon. The primary product serves as a pre-cursor for making silicones, aluminum alloys, photo-voltaics and micro-electronics. Amorphous silica byproduct is sold at lower price to the cement industry as a filler. The reactor is modeled by introducing two major reaction zones. The upper zone is treated as a counter current reactor while the lower zone is treated as a stirred tank (Halvorsen *et al.*, 1991; Halvorsen, 1992; Schei *et al.*, 1998) and (Foss and Wasbø, 2001). The original PDE model represents a hyperbolic PDE system and proved to be very difficult to solve

numerically. We therefore converted the system to parabolic form by including dispersion. This gives “viscosity” (Evans, 2000) and it also allowed us to better match experimental data. The model does not address heat transfer and fluid flow associated with the plasma arc itself. Progress in this direction was made by (Andresen, 1995). Nor do we include models of the electrical control system. A comprehensive treatment of this problem can be found in (Valderhaug, 1992).

The Real Time Optimization (RTO) scheme is based on the idea of using a numerical method to optimize the setpoints using a steady state model which is matched to the process data. Once the optimal setpoints have been found we stabilize the setpoints using a dynamic controller. In this work we achieve the first objective by using a novel interior point Sequential Quadratic Programming (SQP) algorithm with trust region (Arora, 2003). Christofides (Christofides, 2000) reviews different approaches for control of nonlinear PDE systems. We chose to use inventory control which has the

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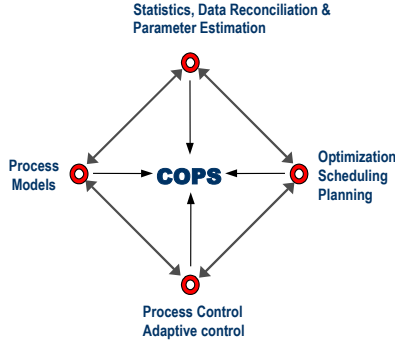


Fig. 1. Real Time Optimization strategy .

advantage that it gives a very simple feedback structure and that stability can be proven using a straightforward Lyapunov argument (Farschman *et al.*, 1998) .

2. RTO - A BIRD'S EYE VIEW

The purpose of the 5 year **COPS Control and Optimization of Silicon** study was to investigate if it was feasible and practical to apply on-line optimization and control to an industrial silicon production process. The concept we used, briefly outlined in Figure 1, consists of four basic elements:

- (1) The process models (dynamic and static material balances).
- (2) A method to reconcile the model to process data and estimate process parameters and states.
- (3) Tools for process optimization to find best operating conditions (setpoints).
- (4) Process control methods to stabilize the process at the optimal operating points.

Points 2-3 are executed at regular intervals. In a brief trial we updated model parameters once every seven days whereas the sampling time for feedback control was 2 hours. The trial period showed that optimization based control methods hold the potential of improving the silicon yield.

3. PROCESS CHEMISTRY

A silicon reactor can use up to 30 MW of AC power delivered through consumable graphite electrodes. Experimental studies indicate that approximately 60% of the energy is distributed throughout the furnace by resistance heating while the remaining 40% is transferred via a plasma arc in the lower part of the furnace. In this study we represent the silicon reactor as a moving bed with countercurrent gas/liquid and solid flow approximating the upper reactor and

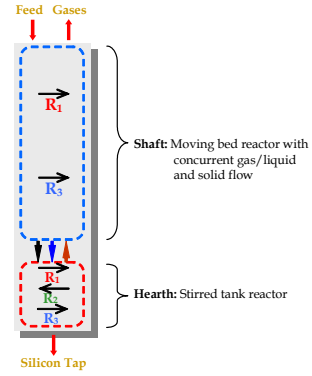
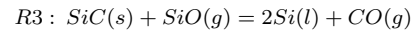
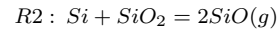
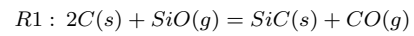


Fig. 2. Modeling approach.

a stirred tank approximating the lower reaction zone (Figure 2).

Chemistry: We used three independent reactions to approximate the reaction chemistry



The temperature is lowest at the top of the reactor where the endothermic reaction ($R1$) predominates by converting C to SiC. The temperature is highest close to the electric arc towards the bottom of the reactor. Here SiO gas is produced via reaction $R2$ and silicon is produced via reaction $R3$. Experimental data shows that no unreacted C appears in the product.

Kinetics: Kinetic expressions are derived on the basis that the reaction rate is proportional to the deviation from the equilibrium partial pressure. The total furnace pressure is assumed constant at 1 atm so that $p_{SiO} + p_{CO} = 1$. Therefore, the deviation from equilibrium pressure for this system is expressed according to:

$$\frac{p_{CO} + \Delta p_j}{p_{SiO} - \Delta p_j} = K_j, \quad j = 1, 2 \quad (1)$$

The equilibrium constant K_j for reaction j is calculated from the JANAF tables (Stull and Prophet, 1985). Per definition we have

$$p_{SiO} = \frac{G_{SiO}}{G_{SiO} + G_{CO}} \quad (2)$$

where G_i represents the gas flux. According to these equations, the deviation from equilibrium pressure (Δp_i) is determined uniquely for a specific temperature and gas pressure. The complete rate expression for reaction $R1$ has the form (Levenspiel, 1999)

$$R_i = \begin{cases} 0 & \Delta p_i \leq 0 \\ a_i c_s \Delta p_i e^{-E_i/RT} & \Delta p_i > 0 \end{cases} \quad (3)$$

where a_i is the rate constant, c_s is the local concentration of solid/liquid, Δp_i is the deviation from equilibrium pressure, E_i is the activation energy, R is the molar gas constant and T is the absolute temperature.

The Shaft Mass Balance Equations: The rate of change of solid concentration depends on convective flow, reaction and dispersion due to non-ideal flow in the vertical direction. Radial effects are not considered so the concentration expresses a mean concentration over the furnace's cross-section.

The solid-phase conservation equation for C , SiC and SiO_2 can now be written so that:

$$(1 - \nu) \frac{\partial c_C}{\partial t} + \nu_s \frac{\partial c_C}{\partial z} - D_{disp} \frac{\partial^2 c_C}{\partial z^2} = -2R_1$$

$$(1 - \nu) \frac{\partial c_{SiC}}{\partial t} + \nu_s \frac{\partial c_{SiC}}{\partial z} - D_{disp} \frac{\partial^2 c_{SiC}}{\partial z^2} = R_1 - R_3$$

$$(1 - \nu) \frac{\partial c_{SiO_2}}{\partial t} + \nu_s \frac{\partial c_{SiO_2}}{\partial z} - D_{disp} \frac{\partial^2 c_{SiO_2}}{\partial z^2} = R_1 - R_3$$

where t is the time, z is the vertical shaft location, ν is the bed porosity, c_i is the local solid concentration, v_s is the solid velocity and D_{disp} is the solid phase dispersion coefficient. The dispersion coefficient for solids represents mixing, non-uniform packing and size distribution and non-uniform flow (Froment and Bischoff, 1990; Levenspiel, 1999). Dispersion converts the hyperbolic equations to parabolic form. Due to their shock dissipation properties, parabolic PDEs are much easier to handle numerically than hyperbolic-type equations used in the previous silicon model studies (Silebi and Schiesser., 1992; Evans, 2000).

The conservation equation for Si liquid is:

$$\nu \frac{\partial l_{Si}}{\partial t} + \frac{\partial \nu_s l_{Si}}{\partial z} - D_{l,disp} \frac{\partial^2 l_{Si}}{\partial z^2} = 2R_3$$

where l_i is the local liquid concentration, v_l is the local liquid velocity and $D_{l,disp}$ is the liquid phase dispersion coefficient. The conservation equations for SiO and CO gases are:

$$\nu \frac{\partial g_{SiO}}{\partial t} + \frac{\partial \nu_g g_{SiO}}{\partial z} - D_{g,disp} \frac{\partial^2 l_{SiO}}{\partial z^2} = -R_1 - R_3$$

$$\nu \frac{\partial g_{CO}}{\partial t} + \frac{\partial \nu_g g_{CO}}{\partial z} - D_{g,disp} \frac{\partial^2 l_{CO}}{\partial z^2} = R_1 + R_3$$

where g_i is the local gas concentration, v_g is the local gas velocity and $D_{g,disp}$ is the gas phase dispersion. The 6 coupled PDEs describe above give the dynamics of the reactor shaft.

The Hearth Mass Balance Equations: The dynamic mass balance equations for solid and liquid phase species in the hearth are approximated as a stirred tank reactor:

$$\frac{dM_C}{dt} = -(\nu_s c_C)_0 - 2R_1$$

$$\frac{dM_{SiC}}{dt} = -(\nu_s c_{SiC})_0 + R_1 - R_3$$

$$\frac{dM_{Si}}{dt} = -(\nu_l c_{Si})_0 - \kappa_{tap} M_{Si} - R_2 + 2R_3$$

$$\frac{dM_{SiO_2}}{dt} = -(\nu_s c_{SiO_2})_0 - R_2$$

where M_i is a solid/liquid concentration, $(\cdot)_0$ represents a shaft-hearth interface flux, and κ_{tap} is a proportionality constant expressing the amount of Si liquid removed during continuous tapping (product withdrawal). Similarly, dynamic mass balance equations are written for the gas phase species yielding:

$$\frac{dG_{SiO}}{dt} = -(G_{SiO})_0 - R_1 + R_2 - R_3$$

$$\frac{dG_{CO}}{dt} = -(G_{CO})_0 - R_1 + 2R_3$$

where G_i refers to the gas flux.

Boundary Conditions: Boundary conditions for flow reactors have been discussed extensively in the literature (Danckwerts, 1953; Wehner and Wilhelm., 1956; Pearson, 1959; Bischoff, 1961). The appropriate boundary conditions for our system are given by

$$c_C(L, t) = c_{C,0}, \quad \frac{\partial c_C(0, t)}{\partial z} = 0$$

$$c_{SiC}(L, t) = c_{C,0}, \quad \frac{\partial c_{SiC}(0, t)}{\partial z} = 0$$

$$c_{SiO_2}(L, t) = c_{SiO_2,0}, \quad \frac{\partial c_{SiC}(0, t)}{\partial z} = 0$$

$$Q_{Si}(L, t) = 0, \quad G_{SiO}(0, t) = (G_{SiO})_0$$

$$G_{CO}(0, t) = (G_{CO})_0$$

which corresponds to Hulburt's conditions. We note that Danckwerts' approach is correct, but we use instead the Hulburt conditions since these adequately approximate a system with small dispersion coefficient and are easy to implement. Boundary conditions for the solid phase concentration reflect the inlet charge concentration of carbon and quartz. The boundary conditions for the liquid-phase flux equations consist in specifying a zero flow conditions at the shaft top.

Solution Strategy: We used the method of lines (MOL) (Silebi and Schiesser., 1992) to convert the PDE's and the boundary conditions to a semi-explicit set of Differential and Algebraic Equations (DAEs). To improve numerical stability, we used a fourth order biased upwind difference and we used a second generation DAE solver called DASPK (Brown *et al.*, 1994). In this method the linear system is solved by dense direct or banded direct, Gaussian elimination with partial pivoting via LINPACK. The iterative method solves the linear system using a preconditioned Generalized Minimal Residual (GMRES) iterative method, a Krylov subspace projection method that solves the system inexactly until convergence.

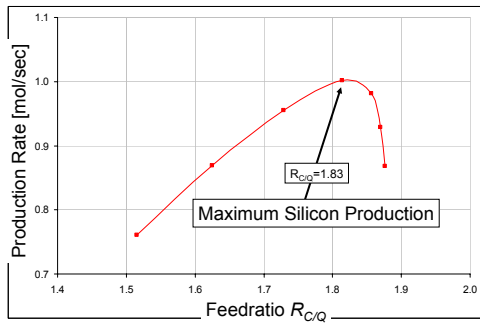


Fig. 3. Production rate vs carbon and quartz ratio.

4. MODEL PARAMETER ESTIMATION

The unknown model parameters were matched to steady state operating conditions obtained by filtering and averaging monthly or weekly data using 2 hour sampling interval. The quadratic objective function:

$$\min_{\theta \in \Theta} \sum_{k=1}^N \|y(k) - h(x(k), z(k), \theta)\|^2$$

subject to

$$0 = f(x, z, \theta)$$

was minimized. y refers to plant measurements, z is a vector of unmeasured model states, θ is a vector of model parameters, Θ the feasible set, and h, f are functions relating states to measurements and steady state relations (the right hand side of the DAE system described above) and boundary conditions. A comprehensive treatment of parameter estimation can be found in (Beck and Arnold, 1977; Bard, 1974). We used an interior point, trust-region SQP method to fit these parameters for multiple time periods in order to see how the algorithm could track time-varying parameters (Arora, 2003). The dispersion coefficient and solids velocity were estimated in a separate experiment (Ruszkowski, 2003). A set of nominal parameters is seen in the table below.

Description	Parameter/Unit	Nominal Value
Furnace height	L [m]	2.0
Solid velocity	ν_s [m/s]	-5.0x10E-5
Dispersion	D_{disp} [m ² /s]	8.0x10E-6
Description	Parameter/Unit	Nominal Value
Shaft R1 rate	a_{1s} [s ⁻¹ atm ⁻¹]	2.0x10-E4
Shaft R3 rate	a_{3s} [s ⁻¹ atm ⁻¹]	5.0x10-E4
Hearth R1 rate	a_{1h} [s ⁻¹ atm ⁻¹]	5.0x10-E2
Hearth R2 rate	a_{2h} [s ⁻¹ atm ⁻¹]	4.1x10-E3
Hearth R3 rate	a_{3h} [s ⁻¹ atm ⁻¹]	5.0x10-E2
Effective area	A_{eff} [m ²]	55.0
Top temp.	T_s [K]	1624.0
Hearth temp.	T_h [K]	2244.0

5. PROCESS DYNAMICS

Figure 3 shows how carbon availability influences the production rate and motivates the use of RTO

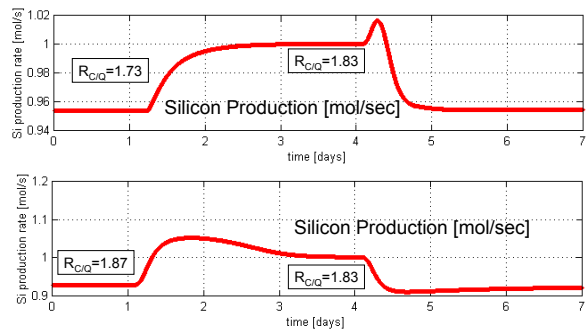


Fig. 4. Low carbon to optimal and back (top). High carbon to optimal and back (bottom).

for this process. As we increase the carbon to Quartz ratio $R_{C/Q}$ in the feed from about 1.6 to about 1.8 the production rate of silicon increases and reaches a maximum. Increasing $R_{C/Q}$ further leads to a rapid decrease in the production rate and the model shows that silicon carbide (SiC) starts to build up in the reactor. SiC comes in different crystalic forms. The β -carbide reacts quite readily whereas the α -carbide is not reactive at all and builds up over time if there is too much carbon present. It is therefore very important to control the reactor to avoid production of β -carbide since this may lead to shut-down.

To illustrate the dynamic behavior of the reactor we performed a series of simulations for various feed ratios ($R_{C/Q}$) at nominal parameter values and under the constraint that the reactor volume was kept constant. Figure 4 shows that if $R_{C/Q}$ is high then the dynamics correspond to a locally linear system with a right half plane zero which gives an “inverse response” close to the optimal point (Bogle and Kuhlmann, 1961). The reason for observing an inverse response in the silicon furnace is rapid release of silicon from the build-up of SiC and gradual ramp-up of SiO gas production. However, after a while the SiO production dynamics overwhelm the Si metal production and the process settles to a lower Si production rate and a higher SiO effluent gas flux. Similar has been reported using a compartmental model of the silicon reactor (Floor-Lund *et al.*, January; Floor-Lund *et al.*, n.d.).

The major theoretical conclusion is that it is very difficult (impossible) to control the system well using feedback from the silicon production since the process is not controllable with smooth feedback at the desired point of operation.

6. RTO AND INVENTORY CONTROL

Inventory control allows the transformation of complex control problems into simpler ones using passivity theory by focusing on inventories

rather than point measurements (Farschman *et al.*, 1998). It is easy to show that for transport-reaction systems

$$\frac{\partial z_i}{\partial t} + \nu \frac{\partial z_i}{\partial z} - \sum_{j=1}^n D_{ij} \frac{\partial^2 z_i}{\partial z^2} = \sigma_i, \quad i = 1, \dots, n$$

the passive pair used for inventory control are :

$$u(z, m, d) = (\bar{f}(0) - \bar{f}(L)) + \int_0^L \bar{\sigma} dx \quad (4)$$

$$y = (v - v^*) \quad (5)$$

where $f(\cdot)$ are the boundary fluxes σ_i is the production term. v is the vector of inventories with * denoting a set point and overbar denotes a deviation. The inventories are defined so that

$$v_i = \int_0^L z_i dx$$

The silicon process, can be represented by a system of conservation laws of the type described here when we define vectors

$$z = (c_C, c_{SiO_2}, c_{SiC}, l_{Si}, p_{SiO}, p_{CO})^T$$

$$\sigma = (\sigma_C, \sigma_{SiO_2}, \sigma_{SiC}, \sigma_{Si}, \sigma_{SiO}, \sigma_{CO})^T$$

The production terms, σ_i , are defined by equations (3). Passivity of the mapping $u \mapsto y$ is easily verified using the storage function $V = (v - v^*)^T (v - v^*)$.

We now get to the question of choosing input-output pairs. In our application it is natural to focus on inventories in the solid phase since the hold-up of gas and liquid are minimal. We also have only have two control variables (carbon and quartz feedrate). This gives two control objectives that need to be satisfied simultaneously:

- (1) Control overall process holdup with quartz feed input
- (2) Control total elemental carbon holdup with carbon feed input

For this type of material balance control holdup of carbon (M_{Ctotal}) and the total holdup of quartz (M_{total}) are defined as:

$$M_{Ctotal} = \sum_{i=C, SiC} A_{eff} \int_0^L c_i dz + V_h m_i$$

$$M_{total} = \sum_{i=C, SiC, SiO_2} A_{eff} \int_0^L c_i dz + V_h m_i$$

where A_{eff} refers to furnace cross-sectional area of the shaft, V_h the volume of the hearth and

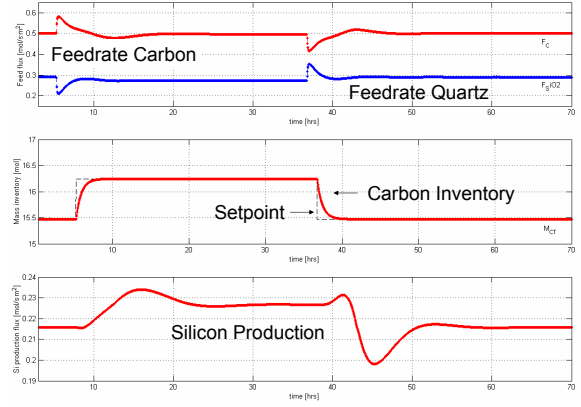


Fig. 5. Undercooked to optimal and back.

c_i and m_i are the concentrations of specie i in the shaft and the hearth respectively. The passivity based 2x2 multivariable feedback feed-forward control system corresponding to equations (4,5) is given by

$$f_C = G_{CO} - K_{c1}(M_{Ctotal} - M_{Ctotal}^*)$$

$$f_Q + f_C = G_{CO} + G_{SiO} + P_{Si} - K_{c2}(M_{total} - M_{total}^*)$$

f_C and f_Q refer to carbon and quartz feed fluxes, respectively, G_{CO} and G_{SiO} to the effluent gas fluxes and P_{Si} to the silicon metal production flux. K_{c1} and K_{c2} are controller gains. The production terms σ are not needed since we use elemental and total balances. Stability of the closed loop control scheme is proven using the storage function (Farschman *et al.*, 1998)

$$H = (M_{Ctotal} - M_{Ctotal}^*)^2 + (M_{total} - M_{total}^*)^2$$

Stability of the zero-dynamics can be proven using the Lypunov function (Alonso and Ydstie, 2001)

$$A = (z - z^*)^T w^*$$

where $w = \partial S(z)/\partial z$ and $S(z)$ is the entropy and * refers to the stationary point consistent with the steady state equations with fixed boundary conditions. The control algorithm can be enhanced by including integral and derivative action.

7. DYNAMIC CONTROL RESULTS

In this section, we briefly present simulated results from using the RTO scheme to stabilize the process. We first matched the model to process data then we optimized the setpoint for the passivity based inventory controller. A typical simulation result is shown in Figure 5. The furnace operated under inventory control in which we restore optimal operation from (i) the undercooked region and (ii) the overcooked state. The inventory converges to its set point without an overshoot or oscillations, and the silicon metal production rate achieves a maximum at the new set point.

8. CONCLUSIONS

In this paper we reviewed how Real Time Optimization and inventory control can be used to control a silicon production process to its optimal steady state operating point. An industrial simulation example was developed using a two-zone model for the silicon furnace. The furnace exhibits three states of operation: the low carbon, the optimal and the high carbon regimes. The process dynamics differ in each of these regimes and it is not controllable at the optimal operating point using only process flow observations/measurements. We developed an inventory control strategy based on total elemental carbon holdup and the total mass holdup. Simulations show that under inventory control, the process can be controlled in a stable manner to the optimal set-point.

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