Minimum Startup Time Control of an Ion Exchange Process used for Water Desalination

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Abstract – **Problem for minimum time control of an ion exchange process for desalination of water is formulated and solved on the basis of an augmented functional of Lagrange. Decomposition method is used to solve the problem in two level calculation structure. Decomposition subproblems solved on the first and second level of the calculating structure are determined.**

Matlab program is developed to implement the method. The program is incorporated in a control system for adaptive control of the process developed in the framework of LabVIEW software.

I. INTRODUCTION

Ion exchange is a chemical process that involves replacement of ions of the same charge from liquid phase to solid phase [2], [4]. In this application, ion exchange resins (little charged beads) are coated with replacement ions H^+ and OH^- for two main phases, cation and anion, of the ion exchange process respectively. The desalination mechanism is to convert the salt into acid using a strong acid cation exchange (cation load column) and subsequently remove the weak acid by absorption using weak anion exchange (anion load column). After a certain period of use resins become exhausted when most of the replacement ions in the resins have been utilized.

In order to replenish the resins a strong solution is used to regenerate the resins into their original form. The basic ion exchange configuration as built in the Department of Chemical Engineering of Cape Peninsula University of Technology consists of four columns, the cation load and regeneration columns and the anion load and regeneration columns.

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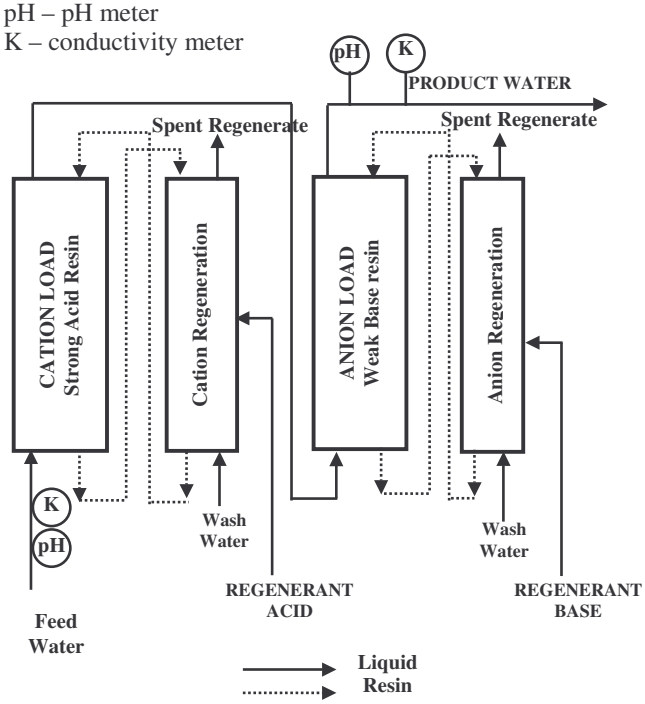

Fig. 1. Basic Ion Exchange Configuration.

Associated with each column is the system of pumps, valves and pipes (Fig.1), which enables the liquid and resins flows to be switched as required at various operation stages. pH (pH) and conductivity (K) sensors are used to determine acidic strength and ion concentration of the solutions at different strategic points. These measurements are in turn used in determining the salt concentration in water being purified and also to determine control actions on the plant (opening and closing of valves).

No methods for optimal control of the ion exchange process are known in the literature. The published papers concern only the process mass balance equations description and simulations [7]. These models are not convenient for the real time control purposes.

The problem for optimal control of an ion exchange process may be formulated as follows: To maintain the operating conditions such that the required quality of

water is produced at constant throughput for the minimum consumption of regenerant chemicals.

It has been established experimentally that the cation exchange column needs about thirty cycles to reach steady state conditions [2], [4], [7]. The starting time is very long. Therefore it is necessary to determine control in order to lead the process for minimum time to the desired steady state operation.

According to this problem the main purpose of the paper is to develop a method for minimum time control calculation and to apply this method for simulation and real time implementation with the pilot plant [6] where pH and conductivity sensors are the measuring devices.

Technically this aim can be formulated using the concentration of salt in the product water and the flow rate of the resin into the column. Flow rate of the resin is very important for the resin balance in the process.

The paper aims to propose a simple model and minimum time control of a counter current continuous ion exchange process, based on the pilot plant built at Cape Peninsula University of Technology.

II. MODEL FORMULATION

The considered ion exchange process is a multistage counter current continuous cyclic process with resin flows coming from the top and the water flows coming from the bottom of the columns according to the cycle times. The time of the up flow periods of the cycles is selected as a control variable. The concentration of the salt in the water in every column stage is selected as a state variable. The mathematical model for the process as developed on the basis of component mass balance equation is:

$$\frac{d(H_n y_n)}{dt} + \frac{d(h_n x_n)}{dt} = (F_{L,n-1} y_{n-1} + F_{R},_{n+1}\, x_{n+1}) - (F_{L,} y_n + F_R, y_n x_n) \quad (1)$$

where F_L is the molar flow rate of the liquid, F_R is the molar flow rate of the resin, y_f is the initial (input) mole fraction of material in liquid phase, y_n is the mole fraction of material in liquid phase, x_n is the mole fraction of material in resin phase, H_n is the liquid hold up, h_n is the resin hold up, N is the number of stages numbered from the bottom to the top. By applying assumptions for equal holdups at every stage, equal resin and liquid flow rates for every stage, linear rate of exchange of ions, it is accepted that

$$x_n = a_n y_n + b_n \quad (2)$$

where a_n and b_n are linearity coefficients of the rate of the ion exchange between the liquid and resin. Using steady state mass balance for the resin flow in every stage the resin flow rate can be represented by the cycle time $TF_R = hd$ (3)

where, h is the resin holdups of the stage, d is the fractional transfer of resin from one stage to another and T is the cycle time. The magnitude of the cycle time is used as a control action in the operation of the plant. As h and d can be accepted constant for every stage then F_R can be expressed by T from (3). That is why, to simplify the calculations and control derivation the flow rate F_R is considered as a control signal.

After selecting the state vector $y(t)=[y_1, y_{2.}...y_N]^T$ the state space model is expressed as

$$\dot{y}(t) = Ay(t) + By(t)F_R + B_1 F_R(t) + Wy_f(t),$$

$$z(t) = Cy(t),\ y(0) = y_0 \quad (4)$$

The model (4) is a bilinear one and therefore characterized by simplicity and better capability to describe the real process. The discrete version of (4) used for modelling and control purposes is given by

$$y(k+1) = [I + \Delta tA]y(k) + \Delta tB\ y(k)\ F_R(k) + \\ + \Delta tB_1\ F_R(k) + \Delta t\, Wy_f(k)$$

$$z(k) = Cy(k),\quad y(0) = y0 \quad (5)$$

$$A = \begin{bmatrix} \frac{F_L}{H+a_1h} & 0 & 0 & ... & 0 \\ \frac{F_L}{H+a_2h} & \frac{F_L}{H+a_2h} & 0 & ... & 0 \\ ... & ... & ... & ... & ... \\ 0 & ... & \frac{F_L}{H+a_{N\ 1}h} & \frac{F_L}{H+a_{N\ 1}h} & 0 \\ 0 & 0 & ... & \frac{F_L}{H+a_Nh} & \frac{F_L}{H+a_Nh} \end{bmatrix}$$

$$B = \begin{bmatrix} \frac{a_1}{H+a_1h} & \frac{a_2}{H+a_1h} & 0 & 0 & ... & 0 \\ 0 & \frac{a_2}{H+a_2h} & \frac{a_3}{H+a_2h} & 0 & ... & 0 \\ ... & ... & ... & ... & ... & ... \\ 0 & 0 & ... & \frac{a_{N\ 1}}{H+a_{N\ 1}h} & \frac{a_{N\ 1}}{H+a_{N\ 1}h} & 0 \\ 0 & 0 & 0 & ... & 0 & \frac{a_N}{H+a_Nh} \end{bmatrix}$$

$$C = [0\ \ 0\ \ ...\ \ 1],\quad W = \left[\frac{F_L}{H+a_1h}\ \ 0\ \ ...\ \ 0\right]^T$$

$$B_1 = \left[\frac{b_2 - b_1}{H+a_1h}\ \ \frac{b_3 - b_2}{H+a_2h}\ \ ...\ \ \frac{b_N - b_{N\ 1}}{H+a_Nh}\right]^T$$

where $A \in R^{NxN}$, $B \in R^{NxN}$, $B_1 \in R^{Nx1}$, $W \in R^{Nx1}$, $C \in R^{1xN}$, $z \in R^{1x1}$ is the model output, $F_R \in R^{1x1}$ is the control input, $y \in R^{Nx1}$ is the state space vector and $y_f \in R^{Nx1}$ is the input disturbance vector.

The model is used in formulation and solution of the minimum time problem. The values of the model parameters are determined on the basis of the column design parameters and experiments [1].

III. MINIMUM TIME PROBLEM FORMULATION AND SOLUTION

The problem for start-up optimal control is formulated in the following way: find the control,

$$u(k) = F_R(k), \quad k = \overline{0, K-1}, \tag{6}$$

which in minimum time $J = K\Delta t$, (7)

leads the system (5), from the initial state to the desired steady state $y(K) = \bar{y}$, (8)

and satisfies constraints $v_{\min}(k) \le v(k) \le v_{\max}(k)$

$$y_{\min}(k) \le y(k) \le y_{\max}(k)$$

$$F_{R\min}(k) \le F_R(k) \le F_{R\max}(k) \tag{9}$$

$$\Delta t_{\min} \le \Delta t \le \Delta t_{\max}$$

where Δt is the sampling period, $K\Delta t$ is the time for reaching the steady state, $v_{\min}(k), v_{\max}(k)$, $v = y, F_R, \Delta t$ are minimum and maximum values respectively for the state, control vectors and for the sampling period, $\bar{y}$ is the desired steady state, K is the number of steps in the optimization interval. The time $K\Delta t$ that is to be minimized is a product of two variables. One of them can be fixed and the other can be minimized. As the sampling period is easier to be included in the model equations and to be minimized, the number of sampling steps will then be fixed constant.

Then the problem for minimization of the startup time is transformed into a problem for minimizing of the sampling period time. The stated problem (6) – (9) is characterized by nonquadratic criterion and bilinear model with the control entering linearly the model equations. The sampling period also enters linearly into the model equations. This means that the solution of the optimal control problem can be singular because the first derivative of the function of Lagrange towards the control variable will not include this variable. To overcome these difficulties an augmented function of Lagrange with a quadratic term for the model equations is introduced:

$$L_a = K\Delta t + \lambda(K)^T [y(K) - \bar{y}] + \mu [y(K) - \bar{y}]^2 +$$
$$+ \sum_{k=0}^{K-1} \{ \lambda(k)^T [y(k+1) - (I + \Delta tA) y(k) -$$
$$- \Delta tBy(k) F_R(k) - \Delta tB_1 F_R(k) - \Delta tWy_f(k)] +$$
$$+ (1/2)\mu [y(k+1) - (I + \Delta tA) y(k) - \Delta tBy(k) F_R(k) -$$
$$- \Delta tB_1 F_R(k) - \Delta tWy_f(k)]^2 \} \tag{10}$$

where $\lambda(k) \in R^{N \times N}$ are the conjugate variables, μ is the penalty coefficient. The problem for minimum time control is solved on the basis of the necessary conditions for optimality of (10). As the model is a bilinear one and the augmented function of Lagrange is used the nonlinear two-point boundary value problem must be solved, which with this type of model requires a lot of complex calculations. In order to overcome these difficulties, time domain decomposition [5] in two-level computing structure is applied, but on the basis of introducing extended coordinating vector of the kind:

$$\lambda(k) = \lambda^l(k), \qquad k = \overline{0, K-1}, \tag{11}$$

$$\rho(k) = y(k+1) = \rho^l(k), \quad k = \overline{0, K-1}, \tag{12}$$

$$\Delta t = \Delta t^l, \tag{13}$$

where l is the index of the coordinating procedure.

The necessary conditions for optimality of (10) towards the problem variables are:

$$\frac{\partial L_a}{\partial y(k)} = e_v(k) = 0, \tag{14}$$

$v = y,\ F_R,\ \rho,\ \lambda,\ \Delta t, \quad k = \overline{0, K-1}$ where

$$\frac{\partial L_a}{\partial y(k)} = 0 = e_y(k) = \tag{15}$$
$$= -\left[(I + \Delta t^l A)^T + \Delta tBF_R(k)\right]\{\lambda^l(k) +$$
$$+ \mu\left[\rho^l(k) - (I + \Delta t^l A) y(k) - \Delta t^l By(k) F_R(k) -\right.$$
$$\left. - \Delta t^l B_1 F_R(k) - \Delta t^l Wy_f(k)\right]\}$$

$$\frac{\partial L_a}{\partial \rho(k)} = 0 = e_\rho(k) = \tag{16}$$
$$= \lambda(k) +$$
$$+ \mu\left[\rho^l(k) - (I + \Delta t^l A) y(k) - \Delta t^l By(k) F_R(k) -\right.$$
$$\left. - \Delta t^l B_1 F_R(k) - \Delta t^l Wy_f(k)\right]$$

$$\frac{\partial L_a}{\partial y(K)} = 0 = e_y(K) = \lambda(K) + \mu\left[y(K) - \bar{y}\right] \tag{17}$$

$$\frac{\partial L_a}{\partial F_R(k)} = 0 = e_{F_R}(k) = \tag{18}$$
$$= -\left[\Delta t^l y(k)^T B^T + \Delta t^l B_1^T\right]\{\lambda^l(k) +$$
$$+ \mu\left[\rho^l(k) - (I + \Delta t^l) Ay(k) - \Delta t^l By(k) F_R(k) -\right.$$
$$\left. - \Delta t^l B_1 F_R(k) - \Delta t^l Wy_f(k)\right]\}$$

$$\frac{\partial L_a}{\partial \lambda(k)} = 0 = e_\lambda(k) = \tag{19}$$
$$= \rho^l(k) - (I + \Delta t^l A) y(k) -$$
$$- \Delta t^l B y(k) F_R(k) - \Delta t^l B_1 F_R(k) - \Delta t^l W y_f(k)$$

$$\frac{\partial L_a}{\partial \Delta t} = 0 = e_{\Delta t} \tag{20}$$
$$= K - (\lambda^l(k)^T + \mu) \cdot$$
$$\cdot \left[A y(k) + B y(k) F_R(k) + B_1 F_R(k) + W y_f(k) \right] +$$
$$+ \rho^l(k) - (I + \Delta t^l A) y(k) -$$
$$- \Delta t^l B y(k) F_R(k) - \Delta t^l B_1 F_R(k) - \Delta t^l W y_f(k)$$

3.1. Two-level Calculating Structure

Solution of (15) – (20) is done in a two level calculating structure, Fig. 2 using decomposition and coordination according to the coordinating variables (11) – (13).

Equations (14) – (20) determine the necessary conditions for optimality of the minimum time control problem. The optimal solution is obtained when these equations are fulfilled. Analytically the values of the coordinating variables are set previously at the second level of the calculating structure and are substituted in (15) – (19). Then the necessary conditions for optimality for the state and control variables can be decomposed fully in time domain. In this way the initial problem is decomposed into $K + 1$ subproblems of the mathematical programming, every subproblem determined at a separate discrete time moment k. Gradient procedures are used to solve these subproblems.

$$y^{l,j+1}(k) = y^{l,j}(k) - \alpha e_y^{l,j}(k), \; k = \overline{0, K-1} \tag{21}$$

$$F_R{}^{l,j+1}(k) = F_R{}^{l,j}(k) - \alpha e_{F_R}^{l,j}(k), \; k = \overline{0, K-1} \tag{22}$$

The solutions of these subproblems depend on the values of the coordinating variables. Then the solutions of the subproblems will be optimal when the values of the coordinating variables are oprimal on the basis of the connection of the solutions of *primal* and *dual* problems. Gradient procedures are used to determine optimal values of the coordinating variables for the conjugate variables λ and the interconnections in time ρ. Analytical solution for the sampling period is obtained

$$\lambda^{l+1}(k) = \lambda^l(k) + \mu e_\lambda^l(k), \quad k = \overline{0, K-1} \tag{23}$$

$$\rho^{l+1}(k) = \rho^l(k) - \lambda^{l+1} / \mu, \quad k = \overline{0, K-1} \tag{24}$$

$$\Delta t = \frac{K - \lambda(K)^T e(K-1) - y(K-1)^T e(K-1) + \mu \bar{y}^T e(K-1)}{\mu e(K-1)^T e(K-1)} \tag{25}$$

where

$$e(K-1) = A y(K-1) + B y(K-1) F_R(K-1) + B_1 F_R(K-1) + W y_f(K-1) \tag{26}$$

When the optimal solution of the coordinating variables is obtained by (23) – (26), then the optimal solution of the initial problem is obtained by the solution of one coordinating problem on the second level and $K + 1$ subproblems on the first level.

3.2. Algorithm for Calculation

The optimal solution of the problems on the first level for every moment k will be determined when, the necessary conditions for optimality (15), (16) are satisfied, which means

$$e_1 = \left\| e_y{}^2(k) \right\|^2 + \left\| e_{F_R}{}^2(k) \right\|^2 \le \varepsilon_1, \quad \varepsilon_1 > 0 \tag{27}$$

In the same way the optimal solution on the coordinating level will be obtained when

$$e_2 = \left\| e_\lambda(k) \right\|^2 + \left\| e_\rho(k) \right\|^2 \le \varepsilon_2, \quad \varepsilon_2 > 0 \tag{28}$$

where ε_1 and ε_2 are criteria for determination of the calculation.

The calculation is organized in a two-level hierarchical structure, Fig.2, according to the following Algorithm:

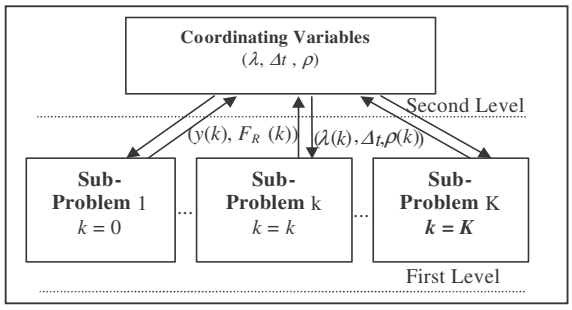

Fig. 2. Two Level Structure for Minimum Startup Time Calculation

1) The values of the coordinating variables are set on the second level on the structure Fig. 2 and sent to the subproblem on the level 1.
2) The subproblems (15), (17), (18), (21), (22) are solved and the obtained results are sent to the second level.

3) Coordination error (28) is checked on the second level. If it is satisfied, the calculations stop. If the condition is not satisfied, new values of the coordinating variables are calculated according to (16), (19), (20), (23) – (26) and are sent to the first level and so on.

A Matlab program is developed to solve the problem for minimum time control calculation according to the Algorithm above. Calculations are carried out for the model of the pilot plant.

IV. SIMULATION AND REAL TIME IMPLEMENTATION OF THE PROBLEM FOR MINIMUM TIME CONTROL

The process is for removing of *NaCl* from wastewater. The values of the process parameters are a = [5.67 4.58 4.32 4.18 4.05 3.4 2.7 2.92], b = [0.0009 0.016 0.016 0.016 0.016 0.01 0.014 0.005], $H=37.62[dm^3]$, $y_f(i)=1.2[g/l], i=\overline{1,N}$ $y_0(i)=2.2[g/l],\ i=\overline{1,N}$, $F_L=2000[dm^3/h]$, $h=28.96[dm^3]$

$y^{sp}=[0.05\ 0.1\ 0.4\ 0.5\ 0.6\ 0.8\ 1.2\ 1.4][g/l]$.

The results from the program for simulation of the process with the proposed control are shown on Fig 3.

The problem for minimum time control is a part of a developed strategy in [1], [3] for control of the ion exchange process. Real time implementation of the minimum time control is done according to Fig. 4.

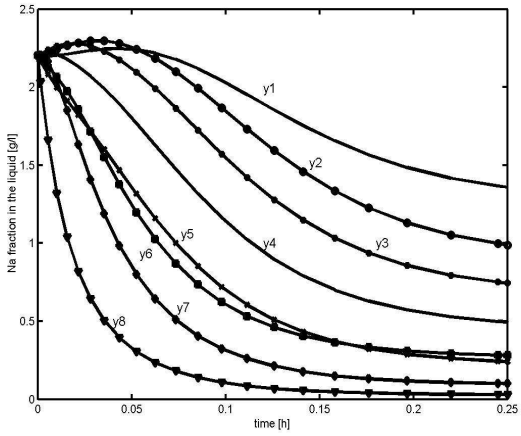

Fig. 3. State trajectories under Minimum Time control.

When the process is started the values of pH and conductivity are measured and sent to I/O card of the PC with LabVIEW software where the concentration is calculated and sent to Matlab program for the minimum time control calculation.

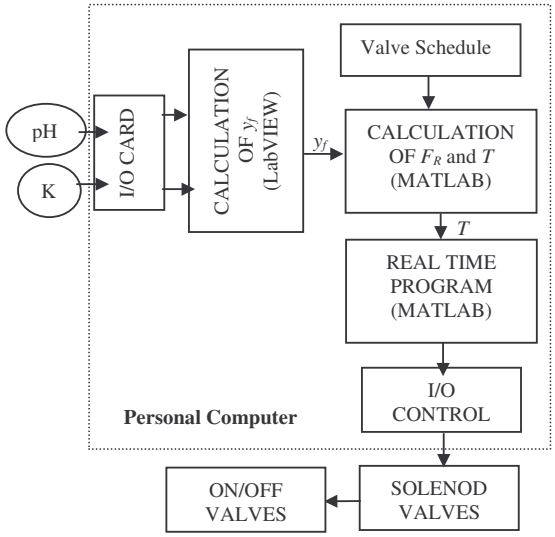

Fig. 4. Real Time Control Implementation of Minimum Time control.

The value of the upflow period T is then calculated according to (3). This value is used in schedule for switching times of the process valves. Then the corresponding ON/OFF output voltage is sent to the solenoid valves controlling the flows diaphragm valves. The values of the column output concentration are measured by output flow pH and conductivity sensors. When the set value of concentration $\overline{y}$ is reached the minimum time control is switched to repetitive optimal control of steady state [6].

V. CONCLUSION

The aim of the research work described in the paper was to develop a model and optimal minimum time control for the ion exchange process for the purposes of real time control implementation using PC. The strategy consists of two types of problems – minimum time start up of the process and two layer optimal control with steady state optimization and steady state stabilization in the presence of slowly varying disturbances.

The calculation of the minimum time control by the proposed decomposition method allows simplification of the type of problems solved on the first and second levels of the calculating structure. The use of an augmented Lagrangian allows the nonconvex optimal control problem to be convexified and correspondingly allows the subproblems gradient procedures to converge to one global solution.

The value of minimum time control depends on the values of the input concentration.

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