HYBRID SIMULATION OF A CONTROL SYSTEM FOR A TUBULAR CHEMICAL REACTOR

INTRODUCTION

These Notes describe the application of hybrid techniques in the simulation of a distributed parameter system--specifically, the control system for a tubular chemical reactor--consisting of a number of partial differential equations. The simulation is performed on the EAI HYDAC® 2400 Hybrid Computing System which combines analog speed with digital memory and accuracy to provide maximum problem solving capability of the available computing facilities.

Figure 1 shows a block diagram of the physical system simulated. This system differs from other design, control or data analysis problems solved on analog computers alone by the chemical process industries (CPI) in that its mathematical description involves partial differential equations (PDE). Since each PDE must be transformed into a set of ordinary differential equations, each of which must be solved simultaneously, the implementation of a large number of almost identical circuits is required and this usually is sufficient to exhaust the analog equipment complement of even the best equipped laboratories.

By means of a different mathematical formulation of the equations--a formulation which requires a function memory capability--this situation can be changed. Hybrid computers have satisfied this requirement for memory and thus enable system analysts to utilize the full power of available computing hardware. In addition, they have provided simple means for implementing logical operations, transport delays, and the transient simulation of stage-wise processes.

Printed in U.S.A. 115

Bulletin No. ALHC 65075

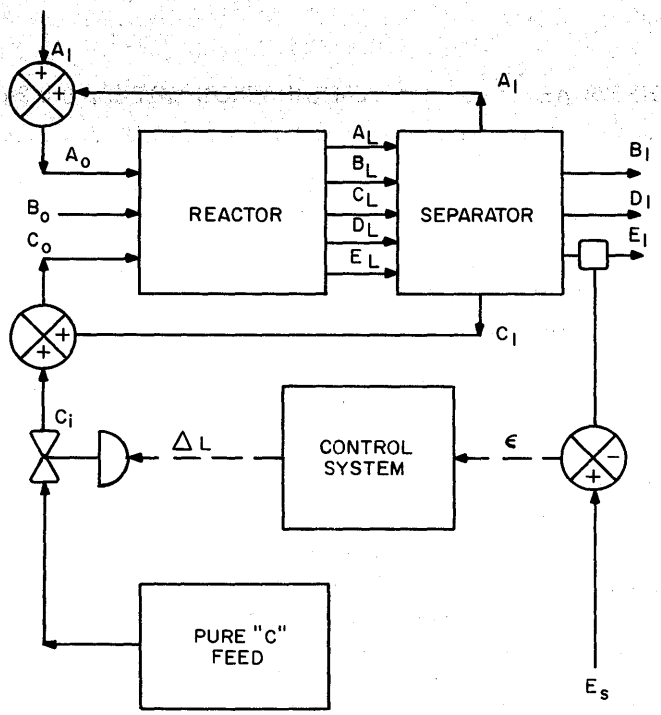

Figure 1: Block Diagram of Physical System

OBJECTIVES

The objectives of this simulation are typical of those encountered in many CPI simulations. These are:

(1) To define the physical system mathematically,

(2) To propose a control system to maintain a constant output product flow rate, and

(3) To determine controller settings for the proposed control system.

Problem definition, organization, programming, and hardware requirements to attain these objectives are presented in detail.

PHYSICAL SYSTEM

The complete system under study, shown schematically in Figure 1, consists of a tubular reactor, a separator, and a control loop. The kinetics of the system are:

$$A + B \underset{k_1}{\overset{k_5}{\rightleftharpoons}} C + D \qquad (1)$$

$$C + B \underset{k_2}{\overset{k_4}{\rightleftharpoons}} E + D \qquad (2)$$

where component E, the desired product, is formed by feeding A, B and C to the reactor. Component D is a waste product which is discarded.

Disturbances (step changes and noise such as valve chatter or low frequency sinusoids) enter the system through the make-up feed stream, A_i, and cause variations in product flow, E_i. The purpose of the control loop is to operate on the flow error, ϵ, using a control system to vary the feed rate of component C. Since B is present in excess (to maintain favorable reactor behavior), variations in C, as in equation (1), have a direct effect on product formation. The control system selected is a conventional three-mode controller.

It has been assumed that the separator is 100% efficient and that its dynamics can be represented by a first-order lag. Sensor and valve dynamics associated with the control loop are assumed negligible and the valve-position-versus-flow relationship is considered to be linear.

MATHEMATICAL MODEL

Kinetics: The rates of conversion for the components are given by:

$$r_a = -k_1\ ab + k_1\ cd \qquad (3)$$

$$r_b = -k_1\ ab + k_3\ cd - k_2\ bc + k_4\ de \qquad (4)$$

$$r_c = k_1\ ab - k_3\ cd - k_2\ bc + k_4\ de \qquad (5)$$

$$r_d = k_1\ ab - k_3\ cd + k_2\ bc - k_4\ de \qquad (6)$$

$$r_e = k_2\, bc - k_4\, de \tag{7}$$

Where a...e are component concentrations, r_a ...r_e are rates of formation, and $k_1 \ldots k_4$ are reaction rate constants.

Reactor Equations: The concentration dependence of components A and E with respect to time and position is expressed by two partial differential equations:

$$\frac{\partial A}{\partial t} + V\,\frac{\partial a}{\partial x} = r_a \tag{8}$$

$$\frac{\partial e}{\partial t} + V\,\frac{\partial e}{\partial x} = r_e \tag{9}$$

where t is time, x is distance from reactor entrance, and V is velocity of mixture through reactor.

These equations can be rewritten in terms of flow rates to obtain

$$\frac{\partial A}{\partial t} + V\,\frac{\partial A}{\partial x} = -k_1\,\frac{AB}{F} + k_3\,\frac{CD}{F} \tag{10}$$

$$\frac{\partial E}{\partial t} + V\,\frac{\partial E}{\partial x} = k_2\,\frac{BC}{F} - k_4\,\frac{DE}{F} \tag{11}$$

$$B = B_o - A_o + A - E \tag{12}$$

$$C = C_o + A_o - A - E \tag{13}$$

$$D = B_o - B \tag{14}$$

Separator Equations: The separator equations, which are first-order lags, are, in transfer function notation,

$$\frac{A_1}{A_L} = \frac{C_1}{C_L} = \frac{E_1}{E_L} = \frac{1}{\tau S + 1} \tag{15}$$

where S is the Laplace operator and τ is the separator time constant.

Control System: The classical transfer function for a three-mode controller is

$$\frac{\Delta \ell}{\epsilon} = K_c \left(\frac{\tau_D\, S + 1}{\alpha \tau_D\, S + 1}\right)\left(\frac{\tau_r\, S + 1}{\tau_r\, S + \frac{1}{K_r}}\right) \tag{16}$$

where τ_D is the derivative time constant, τ_r is the reset time constant, α is derivative gain, K_r is reset gain, K_c is controller gain, and $\Delta \ell$ is the change in percent of valve opening.

Feed and Recycle Equation: Based on the linear valve assumption, the following reactor feed equations are obtained:

$$A_O = A_1 + A_S + f \tag{17}$$

$$C_O = C_1 + C_S + \left(\frac{Cm}{100}\right)^{\Delta \ell} \tag{18}$$

The disturbance, f, can take two forms, viz:

$$\text{a step change, } f = K \tag{19}$$

$$\text{or a sinusoid, } f = K \sin \omega t \tag{20}$$

Computational Model: Since the reactor-separator system is presumed to be operating at its design point when a disturbance is introduced into the system, good scaling dictates that equations be rewritten in perturbation form. The non-linearities in the reactor equations make perturbation variables impractical. However, their form does lend itself to solution by the method of characteristics.

Applying this technique yields

$$-\frac{dA}{dy} = k_1\, AB - k_3\, CD \tag{21}$$

$$-\frac{dE}{dy} = k_4\, DE - k_2\, BC \tag{22}$$

where

$$y = \frac{\gamma x}{F^2} = \frac{x}{\gamma F} \tag{23}$$

These reactor equations, solved in conjunction with the three algebraic equations, (12), (13), and (14), defining B, C and D in terms of A and E are the computational model of the reactor. The controller equation, (16), requires no modification since it is already in perturbation form.

A high-speed computational procedure is required to allow the reactor outlet product flows to be obtained in a semi-continuous manner.

Please send for Application Study: 6.4.2h, Bulletin No. ALHC 65076 for complete details, including results, of this simulation.