International Research Journal of Advanced Engineering and Science
ISSN (Online): 2455-9024

Implementation of a Kalman-Bucy Filter for Estimating Product Concentration of a CSTR Process

Eze Paulinus C.[1], Muoghalu Chidiebere[2], Jonathan Amabikutol E.[3], Aigbodioh Ferdinard A.[4], Okoronkwo Emmanuel A.[3], Ekengwu Bonaventure O.[2]
[1]Electrical and Electronic Engineering, Covenant Polytechnic, Aba, Abia State, Nigeria
[2]Electrical and Electronic Engineering, Chukwuemeka Odumegwu Ojukwu University, Uli, Anambra State, Nigeria
[3]Electrical and Electronic Engineering, Federal University of Technology, Owerri, Imo State, Nigeria
[4]Electrical and Electronic Engineering, Auchi Polytechnic, Auchi, Edo State, Nigeria

Abstract—*This paper has presented the implementation of a Kalman-Bucy filter for estimating product concentration of a continuous stirred tank reactor (CSTR). An ideal operation was assumed such that the chemical reaction taking place in the system was considered a linear continuous time process. A transfer function model for the product concentration considering reactor mass balance is obtained. It is required to estimate and track the product concentration using measurement noise. A Kalman-Bucy filter was developed and implemented in Matlab/Simulink environment. A computer programme using Matlab code for the Kalman-Bucy filter implemented in Matlab/Simulink embedded block function was used for the simulation in this paper. The results obtained showed that the performance of the filter in rejecting the noise and estimating a signal that accurately tracks the input improved as the value of the noise variance was tuned within the range of 0.0001 to 0.1.*

Keywords*— Computer programme, CSTR, Embedded block function, Kalman-Bucy filter, Matlab/Simulink, Product concentration.*

I. INTRODUCTION

Some of the primary factors driving the growth of continuous stirred tank reactor (CSTR) are increasing adoption of sustainable production technique to gain competitive advantage, need of cost cutting and mass production [1]. A CSRT is a system in which reactants are added and products are continuously removed at the same rate with the reactant continuously stirred using internal component [1]. The flow rate, reaction time and dilution rate are basic three parameters that define the nature of CSRT. It has gain wide application in chemical and waste water treatment industries basically due to the fact that it has approximate mixing property. For instance, in chemical industry, it provides perfect mixing of chemicals which are continuously added in the reactor and also gives similar composition of input chemical and output mixture [1].

It is one of the most essential unit operation in chemical industries. Continuous stirred tank reactor (CSTR) shows nonlinear behaviour and its operating is normally wide [2]. The chemical reactions that take place in CSTR are either endothermic or exothermic. During this reaction, energy can either be added or removed so as to keep a constant temperature. It is usually operated in such a way that the well mixed chemical process normally run at steady state.

There are several works in literature that deal with CSTR. Mohd et al. [4] carried-out experimental study on the effect of operating conditions on CSTR performance. The influence of operating conditions on the conversion and specific rate constant was studied. Igbokwe et al. [5] presented the characterization of a five-litre continuous stirred tank reactor. Antonelli and Astolfli [6] designed bounded control laws for the temperature stabilization of a class of continuous stirred tank reactors with exothermic or endothermic reactions using methodologies and tools from Lyapunov theory. Controller design for continuous stirred tank reactor is presented by Prabhu and Bhaskaran [7]. It studied the problem of temperature control of CSRT using adaptive controller. DI Ciccio et al. [8] proposed a novel digital control law for continuous stirred reactor tank. It used the relative degree preservation under sampling as its methodology. Alejandro (2010) presented a problem based learning approach in the analysis of continuous stirred tank chemical reactors with a process control approach.

In this paper, a Kalman-Bucy filter is developed and implemented in Matlab/Simulink to estimate the product concentration of component X in a reactor. The Kalman-Bucy filter is a Kalman filter in continuous time. The design of Kalman-Bucy filter is such that it can be used to estimate unmeasured states of a continuous process, either for controlling one or more of them [3].

II. THEORETICAL BACKGROUND

This section presents the theoretical frame work for developing the dynamic model of the considered continuous stirred tank reactor (CSTR). The state space modelling and representation of the continuous time process. Also in this section, the theoretical concept of a Kalman-Bucy filter is presented.

A. Process Description for Ideal CSTR

In this paper, the reactor mass balance dynamic equation has been considered for estimating the product concentration of a component X in a typical reactor. A model of a CSTR using first principles operational data (Table 1) as stated in [10] has been used for carrying out computer simulation in this work. Fig. 1 shows an irreversible, exothermic chemical reaction taking place in constant volume reactor that is cooled by a single coolant stream [2]. A feed material whose composition is C_{X0} enters the reactor at a temperature, T_{c0} at a constant volumetric flow rate Q. Product is taken out of the system at the same volumetric flow rate Q. A

Eze Paulinus C., Muoghalu Chidiebere, Jonathan Amabikutol E., Aigbodioh Ferdinard A., Okoronkwo Emmanuel A., and Ekengwu Bonaventure O., "Implementation of a Kalman-Bucy filter for estimating product concentration of a CSTR process," *International Research Journal of Advanced Engineering and Science*, Volume 3, Issue 1, pp. 97-100, 2018.

homogeneous mixture is assumed for the liquid content within the reactor.

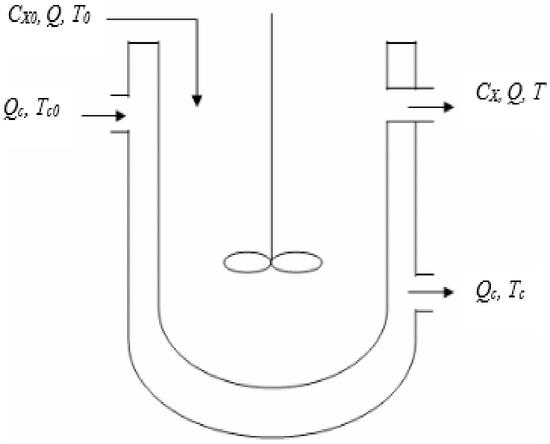

Fig. 1. A typical diagram of a continuous stirred tank reactor.

Fig. 1 shows a jacketed continuous stirred tank reactor (CSTR) in which heat is added or removed as a result of the difference between the jacket fluid and the reactor fluid [2]. Heat transfer liquid is usually pumped through a nozzle that circulates the liquid through the jacket at a high velocity. The coolant flows at a rate, Q_c and at a feed temperature, T_{c0}. The coolant liquid temperature at exit is T_c.

B. *Dynamic Model of reactor Mass Balance*

In order to perform the modelling of the system, assumptions are made so as to obtain a simplified model for an ideal CSTR as follows [2]:

i. The mixing taking place in the reactor and jacket is perfect
ii. Reactor and jacket volume is constant

The dynamic modelling for the process is formulated considering mas balance as in [2]:

$$V\frac{dC_X}{dt} = Q(C_{X0} - C_X) - Vr_X \tag{1}$$

where C_X = product concentration of component X in the reactor, r_X = rate of reaction per volume, and V = volume of CSTR

The rate of reaction per volume is usually expressed using Arrhenius equation [2].

$$r_X = k_o \exp\left(\frac{-E}{RT}\right)C_X \tag{2}$$

where k_o = reaction rate constant, E = activation energy, R = ideal gas constant, and T = reactor absolute temperature in Kelvin.

Rearranging Eq. (2) and taking the Laplace transform gives the transfer function as in Eq. (3):

$$\frac{C_X(s)}{C_{X0}(s)} = \frac{Q}{Vs + Q + k_o \exp\left(\frac{-E}{RT}\right)} \tag{3}$$

Table 1 shows the parameters and values used for simulation in this paper.

TABLE 1. Steady state operating data [10].

Serial No.	Physical Parameters	Symbols	Values
1	Reaction rate constant	k_o	$7.2\times10^{10}\ \text{min}^{-1}$
2	Feed flow rate	Q	100 l/min
3	Reactor temperature	T	441.2 K
4	CSTR volume	V	100 l
5	Activation energy term	E/R	1×10^{4} K

Substituting the values of the parameters in Table 1 into Eq. (3) gives the process transfer function as:

$$G_p(s) = \frac{1}{s+1} \tag{4}$$

C. *The Kalman-Bucy Filter*

Given the inputs and measured output, assumptions are made on the state and output noise. The Kalman-Bucy filter is used to estimate unmeasured states (assuming that they are observable) and the actual outputs of the process. Fig. 2 shows the estimated states $\hat{x}$, and the estimated measured output $\hat{y}$.

Fig. 2. Block diagram of input-output relation of the Kalman-Bucy filter.

A differential Riccati equation to be integrated through time is used by the Kalman-Bucy filter unlike the Kalman filter that uses a predictor-corrector algorithm to update the state estimates. The filter update equations are stated as:

$$K = PC^T R^{-1} \tag{5}$$

$$\dot{\hat{x}} = A\hat{x}(t) + Bu((t) + G(y(t) - C\hat{x}(t)) \tag{6}$$

$$\dot{P} = AP + PA^T - KRK^T + Q \tag{7}$$

In the above equations, K is Kalman-Bucy filter observer gain matrix which makes the observer sensitive to sensor noise, P is an estimate of the covariance of the measurement error and satisfies the Riccati equation, C^T is the transpose of the measurement matrix C, R is a weighting matrix of measurement (sensor) noise, Q is a weighting matrix of process (state) noise, A is the system matrix, and B is the input matrix. For the filter implementation, both $\hat{x}$ and $\dot{P}$ must be integrated through time.

III. METHOD

A. *State Space Representation*

The state space representation of the reactor mass balance equation of a CSTR process is presented assuming a linear continuous time process with input and measurement noise as shown in Fig. 3.

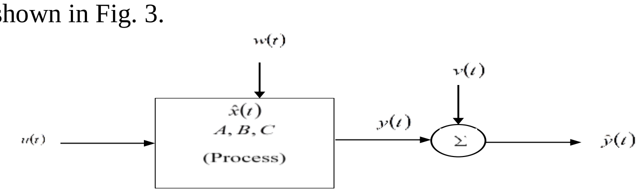

Fig. 3. Linear continuous-time process with input and output noise.

Eze Paulinus C., Muoghalu Chidiebere, Jonathan Amabikutol E., Aigbodioh Ferdinard A., Okoronkwo Emmanuel A., and Ekengwu Bonaventure O., "Implementation of a Kalman-Bucy filter for estimating product concentration of a CSTR process," *International Research Journal of Advanced Engineering and Science*, Volume 3, Issue 1, pp. 97-100, 2018.

$$\dot{x} = Ax + Bu + w \quad (8)$$

$$y = Cx \quad (9)$$

$$\hat{y} = y + v \quad (10)$$

where u is the vector of inputs, X is the actual states vector, y is the actual process outputs vector, $\hat{y}$ is a vector of the actual process outputs, w and v are state and output noise respectively. In this paper, the state or process and output noise are assumed to be zero Gaussian.

The process, Eq. (4), considered in this paper is a first order system given by the following state space equation:

$$\dot{x} = -x + u \quad (11)$$

$$y = x \quad (12)$$

where $A = -1$, $B = 1$, and $C = 1$

The complete programme for the computer simulation in Matlab/Simulink environment is shown in Fig. 4. It should be noted that only the estimated output result is presented in this paper.

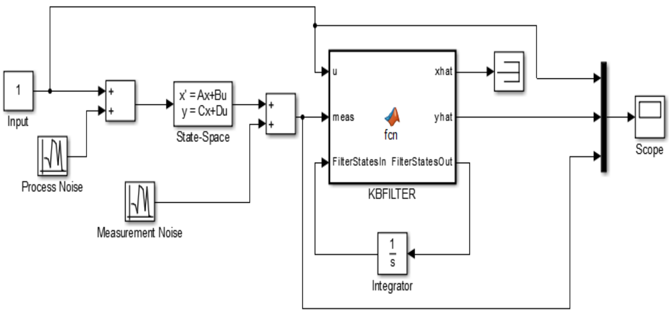

Fig. 4. Complete programme for the simulation.

IV. Simulation Results and Discussion

A. Simulation Results

Simulations are performed considering different selected or tuned values for the variance σ^2 of the process noise and the variance of the measurement noise. The values were selected within the range of 0.0001 to 0.1. The simulation results obtained are shown in Fig. 5, 6, 7, and 8.

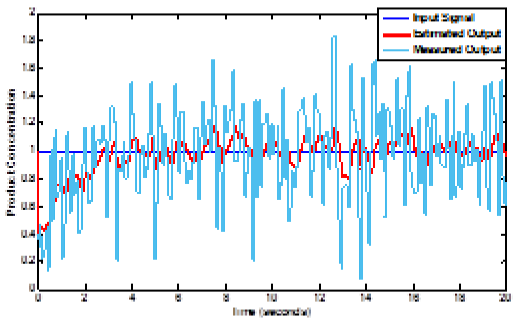

Fig. 5. Step Response, σ^2 = 0.1.

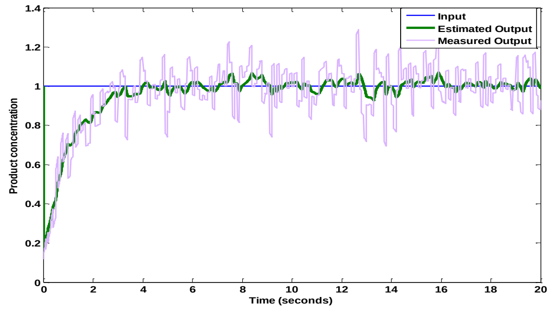

Fig. 6. Step Response, σ^2 =0.01.

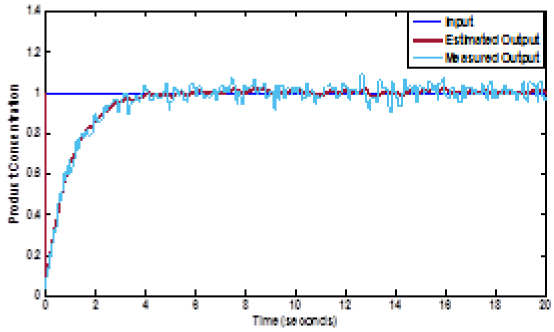

Fig. 7. Step Response, σ^2 =0.001.

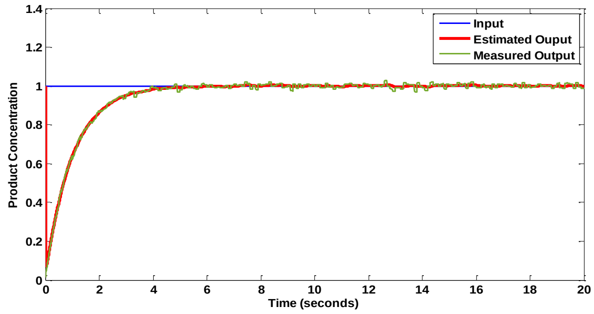

Fig. 8. Step Response σ^2 =0.0001.

B. Discussion

In this work, two sources of zero-mean Gaussian noise are made to enter the system. The input is corrupted with process noise and the output corrupted with measurement noise. The variance of the process noise and that of the measurement noise were tuned within the range of 0.0001 to 0.1. In Fig. 5, the variance of the process noise and measurement noise were tuned to 0.1. It can be seen that the estimated signal tracks the referenced input signal but is highly corrupted by noise. In Fig. 6, the variance of the process noise and measurement noise were tuned to 0.01. It can be seen that the estimated signal tracks the referenced input and is less corrupted by noise than the result of Fig. 5. In Fig. 7, the process noise and the measurement noise have their variance tuned to 0.001. The plot shows that the estimated noise tracks the referenced input with improved noise rejection. In Fig. 8, the estimated signal tracks the referenced input with well improved noise rejection. This shows that by tuning the variance of the process noise and measurement noise, within the range considered, the

Eze Paulinus C., Muoghalu Chidiebere, Jonathan Amabikutol E., Aigbodioh Ferdinard A., Okoronkwo Emmanuel A., and Ekengwu Bonaventure O., "Implementation of a Kalman-Bucy filter for estimating product concentration of a CSTR process," *International Research Journal of Advanced Engineering and Science*, Volume 3, Issue 1, pp. 97-100, 2018.

product concentration of a continuous stirred tank reactor (CSTR) system can be estimated using Kalman-Bucy filter.

V. CONCLUSION

This work has presented the implementation of a Kalman-Bucy filter for estimating product concentration in Simulink. The work considered a typical continuous stirred tank reactor (CSTR). Assuming ideal operation, the chemical reaction process taking place in the system was considered as a linear continuous time process. A model of a reactor mass balance was used in this work to obtain a transfer function for the product concentration which is to be estimated using measurement noise. A Kalman-Bucy filter algorithm was developed and implemented in Matlab/Simulink environment. A computer programme using Matlab code for the Kalman-Bucy filter implemented in Matlab/Simulink embedded block function was used for the simulation in this paper.

The input and the output were corrupted with zero-mean Gaussian noise whose variance is tuned within the range of 0.0001 to 0.1. The performance of the designed filter was presented in terms of the input signal, estimated output and measured output as shown in the plots in Fig. 5, 6, 7, and 8. It can be seen from the plots that the performance of the filter in rejecting the noise and estimating a signal that accurately tracks the input improves as the value of the noise variance is tuned within the range of 0.1 to 0.0001.

REFERENCES

[1] Persistence Market research, “Continuous flow stirred tank reactor (CSTR) market: Global industry analysis and forecast 2016-2026” https://www.persistencemarketresearch.com/market-research/continuous-flow-stirred-tank-reactor-market.asp
[2] Anonymous, “Mathematical modeling of a continuous stirred tank reactor,”
[3] Goddard Consulting, “A simple Kalman-Bucy filter in simulink” hppt://www.goddardconsulting.ca/simulink-kalman-bucy-filter
[4] M. Danish, M. K. Al Mesfer, and M. M. Rashid, “Effect of operating conditions on CSTR Performance: an experimental study,” *Int. Journal of Engineering Research and Applications*, vol. 5, issue 2, pp. 74-78, 2015.
[5] P. K. Igbokwe, J. T. Nwabanne, and S. W. Gadzama, “Characterization of a 5 litre continuous stirred tank reactor,” *World Journal of Engineering and Technology*, vol. 3, issue 2, pp. 25-40, 2015.
[6] R. Antonelli and A. Astolfi, “Continuous stirred tank reactors: Easy to stabilize,” *Automatica*, vol. 39, issue 10, pp. 1817-1827, 2003
[7] K. Prabhu and V. M. Bhaskaran, “Controller design for continuous stirred tank reactor using adaptive control,” *Research Journal of Applied Sciences*, vol. 9, issue 8, pp. 489-495, 2014.
[8] M. P. Di Ciccio, M. Bottini, and P. Pepe, “Digital control of a continuous stirred tank reactor,” *Hindawi Publishing Corporation, Mathematical Probles in Engineering*, vol. 2011, Article ID 439785, pp. 1-18, 2011.
[9] R. Alejandro, Rosario C. P. and Juan B. G., “Problem based learning (PBL): analysisof continuous stirred tank chemical reactors with a process control approach,” *International Journal of Software Engineering and Application (IJSEA)*, vol. 1, no. 4, pp. 54-73, 2010.
[10] M. Pottman and D. E. Seborg, “Identification of non-linear process using reciprocal multiquadratic functions,” *J. Process Control*, vol. 2, issue 4, pp. 189-203, 1992.