Effect of Random Noise, Quasi Random Noise and Systematic Random Noise on Unknown Continuous Stirred Tank Reactor (CSTR)

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Abstract

Continuously stirred tank reactors (CSTRs) play a big role in chemical engineering and in industries nowadays. Therefore, it is important and necessary to make sure CSTRs work successfully by avoiding disturbance from external factors. In this paper, we look at the impact of different kind of uncertainties (errors) to the model fitting and the parameter estimation of the CSTR’s, for both cases of exothermic and endothermic reactors by taking into consideration of high and low variances of noise into concentration and temperature of the model. Two parameters, activation energy $E$ and pre-exponential Arrhenius reaction rate $k_0$ have been estimated and investigated, due to their sensitivities to the system facilitated by the guessed noisy data and by using Minimization Assimilation Method (MAM). Results showed that, the increase of noise in measurements affects activation energy $E$ much more than the pre-exponential Arrhenius reaction rate $k_0$ for all types of noise as $k_0$ converges to its guessed values. Also, from the results obtained, the endothermic CSTR is more sensitive than the exothermic CSTR for any kind of noise according to much deviation observed in its estimated activation energy values. Furthermore, quasi random noise has provided closer values for parameter estimation compared to the remaining types of noise but with negative activation energies for both cases (exothermic and endothermic).

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Keywords: CSTR, Exothermic, Endothermic, Random noise, Systematic random noise and Quasi random noise

1 Introduction

Many years ago, continuously stirred tank reactor was used for waste treatment only but currently, it is used in chemical engineering to produce products from the given input of substances. For instance, the treatment of waste by producing organic fertilizers [6], electricity from biogas [6], production of chemical products (eg: alcohols) [8], polymerization [1], etc. Based on the dynamical behaviour of the CSTR, it is better to understand how it operates for designing controllers [10]. Some methods are currently used by different authors to study the steady states and to prove their effectivenesses on parameter estimation of the CSTR such as Approximate Expectation Maximization (AEM), Approximate Maximum Likelihood Estimate (AMLE) and the Continuously Time Stochastic Modelling (CTSM) [2], sigma point method in [9] and the Extended Kalman Filter method. The Extended Kalman Filter method is very famous method for non-linear systems and was used in [11] to estimate the valve constants ($k_{11}, k_{22}$) for the two communicating tanks-in-series process, the temperature of reaction mixture and the pre-Arrhenius reaction rate (frequency factor ($k_0$)) for CSTRs. In their work they wanted to apply the Extended Kalman Filter method for the purpose of linearisation of the two CSTR models around the Kalman Filter estimate. The estimation of the parameters and states of the process were observed by adding white noise to the models. Simulations and parameter estimation results showed that the Extended Kalman Filter algorithm gives small deviation from the true solutions. Also, the estimated parameters converge with the minimum time for different proposed initial values.

There is a shortage of literature found discussing some similar works which may take into consideration of all three kinds of noise. Again, unlike those above methods, in this paper we are using MAM to estimate parameters and to study the effect of high and low different types of noise on concentration and temperature for both models as they include parameters under investigation. We chose to use MAM estimator because it is among the methods that provides the accuracy for parameter estimation for non-linear dynamical processes.

The goal of this work is to track the influence of three kinds of noise on CSTRs through parameter estimation and simulation. We firstly, track the influence of random noise which is the Gaussian distribution noise on CSTRs and may get into the system randomly, mathematically defined as $R.E = (x_i - \bar{x})$ [3]. Secondly, we look at the impact of quasi random noise which is like sobol sequence on CSTRs. Quasi random noise has the property of low-discrepancy means points are generated in a correlation procedure and are
located in a such way that the next point to be generated knows where all previous ones are located [7]. Finally, we investigate the effect of systematic random noise which is bias noise or determinate noise with systematic pattern distribution on CSTRs, mathematically defined as $S.E = \bar{x} - \mu$ [3]. This kind of noise may occur in measurements from non-calibrated measurement instrument and hence can be measured, adjusted and corrected [3]. One can also show how internal noise sources can be transferred to the output terminals of a process, where the noise becomes observable to the outside world.

The paper will proceed as follows: Section 1 motivates the ideas behind the CSTR, while the Section 2 describes the model formulation. Section 3 points out parameters to be estimated and the source of data that is going to be used and the tools as well. Section 4 which is the main part of this paper covers the simulations and the interpretation of the graphs. Section 5 is the discussion of the results obtained whilst the last section includes conclusion and dedication for further work.

2 Model framework

To describe the dynamic behaviour of the CSTR with exothermic or endothermic reactions, we have to take care of the mass component balance and energy component balance [12]. Inside the CSTR, a reaction will produce new components (products) while on the other hand, reduces the concentration of the reactants. This process may cause exothermic reactions (which release heat energy) or endothermic reactions (which acquire heat energy) [12]. The schematic diagrams in Figure 1 and Figure 2 for both tanks are constructed based on a diagram found in [5].

![Figure 1: Graph describing the exothermic process with the cooling Jacket.](image-url)
Therefore, both models for exothermic and endothermic reactions inside the tank with cooling and heating jackets are respectively derived by using the mass balance and conservation of the energy for which the reaction rate \( k \) depends on temperature and pre-exponential Arrhenius reaction rate \( k_0 \) according to Arrhenius equation

\[
k = k_0 e^{-\frac{E}{RT}}
\]

and are as follow,

\[
\begin{align*}
\frac{dT(t)}{dt} &= \frac{F}{V} (T_{in} - T(t)) - \frac{(\Delta H)k_0 e^{-\frac{E}{RT}}C(t)}{\rho C_p} - \frac{UA}{\rho V C_p} (T(t) - T_c(t)) , \\
\frac{dT_H(t)}{dt} &= \frac{F_H}{V_H} (T_{Hin} - T(t)) - \frac{UA}{\rho_H C_p C_{pH}} (T_H(t) - T(t)) , \\
\frac{dC(t)}{dt} &= \frac{F}{V} (C_{in} - C(t)) - k_0 e^{-\frac{E}{RT}}C(t) .
\end{align*}
\]

(1)

Where \( T(t), T_c(t) \) in \(^oK\) and \( C(t) \) in \( \text{mole} \text{m}^{-3} \) are variables which represent the temperature, temperature of the cooling jacket and the concentration inside of the exothermic tank at time \( t \) respectively.

And

\[
\begin{align*}
\frac{dT(t)}{dt} &= \frac{F}{V} (T_{in} - T(t)) + \frac{(\Delta H)k_0 e^{-\frac{E}{RT}}C(t)}{\rho C_p} + \frac{UA}{\rho V C_p} (T_H(t) - T(t)) , \\
\frac{dT_H(t)}{dt} &= \frac{F_H}{V_H} (T_{Hin} - T(t)) - \frac{UA}{\rho_H C_p C_{pH}} (T_H(t) - T(t)) , \\
\frac{dC(t)}{dt} &= \frac{F}{V} (C_{in} - C(t)) - k_0 e^{-\frac{E}{RT}}C(t) .
\end{align*}
\]

(2)

Where \( T(t), T_H(t) \) in \(^oK\) and \( C(t) \) in \( \text{mole} \text{m}^{-3} \) represent the temperature, temperature of the heating jacket and the concentration inside of the endothermic tank at \( t \) successively.

Constants that are in systems of equation (1) and equation (2) are explained in Table 1.
Table 1: Table Constants and Parameters

<table>
<thead>
<tr>
<th>Constants</th>
<th>Descriptions</th>
<th>Values</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R$</td>
<td>Gas law constant</td>
<td>8.314</td>
<td>$N m^2 s^{-1}$</td>
</tr>
<tr>
<td>$T_{\text{mean}}$</td>
<td>Mean of temperature</td>
<td>298.15</td>
<td>$^oK$</td>
</tr>
<tr>
<td>$k_0$</td>
<td>Pre-exponential Arrhenius reaction rate</td>
<td>to be estimated</td>
<td>$\text{mole} m^{-3}$</td>
</tr>
<tr>
<td>$E$</td>
<td>Activation energy</td>
<td>to be estimated</td>
<td>$J$</td>
</tr>
<tr>
<td>$F$</td>
<td>Volumetric flow rate in or out of tank</td>
<td>$130 \times 10^{-6}$</td>
<td>$\text{m}^3 s^{-1}$</td>
</tr>
<tr>
<td>$V$</td>
<td>Volume of reactor</td>
<td>$110 \times 10^{-6}$</td>
<td>$\text{m}^3$</td>
</tr>
<tr>
<td>$\Delta H$</td>
<td>Enthalpy for the endothermic and exothermic</td>
<td>$10043 \times 10^2$ and $-10043 \times 10^2$</td>
<td>$\text{J} \text{mole}^{-1}$</td>
</tr>
<tr>
<td>$C_{\text{in}}$</td>
<td>Concentration of substance flows into tank</td>
<td>316.8</td>
<td>$\text{mole} m^{-3}$</td>
</tr>
<tr>
<td>$t$</td>
<td>Time interval</td>
<td>$[0 : 20]$</td>
<td>s</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Density of the substance in reactor</td>
<td>1000</td>
<td>$\text{kg} m^{-3}$</td>
</tr>
<tr>
<td>$c_p$</td>
<td>Heat capacity of reactor</td>
<td>4186</td>
<td>$\text{kg} \text{oK}^{-1}$</td>
</tr>
<tr>
<td>$T_{\text{in}}$</td>
<td>Temperature of the substance flows into tank</td>
<td>$25^oC = 298.35^oK$</td>
<td>$^oK$</td>
</tr>
<tr>
<td>$U$</td>
<td>Heat transfer coefficient</td>
<td>10000</td>
<td>No unit</td>
</tr>
<tr>
<td>$A$</td>
<td>Heat transfer area</td>
<td>0.015</td>
<td>$m^2$</td>
</tr>
<tr>
<td>$F_H$</td>
<td>Volumetric flow rate of the heating substance</td>
<td>$465 \times 10^{-7}$</td>
<td>$\text{m}^3 s^{-1}$</td>
</tr>
<tr>
<td>$V_H$</td>
<td>Volume of the heating jacket</td>
<td>$50 \times 10^{-6}$</td>
<td>$\text{m}^3$</td>
</tr>
<tr>
<td>$\rho_H$</td>
<td>Density of the heating substance</td>
<td>1000</td>
<td>$\text{kg} m^{-3}$</td>
</tr>
<tr>
<td>$c_{\rho H}$</td>
<td>Heat capacity of heating jacket</td>
<td>4186</td>
<td>$\text{kg} \text{oK}^{-1}$</td>
</tr>
<tr>
<td>$T_{H\text{in}}$</td>
<td>Temperature of the heating substance</td>
<td>288.15</td>
<td>$^oK$</td>
</tr>
<tr>
<td>$T_{c}(t)$</td>
<td>Temperature of cooling Jacket at time $t$</td>
<td>to be computed</td>
<td>$^oK$</td>
</tr>
<tr>
<td>$\rho_c$</td>
<td>Density of the cooling substance</td>
<td>1000</td>
<td>$\text{kg} m^{-3}$</td>
</tr>
<tr>
<td>$c_{\rho c}$</td>
<td>Heat capacity of the cooling Jacket</td>
<td>4186</td>
<td>$\text{kg} \text{oK}^{-1}$</td>
</tr>
<tr>
<td>$F_c$</td>
<td>Volumetric flow rate of the coolant</td>
<td>$465 \times 10^{-7}$</td>
<td>$\text{m}^3 s^{-1}$</td>
</tr>
<tr>
<td>$V_c$</td>
<td>Volume of the cooling Jacket</td>
<td>$50 \times 10^{-6}$</td>
<td>$\text{m}^3$</td>
</tr>
<tr>
<td>$T_{\text{cin}}$</td>
<td>Temperature of the cooling substance</td>
<td>288.15</td>
<td>$^oK$</td>
</tr>
</tbody>
</table>

3 Estimation of parameters

Data: We assume real activation energies ($E$) and pre-exponential Arrhenius reaction rates ($k_0$) for generating data from models, which in turns the noise is added to the concentration and temperature data for proving guessed parameters of models. Therefore, the noisy data is used to estimate back the parameters and fitting models. Several results of estimated parameters and their difference from guessed parameters were noted during simulation period using Scilab codes. Deviation of estimated solutions from guessed solutions (residuals), its squared with the mean squared residuals were plotted to observe their variations as one of the analysis method. Finally, residuals are analysed through plots and their variations are observed. Parameters to be estimated are $E$ and $k_0$ and we use the MAM to estimate these parameters.
4 Numerical simulations

This section shows results achieved by doing simulations and parameter estimation. Since we are dealing with two cases, the exothermic continuously stirred tank reactor and endothermic continuously stirred tank reactor, together with three types of noise, results are categorized into six subsections. Performing our simulations we chose the values of parameters according to our guessed parameters. We have fixed the guessed parameters to be $k_0 = 0.9$, $E = 0.5$ for the exothermic CSTR case and $k_0 = 0.4$, $E = 0.5$ for the endothermic CSTR case. We have run our simulations 5 times by guessing the values of parameters. These guesses were chosen based on the following criteria: by guessing higher values than the fixed parameters, higher values than the fixed parameters but closer, less values than the fixed parameters but closer, small values compared to the fixed parameters and the final guess become fixed parameters. The highest guess of values is $[1, 1]$ for all cases of the exothermic and endothermic CSTR. Higher but closer guess values are $[1, 0.6]$ and $[0.5, 0.6]$ for the exothermic and endothermic cases respectively. Less but closer guesses are $[0.8, 0.4]$ for exothermic case and $[0.3, 0.4]$ for endothermic case. A very less guess of values is $[0.1, 0.1]$ for all cases whereas the last guesses are $[0.9, 0.5]$ and $[0.4, 0.5]$ for the exothermic and endothermic CSTRs respectively where the first value in bracket represents the guess for pre-exponential Arrhenius reaction rate while the second is the guess for activation energy.

The simulations were facilitated by the constants values and the parameters that are described in Table 1.

4.1 Random noise effect on the exothermic CSTR

For $\sigma = 2$, the fitted curves and the residuals graphs are as shown in Figure 3.
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Figure 3: plots (1), (2) and (3) respectively show the model fitting, residuals and squared residuals of exothermic CSTR model. $\sigma = 2$ and the fixed parameters $k_0 = 0.9$ and $E = 0.5$ are involved in numerical simulations. Estimated parameters are $k_0 = 0.8853$ and $E = 377.2327$.

From Figure 3, the result shows that the estimated pre-exponential Arrhenius reaction rate approaches the fixed value with the difference of 0.0147 while the activation energy is too far from its estimated value. In sub-plot (2), more residuals of temperature are above zero in a scale of $[-0.4, 1.59]$, which indicates that more temperature observations are greater than the estimated temperature of the reactor. This is not the case for concentration residuals since almost 50% of the observations are greater than the estimated concentration while almost the other 50% are lower in the range $[-0.9, 1.1]$. The difference between the observations and the estimated values is not very significant since the scale of residuals is small. In sub-plot (3), the squared residuals are varying in the range $[0, 1.34]$ and $[0, 2.49]$ with the mean values of 0.34584 and 0.5917550 for the concentration and temperature respectively. We cannot observe the squared residuals of the cooling temperature on the squared residuals graph because they are around 0 with a very small mean value of 0.00082698. Hence, the results are quite good as the variation of residuals is at a low scale with small mean values. Therefore, the data is fitting the model well.

We now repeat the above simulations when $\sigma = 10$. The results are as shown in Figure 4.
In Figure 4, the estimated pre-exponential Arrhenius reaction rate is greater but converges to its fixed value with the difference of 0.0044 while the activation energy becomes negative and diverges from its fixed value. The negative value for the activation energy, physically indicates that the reaction cannot be stopped, unless the reactants are kept away from the tank. In sub-plot (2), the scale of concentration and the temperature residuals becomes high and ranges between $-5$ and $5$. This implies that the significance of the difference between the observations and the estimated values of the temperature and concentration is considerable. In sub-plot (3), the squared residuals of the concentration vary in $[0, 24.53]$ with the mean value of 7.8652, and the squared residuals of the temperature range from 0 up to 24.74 with the mean value of 7.8723. The squared residuals of the cooling temperature vary near zero with the mean value of 0.000023. Hence, the variation and mean values of the squared residuals of the concentration and temperature increase. This is the reason why the data does not fit the model well.
4.2 Random noise effect on the endothermic CSTR

Figure 5: Sub-plots (1), (2) and (3) respectively represent the model fitting, residuals and squared residuals of the endothermic CSTR model. The level of noise is $\sigma = 2$ and the fixed parameters involved in numerical implementation are $k_0 = 0.4$ and $E = 0.5$. Estimated parameters from Minimization Assimilation method become $k_0 = 0.3948$ and $E = 485.69$.

The results obtained from Figure 5 also look good as the pre-exponential Arrhenius reaction rate is closer to its fixed value with only a difference of 0.0052, although the activation energy does not converge. It is however among the smallest values compared to the estimated activation energies obtained in this work. In sub-plot (2), the scale of concentration residuals is $[-0.8, 1.7]$ while the temperature residuals are skewed and almost a half of them are greater than zero on a scale of $[-0.4, 1.58]$. The difference between the observations and the estimated values of the concentration and the temperature is not high. The squared residuals of the concentration range between 0 and 1.31 with the mean value of 0.3028747 and the squared residuals of the temperature vary in the range $[0, 2.4]$ with the mean value of 0.5334537. The mean value of the squared residuals of the heating temperature is 0.00029228. Fortunately, good fitting can be seen in Figure 5, as most of the data points are in a margin of fitting the curves.

The fitting model and the residuals graphs of CSTR with the endothermic reaction when $\sigma = 10$ are as represented in Figure 6.
Figure 6: Graphs representing the endothermic CSTR model. Sub-plot (1) points out both fitting concentration and temperature curves. Sub-plot (2) shows the residuals while sub-plots (3), (4) and (5) show the squared residuals. The experimental parameters are $k_0 = 0.4$ and $E = 0.5$ whilst estimated parameters are $k_0 = 0.3782$ and $E = 3606.8$. The level of random noise is given by $\sigma = 10$.

The result shows that the variability in the pre-exponential Arrhenius reaction rates has increased slightly with the difference of 0.0218 and the estimated activation energy remains large compared to the results obtained in Figure 5. The range of residuals has also increased and becomes $[-5, 5]$ for both temperature and concentration. Almost half of the residuals are above zero while the other half are below zero. This implies that almost 50% of the observations are greater than the estimated values while the other 50% are less than the estimated temperature and concentration solutions. The difference between observations and the estimated values is significant since more of the residuals are not around zero. The residuals of concentration squared vary in the range $[0, 25]$ with the mean value of 7.7814381 whereas the squared residuals of temperature vary between 0 and 24.8 with the mean value of 7.8997289, as can be seen in sub-plots (4) and (5) of Figure 6. The obtained mean value of the squared residuals of the heating temperature is 0.000086324, which is very small and negligible. Few data points among hundred fit the model while others are far away from the model.

4.3 Quasi random noise effect on the exothermic CSTR

The fitted curves and the residual graphs of the exothermic CSTR when $\sigma = 2$ are represented in Figure 7.
As the previous case of the exothermic CSTR, the estimated parameters are computed using the fminsearch function in scilab. The obtained estimated pre-exponential Arrhenius reaction rate is greater than its experimental parameter but converges to its fixed value $k_0 = 0.9$ with the small difference of 0.0006. The estimated activation energy is negative and greater than its fixed value in absolute value. However, it is the closest result in absolute value obtained compared to the other results obtained in this research. To quantify how good the fit is in Figure 7, we based on the variation of the residuals and the squared residuals of the components (variables) of the models. In sub-plot (2), the concentration and temperature residuals are located in a range of $[-4.5, 4.85]$, but more of them are accumulated in interval $[-1, 1]$. Therefore, not much deviation between observations and estimated values were observed. Again, the squared residuals of the concentration vary in the range of 0 and 23.2 with the mean value of 3.6297, while the squared residuals of the temperature vary in a range of $[0, 23.4]$ with the mean value of 3.63. The squared residuals of cooling temperature vary around zero with a negligible mean value of 0.0000020521 as it could not be seen on the squared residuals graph. An enormous number of data points among a hundred fit the curves.
Figure 8: Graphs showing the fitted curves of exothermic CSTR model. Sub-plot (1) shows the fitted temperature and concentration. Sub-plot (2) represents the residuals while sub-plot (3) shows the squared residuals of concentration and temperature. The fixed parameters are $k_0 = 0.9$, $E = 0.5$ and the estimated parameters become $k_0 = 0.903$, $E = -131.54$. The noise level is determined by $\sigma = 10$.

From Figure 8, the simulations show that the pre-exponential Arrhenius reaction rate converges to its fixed value with the difference of 0.003 while the activation energy becomes high in the negative sense. The squared residuals of the concentration and temperature vary in intervals $[0, 580.4]$ and $[0, 585.3]$ with the mean values of 90.74 and 90.75 respectively, as seen in sub-plot (3). The squared residuals of the cooling temperature vary around 0 but with the mean value of 0.0000509, which cannot be seen on the squared residuals graph. The scale of residuals has increased from $-22$ to $24$ with more of them between $[-5, 5]$. Therefore, the difference between the observations and the estimated values is large as may be viewed in Figure 8. As a consequence, a small number of data points among a hundred fit the concentration and temperature curves.

### 4.4 Quasi random noise effect on the endothermic CSTR

The endothermic CSTR fitted curves, residual graphs and its estimated parameters with $\sigma = 2$ and $\sigma = 10$ are visualized in Figure 9 and Figure 10 respectively.
Figure 9: Graph (1) represents the model fitting, graph (2) represents the residuals, graphs (3) and (4) show the squared residuals of concentration and temperature respectively. Level of noise is $\sigma = 2$ and the experimental parameters involved in numerical simulations are $k_0 = 0.4$ and $E = 0.5$. Estimated parameters from Minimization Assimilation method become $k_0 = 0.4008$ and $E = -144.1007$.

Figure 10: Sub-plot (1) represents the model fitting, sub-plot (2) represents the residuals while sub-plots (3) and (4) show the squared residuals of concentration and temperature respectively. Level of noise is $\sigma = 10$ and the experimental parameters involved in numerical simulations are $k_0 = 0.4$ and $E = 0.5$. Estimated parameters from Minimization Assimilation method become $k_0 = 0.4037$ and $E = -705.8411$. 
It is clear that the values of the estimated activation energy has increased in the absolute value compared to the result obtained from Figure 9. However, the pre-exponential Arrhenius reaction rate converges to its fixed value with the difference error of 0.0037. The difference between the observations and the estimated solutions is significant as the concentration and temperature residuals vary between $-22$ and $24$ with most of them accumulated in $[-5, 5]$. The variations of squared residuals of the concentration and temperature become $[0, 580.2]$ and $[0, 585.2]$ with the mean values of $90.7415$ and $90.7572$ respectively, and hence slightly increase. The mean value of the squared residuals of the heating temperature for this case is $0.00001911$, which allows the squared residuals of the heating temperature to be around zero and negligible. Consequently, the data points do not fit the model well compared to the fitted curves in Figure 9. This is the negative impact of high variability in the numerical solutions caused by the increase of the quasi random noise.

4.5 Systematic random noise effect on the exothermic CSTR

Figure 11 indicates the fitted exothermic CSTR models with systematic random noise produced by $\sigma = 2$, as well as the residuals on sub-plots (2) and (3).

Figure 11: Graphs representing the fitted curves of exothermic CSTR model. Sub-plot (1) shows the fitting temperature and concentration curves. Sub-plots (2) and (3) respectively show the residuals and squared residuals. The fixed parameters involved in data Assimilation are $k_0 = 0.9$, $E = 0.5$ and the obtained estimated parameters are $k_0 = 0.8893$, $E = 65.5958$. The level of systematic noise is determined by $\sigma = 2$. 
The results show that the parameter for the activation energy does not converge to the fixed value. Nevertheless, it is the second among the smallest estimated activation energy values in this research. The pre-exponential Arrhenius reaction rate converges to the fixed parameter with the difference error of 0.0107. The concentration residuals are spreading in a range of $[-0.7, 1.2]$, but more among them are accumulated in $[-0.5, 0.5]$. On the other hand, the temperature residuals are varying in a range of $[0.2, 2.14]$ with a big number of them in the scale of $[0.5, 1.5]$. Therefore, small differences between solutions of concentrations, temperatures and their estimated values are experienced in a system. From sub-plot (3), the squared residuals of the concentration vary in the range $[0, 1.5146]$ with the mean value of 0.349 while the squared residuals of the temperature range from 0 up to 4.5929 with the mean value of 1.6231. The squared residuals for the cooling temperature are varying around zero with the mean value of 0.0045. As the residual values and their mean values are small, then, all hundred data points fit the model as it is shown in Figure 11.

The same fitted and residual graphs but different standard deviation $\sigma = 10$, are shown in Figure 12.

![Figure 12](image-url)

Figure 12: Graphs representing the fitted curves of exothermic CSTR model. Sub-plot (1) shows the fitting temperature and concentration curves. Subplots (2) and (3) respectively show the residuals and squared residuals. The fixed parameters involved are $k_0 = 0.9$, $E = 0.5$ and estimated parameters are $k_0 = 0.847$, $E = 364.97$. The level of systematic random noise is determined by $\sigma = 10$.

In Figure 12, the result shows that the activation energy becomes large compared to its fixed parameter, but the pre-exponential Arrhenius reaction rate
seems to converge since the only difference from its estimated value is 0.053. From these estimated values, we can say that they become large compared to the results obtained in Figure 11. In sub-plot (1) of Figure 12, variability of noisy data increased in the fitting models. The scale of concentration residuals has increased from $-3.5$ to $6.15$ with an accumulation of them in the range $[-2, 2]$ while the residuals of temperature increase the scale from 0 up to 10.7 with more accumulation in $[3, 8]$. Hence, the difference between the observations and the estimated values becomes big. From sub-plot (3), the squared residuals of concentration are varying in $[0, 37.878]$ with the mean value of 8.7 and the squared residuals of the temperature are varying in a range of $[0, 114.81]$ with the mean value of 40.6 while the squared residuals of the cooling temperature vary around zero with the mean value of 0.112. Hence, the mean values of the squared residuals for the concentration and the temperature have increased. Therefore, a large number of data points does not fit the model well.

4.6 Systematic random noise effect on the endothermic CSTR

For $\sigma = 2$ also we want to find out the effect of this kind of noise on the endothermic CSTR and the fitted curves and residuals graphs are as show in Figure 13.

Figure 13: Graphs showing the fitted curves and residuals graph of endothermic CSTR model. Sub-plot (1) shows the fitted curves, sub-plots (2) and (3) represent the residuals and squared residuals respectively. In this case, the experimental parameters are $k_0 = 0.4$ and $E = 0.5$ while the estimated parameters become $k_0 = 0.388$ and $E = 1173$. Level of noise is given by $\sigma = 2$. 
In Figure 13, the rate of reaction converges to the fixed parameter with the
difference error of 0.012 but the activation energy diverges from its fixed value.
In sub-plot (2), the concentration residuals are oscillating between −0.8 and
1.6 with much accumulation in a range of [−0.5, 1] while the scale of the tem-
perature residuals is varying in [0.1, 2.1] with much accumulation in [0.5, 1.9].
Hence, there is no big difference between the observations (concentration and
temperature) and their estimated values. The plot of squared residuals shows
that the squared residuals of the concentration are varying in [0, 1.35] with the
mean value of 0.370099, while the squared residuals of temperature are varying
in [0, 4.65] with the mean value of 1.561065. The mean value of the squared
residuals of the heating temperature becomes 0.0015, which is very small. As
a result, the data points fit the model well.

Lastly, we show the effect of systematic random noise on the endothermic
CSTR model when the level of noise raised up to σ = 10.

Figure 14: Graphs showing the fitted curves and residuals graph of the en-
dothermic CSTR model. Sub-plot (1) shows the fitted curves, sub-plots (2)
and (3) represent the residuals and squared residuals respectively. In this case,
the experimental parameters are \( k_0 = 0.4 \) and \( E = 0.5 \) while the estimated
parameters become \( k_0 = 0.3442 \) and \( E = 5352.8 \). Level of noise is given by
\( \sigma = 10 \).

From Figure 14, the estimated activation energy \( E \) becomes very large,
while \( k_0 \) has known deviation of 0.0558 from its fixed value. In sub-plot (2),
the concentration residuals are oscillating in interval \([-4, 5.63]\), with more
accumulation in a scale of \([-2, 3]\) while the temperature residuals are bounded
in \([0.9, 10.73]\) with high accumulation in \([2, 9]\). Hence, most of the observations
are different from the estimated values. Also, the squared residuals of the
concentration are varying in a range of $[0, 31.7]$ with the mean value of 10.0174 whilst the squared residuals of the temperature are spreading in $[0, 115]$ with the mean value of 47.332562. The squared residuals of the heating temperature are oscillating around zero and its mean value becomes 0.0474. The range of residuals has increased and the squared residuals for concentration and temperature of the process have increased. The impact corresponds to much deviation in the model fitting as observed in Figure 14.

5 Discussions of results

The effect of 3 different kinds of noise (Random, Quasi and systematic) with different levels ($\sigma = 2, \sigma = 10$) on both exothermic and endothermic processes has been discussed in section 4. Based on simulations and parameter estimation results, it has been shown that the increase of any kind of noise into tanks alters the behaviour of the tanks. For instance, it highly changes the parameters of the models in both negative and positive directions. This causes much deviation of estimated solutions from true solutions as shown in residuals and squared residuals graphs. Furthermore, one of the tanks is more influenced by noise and that is the tank which requires endothermic reaction. More founding and explanations are summarized in Table 2.
6 Conclusion

In this paper, numerical simulations and the parameter estimation of CSTRs based on exothermic and endothermic reactions have been discussed using the Minimization Assimilation method (Least squares method). We introduced...
three types of noise with different levels $\sigma = 2$ and $\sigma = 10$ to the numerical solutions obtained by fixing parameters of the model, in order to generate six different kinds of data, taken as observations or measurements of the continuously stirred tank reactors (exothermic and endothermic CSTRs) at time $t$. This noise data helped us to simulate and estimate the parameters, where the increase of noise into the system has an impact on the parameter estimation and the model fitting as shown in simulation part. The different parameters were fixed to be $k_0 = 0.9$ and $E = 0.5$ for the CSTR with exothermic reactions and $k_0 = 0.4$, $E = 0.5$ for the CSTR with endothermic reactions and have been compared with their estimated parameter values.

The influence of noise on the parameter estimation and the fitting model for continuously stirred tank reactors was tracked, by observing the difference between the experimental parameter values and the estimated ones. The best fitting was determined by computing the variation of residuals, squared residuals and their mean values in the system. The smaller the variation and the mean values of residuals, the best fit the model. The results show that the Minimisation Assimilation Method seems to fail to provide convergent activation energies though, the pre-exponential Arrhenius reaction rate converges. Moreover, the increase of noise into the system influences the activation energy more than the pre-exponential Arrhenius reaction rate. The activation energies of endothermic CSTR show the behaviour of being influenced by the noise more than the ones of exothermic CSTR. The fact that the method failed to provide convergent values for activation energy has not, to our knowledge, been explained as our system is not identifiable. The challenge we faced in this research is to test whether our estimated parameters are robust, since this one requires the exact and real data from any known system. Therefore, the loss of information may have resulted from guessing the parameters. Further work needs to be done on this challenge by using real measurements from the known process as the case of study or by considering the other methods to prove these parameters.

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References


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