A mathematical model for the biological treatment of industrial wastewater in a reactor cascade

Rubayyi Turki Alqahtani  
*University of Wollongong, rtaa648@uowmail.edu.au*

Mark I. Nelson  
*University of Wollongong, mnelson@uow.edu.au*

Annette L. Worthy  
*University of Wollongong, annie@uow.edu.au*

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A mathematical model for the biological treatment of industrial wastewater in a reactor cascade

Abstract
Many industrial processes, particularly in the food industry, produce slurries or wastewaters containing high concentrations of biodegradable organic materials. Before these contaminated wastewaters can be discharged, the concentration of the biodegradable organic pollutant must be reduced. One way to do this is to pass the wastewater through a bioreactor containing biomass which grows through consumption of the pollutant. Anaerobic conditions are often favoured for the processing of waste materials with high levels of biodegradable organic pollutants as these can be removed with low investment and operational costs. We investigate the steady state effluent concentration leaving a cascade of two reactors. Our particular concern is the improvement in performance that can be achieved through the use of one or two recycling units. With even one settling unit, various configurations can be utilized. For instance, the unit can be placed after the first reactor and recycle back to the feed stream of the reactor. Alternatively, the unit can be placed after the second reactor and recycle back to the feed stream of this reactor. Finally, the settling unit can be placed after the second reactor and recycle back to the feed stream of the first reactor. Which of these configurations minimizes the effluent concentration leaving the cascade? Surprisingly, we find that in the general the first of these configurations produces the best results and the third configuration, which is the one more often mentioned in the literature, the worst.

Keywords
cascade, mathematical, continuous, analysis, flow, bioreactor, models, governed, contois, kinetics, two, reactor

Disciplines
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A MATHEMATICAL ANALYSIS OF CONTINUE FLOW BIOREACTOR MODELS GOVERNED BY CONTOIS KINETICS: A TWO- REACTOR CASCADE

Rubayyi T Alqahtani*, Mark I Nelson and Annette L Worthy.

School of Mathematics and Applied Statistics, University of Wollongong, Wollongong, NSW 2522 Australia

*Email: rtaa648@uow.edu.au

ABSTRACT

We analyse a model for the biological treatment of wastewater that is based upon Contois kinetics rather than the more commonly used Monod kinetics. The former growth rate law has increasingly been found to model the degradation of biodegradable organic materials. In particular, we investigate the steady state effluent concentration leaving a cascade of two reactors. Our particular concern is the improvement in performance that can be achieved through the use of one or two recycling units. With even one settling unit various configurations can be utilized. Combinations of reactors and recycle units are investigated. Surprisingly, we find that in general the performance of the reactor cascade with perfect recycle around each reactor does not produce the best performance. Also, contrary to what has been written in literature, the performance of a reactor cascade with recycle around the whole cascade does not always produce the best performance. Application of these results will lead to an improvement in the performance of reactor cascades for processes controlled by Contois kinetics.

Keywords: reactor cascade; Contois growth kinetics; Stirred tank; Water treatment.

INTRODUCTION

Many industries discharge polluted wastewater containing a large number of harmful compounds. Serious damage may result to many life forms. A solution to this problem is to clean the wastewater prior to discharge. An avenue to do this is to pass the polluted wastewater through a reactor containing biomass. The biomass grows through consumption of the pollutant. As result of growth of the biomass, more biomass and products are produced. These products are a mixture of carbon dioxide, methane, water and biological compounds.

Many models for biological wastewater use Monod kinetics. However, the Contois model (Contois, 1959) has increasingly been found to model the degradation of biodegradable organic materials (Hu et al, 2002, Nelson and Holder 2009).

In this paper, we study the behaviour of a cascade with two reactors using the Contois model (1959). Only a few studies have used the Contois model to simulate the growth bioreactor (Nelson et al. 2008), (Nelson & Holder 2009). Nelson et al (2008) investigated the behavior of a single reactor with recycle. In this study, the best performance of the reactor is obtained in the case with perfect recycle \( R_t^* =1 \) Nelson and Holder (2009) studied the behaviour of a reactor cascade of N reactor without recycle. They found at high residence times the effluent concentration is given by

\[
S_n^* \approx \frac{1}{\tau_r^n}, \quad \text{where } \tau_r \text{ is the total residence times of the cascade.}
\]
Bioreactor Geometry

In a bioreactor with recycle, the effluents emerge from the reactor and are fed into a settling unit. Microorganisms settle to the bottom of the tank from which they are recycled into the system. In this paper, we investigate how recycle affects the performance of a reactor cascade with two reactors. Our particular concern is the improvement in performance that can be achieved through the use of one or two recycling units. For instance, a settling unit can be placed after the first reactor with recycle back to the feed stream of this reactor or a unit can be placed after the second reactor with recycle back to the feed stream of this reactor. Finally, the settling unit can be placed after the second reactor with recycle back to the feed stream of the first reactor. The geometries of a two reactors cascade with recycle are demonstrated in Figure 1.

The Dimensional Model

The model for the two reactor configuration is given by the following system of equations.

A. Reactor Cascade With Recycle Around Each Reactor (figure 1a)

\[
\begin{align*}
V \frac{dS_1}{dt} &= F(S_0 - S_1) - \frac{\mu(S_1, X_1)}{\alpha} V X_1, \\
V \frac{dX_1}{dt} &= -FX_1 + V X_1 \mu(S_1, X_1) + R F(C_1 - 1)X_1 - V K_d X_1, \\
V \frac{dS_2}{dt} &= F(S_1 - S_2) - \frac{\mu(S_2, X_2)}{\alpha} V X_2, \\
V \frac{dX_2}{dt} &= F((1 + R_1(1 - C_1))X_1 - X_2) + V X_2 \mu(S_2, X_2) + R_2 F(C_2 - 1)X_2 - V K_d X_2.
\end{align*}
\]

B. Reactor Cascade With Recycle Around Whole Cascade (figure 1b)

\[
\begin{align*}
V \frac{dS_1}{dt} &= F(S_0 - S_1) - \frac{\mu(S_1, X_1)}{\alpha} V X_1 + FR(S_2 - S_1), \\
V \frac{dX_1}{dt} &= -FX_1 + \mu(S_1, X_1) V X_1 - V K_d X_1 + FR(CX_2 - X_1),
\end{align*}
\]
\[ V \frac{dS_i}{dt} = F(S_i - S_i) - \frac{\mu(S_i, X_i)}{\alpha} V X_i + FR(S_i - S_i), \quad (7) \]

\[ V \frac{dX_i}{dt} = F(X_i - X_i) + \mu(S_i, X_i)V X_i - V K_d X_i + FR(X_i - X_i). \quad (8) \]

The specific growth rate is given by

\[ \mu(S_i, X_i) = \frac{\mu_{max} S_i}{K_S X_i + S_i}, \quad (9) \]

This equation defines the specific growth rate of the microorganisms which is known as the Contois model (Contois, 1959).

The total residence time in the reactor cascade is given by

\[ \tau_i = \frac{2V}{F}. \quad (10) \]

In (1)-(8), \( F \) is the flow rate through the reactor cascade (dm³/day⁻¹), \( S_2 \) and \( S_i \) are the substrate concentration in the feed within the second and first reactors (gdm⁻³), \( S_0 \) is the concentration of substrate flowing into the first reactor of the cascade (gdm⁻³), \( K_d \) is the death coefficient (day⁻¹), \( K_i \) is the saturation constant (gdm⁻³), \( X_2 \) is the concentration of the cell mass within the second reactor (gdm⁻³), \( X_1 \) is the concentration of the cell mass within the first reactor (gdm⁻³), \( t \) is the time (day⁻¹), \( V \) is the volume of each reactor in the cascade (dm³), \( \mu \) is the specific growth rate model (day⁻¹), \( \mu_{max} \) is the maximum specific growth rate (day⁻¹), \( \alpha \) is the yield factor and \( \tau_i \) is the total residence time (day⁻¹). The maximum value of concentrating factor \( C_{i,\text{max}} \) is given by

\[ C_{i,\text{max}} = 1 + \frac{1}{R_i} \]

Parameter values for the anaerobic digestion of ice-cream wastewater are given by (Hu et al 2002)

\[ \alpha = 0.2116 \text{ (gVSS) (gCOD)}^{-1}, \quad \mu_{max} = 0.9297 \text{ (day)}^{-1}, \quad K_d = 0.0131 \text{(day)}^{-1} \]

\[ K_s = 0.4818 \text{ (gCOD)(gVSS)}^{-1}. \]

**The Nondimensional Model**

By introducing dimensionless variables: substrate concentration (\( S_i^* = S_i/S_0 \)), \( S_i^* = \frac{S_i}{S_0} \)

microorganism concentration (\( X_i^* = K_s X_i/S_0 \)), \( X_i^* = \frac{K_s X_i}{S_0} \) and time (\( \tau = \mu_{max} t \)) the system of differential equations (1)-(8) can be written in dimensionless form:

**A. Reactor Cascade With Recycle Around Each Reactor (figure 1a)**

\[ \frac{dS_i^*}{dt} = \frac{2}{\tau_i} (1 - S_i^*) - \frac{X_i^* S_i^*}{\alpha (X_i^* + S_i^*)}, \quad (11) \]

\[ \frac{dX_i^*}{dt} = - \frac{2}{\tau_i} X_i^* + \frac{X_i^* S_i^*}{X_i^* + S_i^*} + \frac{2 R_i X_i^*}{\tau_i} - K_d X_i^*, \quad (12) \]
\[
\frac{dS_i^*}{dt} = \frac{2}{\tau_i^*} (S_i^*-S_1^*) - \frac{X_i^*S_i^*}{\alpha^*(X_i^*+S_i^*)}, \quad (13)
\]
\[
\frac{dX_i^*}{dt} = \frac{2}{\tau_i^*} ((1-R_i^*)X_i^* - X_i^*) + \frac{X_i^*S_i^*}{X_i^*+S_i^*} + \frac{2R_i^*X_i^*}{\tau_i^*} - K_d^*X_i^*. \quad (14)
\]

**B. Reactor Cascade With Recycle Around Whole The Cascade (figure 1b)**

\[
\frac{dS_i^*}{dt} = \frac{2}{\tau_i^*} (1-S_i^*) - \frac{X_i^*S_i^*}{\alpha^*(X_i^*+S_i^*)} + \frac{2R}{\tau_i^*} (S_i^*-S_1^*), \quad (15)
\]
\[
\frac{dX_i^*}{dt} = - \frac{2}{\tau_i^*} X_i^* + \frac{X_i^*S_i^*}{X_i^*+S_i^*} - K_d^*X_i^* + \frac{2R}{\tau_i^*} (CX_i^*-X_i^*), \quad (16)
\]
\[
\frac{dS_2^*}{dt} = \frac{2(1+R)}{\tau_i^*} (S_2^*-S_2^*) - \frac{X_2^*S_2^*}{\alpha^*(X_2^*+S_2^*)}, \quad (17)
\]
\[
\frac{dX_2^*}{dt} = \frac{(1+R)}{\tau_i^*} (X_2^*-X_2^*) + \frac{X_2^*S_2^*}{X_2^*+S_2^*} - K_d^*X_2^*. \quad (18)
\]

Here the dimensionless parameters are: \(K_{d}^*\) (death rate \(K_{d}^* = K_{d}/\mu_{max}\)), \(R_{i}^*\) (effective recycle parameter \(R_{i}^* = R_{i}(C_{i}-1)\)), \(\alpha^*\) (yield coefficient \(\alpha^* = K_{i}\alpha\)) and \(\tau_i^*\) (total resident time in each reactor \(\tau_i^* = 2V_{max}/F\)). In model B, there are two additional parameters: \(C\) and \(R\) which define concentration factor and the recycle parameter respectively. In (11)-(18), the main and important experimental control parameter is the residence time, given in (10). For the anaerobic digestion of ice-cream wastewater we have \(\alpha^* = 0.1019\) and \(K_{d}^* = 0.0141\).

**RESULTS**

The steady-state solutions of (11–18)(11–18) (11)–(18) and their stability are determined both analytically and numerically. Steady state diagrams showing the variation of the dimensionless effluent concentration \(S_e^*\) as a function of the dimensionless total residence \(\tau_e^*\) time are plotted. It should be noted that only the stable physical meaningful solutions are presented. In section (A), reactor cascade with recycle around each reactor is considered which described by equations 11-14. In section (B), reactor cascade with recycle around whole cascade is considered which described by equations 15-18.

**A. Reactor Cascade With Recycle Around Each Reactor**

Figure 2 shows the dimensionless effluent concentration \(S_e^*\) in a cascade of two reactors with both perfect recycle around each reactor \((R_i^* = 1)\) and no recycle \((R_i^* = 0)\) and a single reactor with perfect recycle \((R_i^* = 1)\). The performance of the flow reactor with perfect recycle is superior to that of the flow reactor with no recycle but the difference in performance reduces as the dimensionless total residence time increases.
The dimensionless effluent concentration leaving the reactor cascade with perfect recycle decreases more rapidly than the dimensionless effluent concentrations leaving the single reactor with perfect recycle. Comparing the single reactor with perfect recycle and the reactor cascade with no recycle, there are three distinct regions. In the first region, washout occurs in each reactor in the cascade and the effluent concentration leaving the second reactor is the same as the pollutant concentration entering the first reactor in the cascade. In the second region, where the dimensionless total residence time is slightly larger than the washout point for a single reactor, the dimensionless effluent concentration leaving the single reactor is lower than that leaving the cascade reactor with no recycle. In the third region the performance of a single reactor with perfect recycle is superior to the reactor cascade with no recycle. In the third region where the dimensionless total residence time is slightly larger than the washout point for the two reactor cascade, the dimensionless effluent concentration leaving the two reactors cascade is lower than that leaving the single reactor.

Several recycle and reactor configurations are now considered with the aim of minimizing the effluent concentration.

**Recycle Around the Second Reactor**
It can be shown that when there is a settling unit with recycle around the second reactor the dimensionless effluent concentration leaving the cascade is minimized with perfect recycle in the settling unit \((R^*_2 = 1)\).

**Recycle Around the First Reactor**
We consider the performance of a cascade when the dimensionless effective recycle parameter in the first reactor \((R^*_1)\) is varied for a fixed value of the dimensionless effective recycle parameter in the second reactor \((R^*_2)\). Figure (3) shows the performance of the cascade as the value of \(R^*_1\) is varied for two values of \(R^*_2\). In both cases there is an optimal value of \(R^*_1, R^*_1,_{\text{min}}\) at which the dimensionless effluent concentration is minimized.
concentration is minimized. It is observed that, in this figure, $R_{1,\text{min}}^* < 1$. When $R_{2}^* = 0$, there is a critical value of $R_{1}^*$, $(R_{1,\text{max}}^*)$. When $0 < R_{1}^* < R_{1,\text{max}}^*$, recycle has a positive effect upon the dimensionless effluent concentration whereas if $R_{1,\text{max}}^* < R_{1}^* < 1$ then recycle has a negative effect upon the dimensionless effluent concentration. Figure 3 shows that when $R_{2}^* = 0$ the performance of a cascade with perfect recycle around the first reactor ($R_{1}^* = 1$) is inferior to that of a cascade with no recycle around the first reactor ($R_{1}^* = 0$). The critical value $(R_{1,\text{max}}^*)$ only exists for particular value of the dimensionless effective recycle parameter $(R_{2}^*)$. For example, when $\tau_{r}^* = 20$, the critical point $(R_{1,\text{max}}^*)$ only exists when the value of the dimensionless effective recycle parameter $(R_{2}^*)$ is sufficiently small $(0 < R_{2}^* < 0.1)$. In figure 3, the performance of a cascade with perfect recycle around the second reactor $(R_{2}^* = 1$, green line) is superior to that with no recycle $(R_{2}^* = 0$, red line). Figure 3 shows a surprising result namely that the optimal performance of a cascade with recycle around each reactor is not obtained with perfect recycle around each reactor $(R_{1}^* = R_{2}^* = 1)$. It is given instead by $R_{1}^* = R_{1,\text{min}}^*$ and $R_{2}^* = 1$ where the value $R_{1,\text{min}}^*$ must be determined for each value of $\tau_{r}^*$. 

![Figure 3](image.png)

**Fig.3** Dimensionless effluent concentrations as a function of $R_{1}^*$.

$R_{2}^* = 0$ (red line), $R_{2}^* = 1$ (green line), $\tau_{r}^* = 20$.

This outcome is a result of two competing processes. As $R_{1}^*$ increases, the dimensionless microorganisms concentration $(X_{1}^*)$ entering the second reactor (the term $(1-R_{1}^*)X_{1}^*$ in (14)) decreases. At the same time, the substrate concentration $(S_{1}^*)$ entering the second reactor also decreases. These processes have opposing effects upon the dimensionless effluent concentration leaving the second reactor. Over most values of $R_{1}^*$, the later effect dominates and the effluent concentration decreases in the second reactor. However, when $R_{1}^*$ the former affect is close to 1 dominates and the effluent concentration increases. Thus there is a competition in the second reactor
between the benefits of reducing the dimensionless substrate concentration entering the reactor and disadvantages of reducing the dimensionless microorganism concentrations entering the reactor.

**Reactor Configurations.**

In this section, five reactor configurations are considered. These are:

**Configuration a:** No recycling around each reactor \( R'_1 = R'_2 = 0 \).

**Configuration b:** Optimized recycle around the first reactor and no recycling around the second reactor \( R'_1 = R'_{1,\text{min}}, \ R'_2 = 0 \).

**Configuration c:** No recycling around the first reactor and perfect recycling around the second reactor \( R'_1 = 0, \ R'_2 = 1 \).

**Configuration d:** The optimized cascade \( R'_1 = R'_{1,\text{min}}, \ R'_2 = 1 \).

**Configuration e:** Perfect recycling around each reactor \( R'_1 = R'_2 = 1 \).

The comparison of these reactor configurations is demonstrated in Figure 4. The solutions curves in figure 4 split into two bands. The lower band contains the optimized cascade (d), the cascade with optimized recycle around the first reactor and no recycle around the second reactor (b) and the cascade with two perfect recycle units (e). The performance of the optimized cascade (d) performance is marginally superior to that of the others (b) and (e). In fact the solution curves are so close that only two of the three curves can be distinguished. The second band contains the configurations where there is one settling unit around the second reactor (c) and no settling units (a). The performance of the cascade with perfect recycle around the second reactor (c) is slightly superior to the performance of the reactor cascade without recycle (a). For sufficiently small values of the total residence time \( \tau^*_T < 2(1 - K^*_T)^{-1} \), the performance of the optimized reactor cascade with one settling unit (b and c) is significantly better than that of a cascade with no recycle (a). For large value of the total residence time the performance of cascade with no recycle (a) converges to the same performance of the optimized cascade with perfect recycle around the second reactor (c). For large residence time, the performance of the optimized cascade with recycle around the first reactor (b) converges to the same performance of the optimized cascade (d). Consequently, at high total residence time there is little gained in using a cascade with one settling unit compared to using a cascade with no settling units.
Fig. 4  Dimensionless effluent concentration in a cascade of two reactors as function of Dimensionless total residence time where (a) $R_1^* = R_2^* = 0$, (b) $R_1^* = R_{1,\min}^*$, $R_2^* = 0$, (c) $R_1^* = 0$, $R_2^* = 1$, (d) $R_1^* = R_{1,\min}^*$, $R_2^* = 1$ and (e) $R_1^* = R_2^* = 1$.

Table 1 shows the residence time required to achieve a specified dimensionless effluent concentration for various reactor configurations. It can be seen that there is a small gain in optimizing the performance of the cascade compared to having two settling unit with perfect recycle.

**Tab.1**: The dimensionless total residence times that is required to reach specific levels of the dimensionless effluent concentration.

<table>
<thead>
<tr>
<th>Total residence time</th>
<th>Double reactors</th>
<th>Single reactor</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$S_e^*$</td>
<td></td>
</tr>
<tr>
<td>$R_1^* = R_{\min}^<em>$, EMBED Equation. 3 $R_2^</em> = 1$</td>
<td>$R_1^* = 1$, EMBED Equation.3 $R_2^* = 1$</td>
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</table>

**B. Reactor Cascade With Recycle Around the whole Cascades**

Figure 5 shows the dimensionless effluent concentration as a function of the dimensionless total residence time when there is recycle around the whole cascade with $R=0$, 0.2, 0.5 and 1, respectively. It can be seen that there are three distinct regions. Region 1 corresponds to the case when the washout occurs through the reactor cascade. As $R$ increases from 0 to 1, the value of washout point decreases. Region 2 is where the performance of the cascade with recycle is superior to the performance of the reactor.
cascade without recycle. In this region as the recycle parameter ($R$) increases, the performance of the reactor improves. This region finishes when the dimensionless effluent concentration curve with ($R > 0$) intersects the dimensionless effluent concentration with value of $R = 0$.

Fig.5 Dimensionless effluent concentration in a cascade of two reactors with recycles around the cascade as function of dimensionless total residence time. The value of parameters: $R =$ (red) 0, (green) 0.2, (blue) 0.5 and (rose) 1, $C =$ (left) 1, (right) 2.

This intersection point ($t^*_{cr}$) marks the point at which the effect of recycle (R) the reactor performance changes from positive to negative. Region 3 is $t^*_{cr} < t^*_{t}$. This is where recycle has negative effect upon the dimensionless effluent concentration. For a fixed value of dimensionless total residence time, an increase in the recycle parameter ($R$) causes an increase in the dimensionless effluent concentration ($S^*_2$). Figure 5 (right) shows that increasing the concentration factor ($C$) in (16) cause the dimensionless effluent concentration to decreases.

Comparisons between the two reactor configurations.

Figure 6 shows that the dimensionless effluent concentration leaving a cascade with perfect recycle around the second reactor (configuration A) and leaving a reactor cascade with recycle around the whole cascade (configuration B). In this figure the choice of the parameter values ($R = 1, C = 2$) gives the perfect recycle around the second reactor. It can be seen that there are two distinct regions. In the first region, the performance of the reactor cascade with recycle around the whole cascade is superior to the performance of that with perfect recycle around the second reactor. In the second region, the performance of the reactor cascade with recycle around the whole cascade is inferior to the performance of that with perfect recycle around the second reactor.
Fig.6 Dimensionless effluent concentration in a cascade of two reactors with recycles. The value of parameters: $R = 1$, $C = 2$.

Consequently, the choice of reactor configuration depends upon the desired effluent concentration. If the designed effluent concentration is greater than the intersect point ($\tau_i^* < 4.1$) then configuration (B) should be chosen. If the designed effluent concentration is smaller than the intersect point ($\tau_i^* > 4.1$) then configuration (A) should be chosen.

**CONCLUSION**

In this paper we investigated how the use of settling units affects the behavior of a cascade of two reactors. Two recycle configurations are considered: in the first the recycle stream from reactor $i$ ($i = 1, 2$) enters the feed stream of reactor $i$; in the second the recycle stream from the second reactor enters the feed stream of the first reactor. When two settling units are deployed in the first configuration, a surprising result is found that the optimized performance of the reactor cascade occurs with perfect recycle around the second reactor and imperfect recycle around the first reactor. As the total residence time increase to infinity the optimized recycle parameter around the first reactor ($R_{i, \text{min}}^*$) convergences to zero. When only one settling units is employed we found that the performance of the reactor cascade with perfect recycle around the second reactor is inferior to a reactor cascade with optimized recycle around the first reactor at lower total residence times.

We compared the performance of the reactor configuration with recycle around the whole reactor cascade with the performance of the cascade with perfect recycle around the second reactor. We found that at low total residence time the performance of the former is superior. At high total residence time, it is better to have recycle around the second reactor.

Finally it is interesting to consider the question as to whether it is better to have a settling unit or than to have a third reactor.

The decision to either add a third reactor or a settling unit to a cascade of two reactors depends upon the desired effluent concentration. The total residence time required to reach an effluent concentration (0.1, 0.01 and 0.001) in a three reactor cascade without recycle are 3.0521, 3.2345 and 4.3063 respectively. Comparing to the data in the table 1, we reach the conclusion that when the designed effluent concentration is greater than 0.01, then a settling unit should be added to the cascade of two reactors. If the designed
effluent concentration is smaller than 0.01, then the choice of adding one reactor to the cascade should be made.

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REFERENCES

BRIEF BIOGRAPHY OF PRESENTER
Rubayyi is a PhD student in the school of mathematics and applied statistics at Wollongong University. In 2009, he a gained master degree in applied mathematics from Wollongong University with distinction. In 2007, he a gained a bachelor in mathematics from King Saud University with high distinction. He spent a year at King Faisal University as teacher.