Employing fixed point approach in Altering JS-metric space to continuous stirred chemical reactor for solving chemical reaction kinetics

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Abstract: The article examines the existence of solution to a chemical reaction modelled in an adiabatic continuous stirred chemical reactor by employing the fixed point approach in an Altering JS-metric space.

1.Introduction:

Chemical Engineering frequently employs integral equations, in particular for the design and analysis of nuclear reactors. In a chemical reactor, the behaviour of the system is usually expressed by a set of ordinary differential equations (ODEs) [3] or partial differential equations (PDEs) [7]. Nevertheless, these equations may be challenging to analytically solve, particularly if the system behaves nonlinearly or has complicated geometry. An alternative strategy for this issue is by converting those ODEs or PDEs into integral equations that can be solved numerically [2, 5, 6]. Generalised metric spaces [9] are widely employed in chemical engineering to explain systems that display complex behaviour, like systems with fractal-like geometry or non-Newtonian fluids [7]. We have considered an extended metric, Altering JS-metric. This article will examine the applications of integral equations to a chemical reactor in an Altering JS-metric space.

Let the model of adiabatic continuous stirred chemical reactor which processes a chemical reaction be considered. The model can be represented by an integro differential equation given as

$$r'(a) = \gamma_b^a + \int_{k_1}^{k_2} \frac{\partial}{\partial a} \mathcal{F}\big(a, b, r(b)\big) db$$

where $\gamma_b^a = \mathcal{F}(a,b,y)\frac{dy}{da} - \mathcal{F}(a,b,x)\frac{dx}{da}$, $r(a)$is a function that represents steady state temperatureand the factors a, b denotes the reactants number in the presence of impeller (stirrer). On integrating, this equation becomes,

$$r(a) = \int_{k_1}^{k_2} \Gamma\big(a, b, r(b)\big) db, \quad a, b \in [k_1, k_2] \tag{1}$$

which is considered in the space of all continuous real-valued functions defined on the interval$[k_1, k_2]$ and $\Gamma: [k_1, k_2] \times [k_1, k_2] \times \mathbb{R} \longrightarrow \mathbb{R}$ is a continuous non-negative function.

It can be shown through the fixed point methods that this integral equation has a solution which in turn will ensure the solution for the chemical reactor model.

The Altering JS-metric space [8] is utilised to ensure the existence of solution to the system. The following definitions of altering distance function in the sense of Khan and Altering JS-metric space are required for the understanding of further results.

2. Preliminaries:

Definition 2.1. [4] A non-negative map $\omega: [0, \infty) \to [0, \infty)$is an altering distance function if

(1)ω is continuous and monotonically non-decreasing,

(2)$\omega(t) = 0 \Leftrightarrow t = 0$,

(3)$ht^r \leq \omega(t)$; for all $t > 0$ and $h, r > 0$ are constants.

Let Ψ denote the set of all altering distance functions.

For every $r \in S$, let the set $C(J_\phi, S, r)$ be as given below:

$$C(J_\phi, S, r) = \left\{\{r_n\} \subseteq S: \lim_{n\to\infty} J_\phi(r_n, r) = 0\right\}$$

Definition 2.2. [8] Let S be a non-empty set and $J_\phi : S \times S \longrightarrow [0, \infty]$be a function. We say thatJ_ϕ is an Altering JS-metric on S if it satisfies the following axioms. For $r, s \in S$,

(A1)$J_\phi(r, s) = 0 \Longrightarrow r = s$,

(A2)$J_\phi(r, s) = J_\phi(s, r)$,

(A3)there exists $\phi \in \Psi$, and a constant $\lambda > 0$ such that,

$$r, s \in S, \{r_n\} \in C(J_\phi, S, r) \Rightarrow \phi\left(J_\phi(r, s)\right) \leq \limsup_{n\to\infty} \phi[\lambda. J_\phi(r_n, s)]$$

The pair (S, J_ϕ) is said to be an Altering JS-metric space. If the set $C(J_\phi, S, r)$is empty for every element of S, then (S, J_ϕ) becomes an Altering JS-metric space if and only if the axioms (A1) and (A2) are satisfied.

Example 2.3. Consider the set $S = \mathbb{R}$ and the function $J_\phi: S \times S \longrightarrow [0, \infty]$given by

$J_\phi(r, s) = \mid r \mid + \mid s \mid$. Then,

(i) $J_\phi(r, s) = \mid r \mid + \mid s \mid = 0 \Rightarrow r = s = 0$

(ii) $J_\phi(r, s) = \mid r \mid + \mid s \mid = \mid s \mid + \mid r \mid = J_\phi(s, r)$

(iii) It can be observed that the set $C(J_\phi, S, r)$ is non-empty for only $r = 0$ since forany$r \neq 0$, $\lim_{n\to\infty} J_\phi(r_n, r) = \lim_{n\to\infty}[\mid r_n \mid + \mid r \mid] \neq 0$ and hence let $\{r_n\} \in C(J_\phi, S, 0)$ and $s \in S$.

$$\begin{aligned} J_\phi(0, s) &= \mid 0 \mid + \mid s \mid = \mid s \mid \\ &= \lim_{n\to\infty} \mid r_n \mid + \mid s \mid \\ &= \lim_{n\to\infty} [\mid r_n \mid + \mid s \mid] \end{aligned}$$

$$J_\phi(0,s) \le \limsup_{n\to\infty}[| r_n | + | s |]$$

For any positive $\lambda > 1$, we have,

$$J_\phi(0,s) \le \lambda . \limsup_{n\to\infty}[| r_n | + | s |]$$

$$J_\phi(0,s) \le \limsup_{n\to\infty}\{\lambda\, [| r_n | + | s |]\}$$

For any $\phi \in \Psi$, we get,

$$\phi\{J_\phi(0,s)\} \le \phi\left\{\limsup_{n\to\infty} \lambda\, [| r_n | + | s |]\right\}$$

$$\phi\{J_\phi(0,s)\} \le \limsup_{n\to\infty} \phi\{\lambda\, [| r_n | + | s |]\}$$

Then $(\mathbb{R}, J_\phi)$ is an Altering JS-metric space.

Definition 2.4. [1] Banach contraction mapping is a self-map $T : S \to S$ over the completemetricspace (S, d) satisfying the contraction condition:

$$d(Tr, Ts) \le \delta d(r, s), for\ r, s \in S\ and\ \delta \in [0, 1)$$

The Banach type contraction is an extension of the above contraction map in the extended metric space and the subsequent result holds.

Theorem 2.5. Let (S, J_ϕ) be a complete Altering JS-metric space with the iterative sequence $\{r_n\}$in S, defined by $r_n = Tr_{n-1} = T^n r_0, n \in N$ where $r_0 \in S$ and $T : S \to S$ is a Banach type contraction mapping such that $J_\phi(r_0, T^n r_0) < \infty$. Then, the sequence$\{r_n\}$converges to the unique fixed point r of the mapping T.

3. Applications of integral equations in Altering JS-metric space to a chemical reactor

The Altering JS-metric space given below is considered for the model defined.

$$J_\phi(r,s) = | r | + | s | = \sup_{a\in[k_1,k_2]}\{| r\,(a)| + | s(a) |\}, \text{ for } r, s \in S$$

where S is the set of all continuous real-valued functions defined on the interval $[k_1, k_2]$. Then,(S, J_ϕ) is a complete Altering JS-metric space.

Let us consider the integral equation (1). Also consider an operator $T: S \to S$ defined as:

$$Tr(a) = \int_{k_1}^{k_2} \Gamma\big(a, b, r(b)\big)db, \quad a, b \in [k_1, k_2] \qquad (2)$$

where$\Gamma: [k_1, k_2] \times [k_1, k_2] \times \mathbb{R} \longrightarrow \mathbb{R}$ is a continuous non-negative function.

It can be seen that the fixed point of the operator T becomes the solution of the integral equation. Thus, it is enough to prove the existence of the fixed point for the operator T.

Theorem 3.1. Assume that there exists a $\delta > 0$ such that$\delta < \frac{1}{k_2-k_1}$ and $\Gamma\big(a, b, r(b)\big) \le \delta r(b)$almost everywhere. Then the operator T given by equation (2) has a unique fixed point.

Proof.

$$J_\phi(Tr,T^2r)=\sup_{a\in[k_1,k_2]}\left\{\left|\int_{k_1}^{k_2}\Gamma\big(a,b,r(b)\big)db\right|+\left|\int_{k_1}^{k_2}\Gamma\big(a,b,Tr(b)\big)db\right|\right\}$$

$$\leq\delta\sup_{a\in[k_1,k_2]}\left\{\left|\int_{k_1}^{k_2}r(b)db\right|+\left|\int_{k_1}^{k_2}Tr(b)db\right|\right\}$$

$$\leq\delta'\sup_{a\in[k_1,k_2]}\{|r|+|T(r)|\},\qquad \text{where } \delta'=\delta(k_2-k_1)$$

$$\leq\delta' J_\phi(r,Tr)$$

Hence, all the conditions of Theorem 2.5 are satisfied. Thus, the integral operator T has a unique fixed point which in turn implies that the integral equation (1) has a unique solution.

Now, for the system whose model results in the following integral equation, the solution can be ensured as follows.

$$r(a)=g(a)+\int_{k_1}^{k_2}\Gamma\big(a,b,r(b)\big)db,\quad a,b\in[k_1,k_2] \tag{3}$$

where $g:[k_1,k_2]\to(0,\alpha)$, $\alpha$is a real number and $\Gamma:[k_1,k_2]\times[k_1,k_2]\times\mathbb{R}\longrightarrow\mathbb{R}$are continuous non-negative functions.

Let $T:S\to S$ be an integral operator given by

$$Tr(a)=g(a)+\int_{k_1}^{k_2}\Gamma\big(a,b,r(b)\big)db,\quad a,b\in[k_1,k_2] \tag{4}$$

where $g:[k_1,k_2]\to(0,\alpha)$, $\alpha$is a real number and $\Gamma:[k_1,k_2]\times[k_1,k_2]\times\mathbb{R}\longrightarrow\mathbb{R}$ are continuous non-negative functions.Let us prove that equation (3) has a unique solution.

Theorem 3.2. Suppose that $T:S\to S$ be the operator given by equation (4). Assume that$\Gamma\big(a,b,r(b)\big)\leq\alpha\, r(b)$, for every $r\in S$ and $a,b\in[k_1,k_2]$, where α is chosen in such a way that $\alpha<\frac{1}{4v}$, $v=\lceil k_2-k_1\rceil$. Then T has a unique fixed point.

Proof.

$$J_\phi(Tr,Ts)=\sup_{a,b\in[k_1,k_2]}\{|Tr(a)|+|Ts(a)|\}$$

$$=\sup_{a,b\in[k_1,k_2]}\left\{\left|g(a)+\int_{k_1}^{k_2}\Gamma\big(a,b,r(b)\big)db\right|+\left|g(a)+\int_{k_1}^{k_2}\Gamma\big(a,b,s(b)\big)db\right|\right\}$$

$$\leq\sup_{a,b\in[k_1,k_2]}\left\{|g(a)|+\left|\alpha\int_{k_1}^{k_2}r(b)db\right|+|g(a)|+\left|\alpha\int_{k_1}^{k_2}s(b)db\right|\right\}$$

$$= \sup_{a,b\in[k_1,k_2]} \left\{ 2|g(a)| + \left| \alpha \int_{k_1}^{k_2} r(b)db \right| + \left| \alpha \int_{k_1}^{k_2} s(b)db \right| \right\}$$

$$\leq \sup_{a,b\in[k_1,k_2]} \left\{ 2|g(a)| + |\alpha| \left[\left| \int_{k_1}^{k_2} r(b)db \right| + \left| \int_{k_1}^{k_2} s(b)db \right| \right] \right\}$$

$$\leq 2\alpha + \sup_{b\in[k_1,k_2]} \left\{ |\alpha| \left[\left| \int_{k_1}^{k_2} r(b)db \right| + \left| \int_{k_1}^{k_2} s(b)db \right| \right] \right\}$$

$$\leq 2\alpha + \sup_{b\in[k_1,k_2]} \{\alpha[|r(b)|(k_2 - k_1) + |s(b)|(k_2 - k_1)]\}$$

$$= 2\alpha + \alpha(k_2 - k_1) \sup_{b\in[k_1,k_2]} \{|r(b)| + |\, s(b)|\}$$

$$= \alpha(2 + k_2 - k_1) \sup_{b\in[k_1,k_2]} \{|r(b)| + |\, s(b)|\}$$

$$= \delta J_\phi(r,s)$$

Where $\delta = \alpha(2 + k_2 - k_1) < 1$.Hence, it satisfies all the conditions of theorem 2.5 and hence, the operator T has a unique fixed point.

In general, for the n-dimensional integral equation

$$r(a_1, a_2, \dots, a_n) = g(a_1, a_2, \dots, a_n) + \int_{k_1}^{k_2} \int_{k_1}^{k_2} \dots \int_{k_1}^{k_2} \Gamma\big(a, b, r(a_1, a_2, \dots a_n)\big) da_1 da_2 \dots da_n$$

$a_i, a, b \in [k_1, k_2]$ (5)

where $g: [k_1, k_2] \times [k_1, k_2] \times \dots [k_1, k_2](n\ times) \to (0, \alpha)$, $\alpha$is a real number and $\Gamma: [k_1, k_2] \times [k_1, k_2] \times \mathbb{R} \longrightarrow \mathbb{R}$ are continuous bounded non-negative functions.

Let S be the set of all continuous bounded real-valued functionsdefined on$[k_1, k_2] \times [k_1, k_2] \times \dots [k_1, k_2](n\ times)$.Define the Altering JS-metric defined as in the above theorems. Let $T: S \to S$ be the integral operator given by

$$Tr(a_1, a_2, \dots, a_n) = g(a_1, a_2, \dots, a_n) + \int_{k_1}^{k_2} \int_{k_1}^{k_2} \dots \int_{k_1}^{k_2} \Gamma\big(a, b, r(a_1, a_2, \dots a_n)\big) da_1 da_2 \dots da_n$$

$a_i, a, b \in [k_1, k_2]$(6)

where $g: [k_1, k_2] \times [k_1, k_2] \times \dots [k_1, k_2](n\ times) \to (0, \alpha)$, $\alpha$is a real numberand
$\Gamma: [k_1, k_2] \times [k_1, k_2] \times \mathbb{R} \longrightarrow \mathbb{R}$ are continuous bounded non-negative functions.

Theorem 3.3. The operator $T : S \to S$ given by equation (6) has a unique fixed point if

$\Gamma\big(a,b,r(a_1,a_2,\dots a_n)\big) \le \alpha . r(a_1,a_2,\dots,a_n)$ for every $r \in S$ and $a,b,a_i \in [k_1,k_2]$ where α is chosen in such a way that $\alpha < \frac{1}{(n+3)v^n}$ where $v = \lceil k_2 - k_1 \rceil$.

Proof.

$$J_\phi(Tr,Ts) = \sup_{a_i\in[k_1,k_2]} \{|Tr(a_1,a_2,\dots a_n)| + |Ts(a_1,a_2,\dots a_n)|\}$$

$$= \sup_{a_i\in[k_1,k_2]} \left\{ \begin{array}{l} \left| g(a_1,a_2,\dots,a_n) + \int_{k_1}^{k_2}\int_{k_1}^{k_2}\dots\int_{k_1}^{k_2} \Gamma\big(a,b,r(a_1,a_2,\dots a_n)\big) da_1 da_2 \dots da_n \right| \\ + \left| g(a_1,a_2,\dots,a_n) + \int_{k_1}^{k_2}\int_{k_1}^{k_2}\dots\int_{k_1}^{k_2} \Gamma\big(a,b,s(a_1,a_2,\dots a_n)\big) da_1 da_2 \dots da_n \right| \end{array} \right\}$$

$$\le \sup_{a_i\in[k_1,k_2]} \left\{ \begin{array}{l} |g(a_1,a_2,\dots,a_n)| + \left| \int_{k_1}^{k_2}\int_{k_1}^{k_2}\dots\int_{k_1}^{k_2} \Gamma\big(a,b,r(a_1,a_2,\dots a_n)\big) da_1 da_2 \dots da_n \right| \\ + \quad |g(a_1,a_2,\dots,a_n)| \\ + \left| \int_{k_1}^{k_2}\int_{k_1}^{k_2}\dots\int_{k_1}^{k_2} \Gamma\big(a,b,s(a_1,a_2,\dots a_n)\big) da_1 da_2 \dots da_n \right| \end{array} \right\}$$

$$\le \sup_{a_i\in[k_1,k_2]} \left\{ \begin{array}{l} 2g(a_1,a_2,\dots a_n) + \alpha \left| \int_{k_1}^{k_2}\int_{k_1}^{k_2}\dots\int_{k_1}^{k_2} r(a_1,a_2,\dots a_n) da_1 da_2 \dots da_n \right| \\ + \alpha \left| \int_{k_1}^{k_2}\int_{k_1}^{k_2}\dots\int_{k_1}^{k_2} s(a_1,a_2,\dots a_n)\, da_1 da_2 \dots da_n \right| \end{array} \right\}$$

$$\le 2\alpha + \sup_{a_i\in[k_1,k_2]} \left\{ \begin{array}{l} \alpha \left| \int_{k_1}^{k_2}\int_{k_1}^{k_2}\dots\int_{k_1}^{k_2} r(a_1,a_2,\dots a_n)\, da_1 da_2 \dots da_n \right| \\ + \quad \alpha \left| \int_{k_1}^{k_2}\int_{k_1}^{k_2}\dots\int_{k_1}^{k_2} s(a_1,a_2,\dots a_n)\, da_1 da_2 \dots da_n \right| \end{array} \right\}$$

$$\le 2\alpha + \alpha \sup_{a_i\in[k_1,k_2]} \left\{ \begin{array}{l} \left| \int_{k_1}^{k_2}\int_{k_1}^{k_2}\dots\int_{k_1}^{k_2} r(a_1,a_2,\dots a_n)\, da_1 da_2 \dots da_n \right| \\ + \quad \left| \int_{k_1}^{k_2}\int_{k_1}^{k_2}\dots\int_{k_1}^{k_2} s(a_1,a_2,\dots a_n)\, da_1 da_2 \dots da_n \right| \end{array} \right\}$$

$$\le 2\alpha + \alpha \sup_{a_i\in[k_1,k_2]} \{(k_2-k_1)^n |r(a_1,a_2,\dots a_n)| + (k_2-k_1)^n |s(a_1,a_2,\dots a_n)|\}$$

$$\leq 2\alpha + \alpha(k_2 - k_1)^n \sup_{a_i \in [k_1, k_2]} \{|r(a_1, a_2, \dots a_n)| + |s(a_1, a_2, \dots a_n)|\}$$

$$\leq \alpha[2 + (k_2 - k_1)^n] \sup_{a_i \in [k_1, k_2]} \{|r(a_1, a_2, \dots a_n)| + |s(a_1, a_2, \dots a_n)|\}$$

$= \delta J_\phi(r, s)$

where $\delta = \alpha[2 + (k_2 - k_1)^n] < 1$. Hence, it satisfies all the conditions of theorem 2.5 and so,the operator T has a unique fixed point.

4. Conclusion

There are a variety of chemical reactor systems in Chemical Engineering which can be modelled into an integral equation. Here in this article, we presented one such conventional approach for ensuring the existence of solution for a chemical reaction kinetics in a continuous stirred chemical reactor using the fixed point method in an Altering JS-metric space. Overall, we believe that this proposed work provides a valuable tool for researchers and practitioners in the field of chemical engineering to optimize the design and improve the eff iciency of chemical processes.

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