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# Consecutive Chemical Reactions Models via P-Fuzzy Systems

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**Abstract**. In this work we propose a p-fuzzy system to describe the dynamic of a consecutive chemical reaction model, which is given by a system of differential equations. We use Mamdani's method as a fuzzy controller based on a fuzzy rule-based system, whose fuzzy rules represent the direction field of the differential equations. Computational simulations reveal that the numerical solution via p-fuzzy system is similar to those of the classical chemical reactions. Finally, we discuss the capability of the p-fuzzy approach as approximator.

**Keywords**. Chemical Kinetics; Fuzzy Rule-Based Systems; P-Fuzzy Model.

## 1 Introduction

Chemical reactions are basically given by transformations involving one or more substances (reagents) resulting in new substances (products) with different properties of the previous ones [2]. Chemical kinetic deals with chemistry experiments and interprets them in terms of mathematical models. In particular, chemical kinetics studies the chemical reactions, as well as the factors that influence the final result [4]. Some of these factors may be given by concentration, temperature, pressure etc.

The velocity of a reaction can be calculated from the concentrations of the reagents and its orders of reactions, which are determined experimentally. Hence there may be imprecision/uncertainty in obtaining this velocity. The classic models do not consider this fact [5]. In order to describe these uncertainties the fuzzy sets theory can be used [1].

In this paper we focus on consecutive chemical reactions models. Consecutive reactions are reactions in which products are formed as intermediates, which then react further. This type of chemical reaction is described by [2]

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C, \quad \text{with reaction rates } k_1 \text{ and } k_2. \tag{1}$$

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An example of this reaction is the consecutive beta decay of an isotope of Uranium-238 into Neptunium-239 and after that into Plutonium-239, that is, ${}^{238}_{92}\mathrm{U} \xrightarrow{\beta^-} {}^{239}_{93}\mathrm{Np} \xrightarrow{\beta^-} {}^{239}_{94}\mathrm{Pu}$.

In order to describe the dynamic of the reaction (1) (as well as the concentration of the reagents), we design a fuzzy rule-based system. From these fuzzy rules, we determine the dynamic of this model via p-fuzzy system.

This work investigates the application of fuzzy set theory and it describes a simple methodology to study a chemical reagent model which can be used for any expert. We provide simulations in order to illustrate the methodology and we compare it with the analytical solution.

## 2 Mathematical Background

A fuzzy subset of $A$ of a universal set $X$ is characterized by a function $\varphi_A : X \to [0,1]$ called membership function of $A$ such that $\varphi_A(x)$ represents the membership degree of $x$ in $X$ [1]. For notation convenience, we denote $\varphi_A(x)$ by the symbol $A(x)$. Here we focus in a special class of fuzzy sets called fuzzy numbers.

In particular a trapezoidal fuzzy number $A$, denoted by a quadruple $(a; m; n; b)$, with $a, m, n, b \in \mathbb{R}$ and $a \leq m \leq n \leq b$, is defined by the following membership function

$$A(x) = \begin{cases} \frac{x-a}{m-a} & , \text{ if } x \in [a, m), \\ 1 & , \text{ if } x \in [m, n], \\ \frac{b-x}{b-n} & , \text{ if } x \in (n, b], \\ 0 & , \text{ otherwise} \end{cases} .$$

In case where $m = n$, we speak of triangular fuzzy number and it is denoted by the triple $(a; m; b)$ instead of $(a; m; m; b)$ [1].

Fuzzy Rule-Based Systems (FRBS) are organized in four components: a *fuzzification* module, a fuzzy rule-base, a fuzzy inference method, and a *defuzzification* module [6,7,10].

In the fuzzification module, real-valued inputs are translated into fuzzy sets of their respective universes. In the general case, expert knowledge plays an important role to build the membership functions for each fuzzy set associated with the inputs [6].

We consider a fuzzy rule-base given by a collection of fuzzy conditional rules of the form "if $x_1$ is $A_{i1}$ and $x_2$ is $A_{i2}$ then $y$ is $B_i$", for $i = 1, \ldots, r$, where $A_{ij}$ and $B_i$, $i = 1, \ldots, r$ and $j = 1, 2$, are fuzzy sets that represent linguistic terms. These linguistic terms $A_{ij}$ and $B_i$ are called by antecedents and consequent of each fuzzy rule, respectively [9].

In this work we use the Mamdani method as canonical inclusion fuzzifier. For a given input $(x_1, x_2)$, the Mamdani method produces the following output $B$:

$$B(y) = \max_{i=1,\ldots,r} \min\{\, A_{i1}(x_1)\,,\, A_{i2}(x_2)\,,\, B_i(y)\,\},\ \forall y \in \mathbb{R}\,. \tag{2}$$

The defuzzification module consists of representing a fuzzy set by a real value [6].

A *partially* fuzzy system or, for short, a $p$-fuzzy system, is a dynamical system where the direction field is given by FRBS based on a partially a priori known of the direction field. Furthermore, the state variables and their variations are considered linguistic.

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Thus, the state variables are correlated to their variations by means of fuzzy rules where the state variables are the input and the variations are outputs. Since in such methodologies, processes of defuzzification are expected, the final solution of a $p$-fuzzy system is deterministic [8, 9].

In this work we use $p$-fuzzy systems to deal with autonomous initial value problems (IVPs) of the form

$$\begin{cases} \dfrac{dx_1}{dt} = f_1(x_1, x_2, x_3)\,, & x_1(0) = (x_1)_0\,, \\ \dfrac{dx_2}{dt} = f_2(x_1, x_2, x_3)\,, & x_2(0) = (x_2)_0\,, \\ \dfrac{dx_3}{dt} = f_3(x_1, x_2, x_3)\,, & x_3(0) = (x_3)_0\,. \end{cases} \tag{3}$$

where the functions $f_1, f_2$ and $f_3$ are partially known.

In order to obtain the solution of the IVP (3) via $p$-fuzzy system or at least an approximation of it, without knowing the field $f_1, f_2$ and $f_3$ explicitly, we take into account the qualitative information available to design a fuzzy rule-base which represents the properties that characterize the phenomenon [3].

The analytical solution $(x_1(t), x_2(t), x_3(t))$ of (3) can be estimated by a sequence $(X_1(n), X_2(n), X_3(n))$ of a $p$-fuzzy system obtained by means of numerical methods for the ordinary differential equations (ODE) such as Euler's method, which is computed by

$$X_i(n+1) = X_i(n) + h\, F_i(n) \tag{4}$$

for $i = 1, 2, 3$, where $h$ is the step (in time) and $F_i(n) = F_i(X_1(n), X_2(n), X_3(n))$ are variations rates obtained by FRBSs. Thus we can rewrite (3) as follows:

$$\begin{cases} \dfrac{dX_1}{dt} = \mathrm{FRBS}_{F_1}\,, & X_1(0) = (x_1)_0\,, \\ \dfrac{dX_2}{dt} = \mathrm{FRBS}_{F_2}\,, & X_2(0) = (x_2)_0\,, \\ \dfrac{dX_3}{dt} = \mathrm{FRBS}_{F_3}\,, & X_3(0) = (x_3)_0\,. \end{cases} \tag{5}$$

In general a Mamdani fuzzy controller yields a function $F_i = f_r^*$ (for any $i = 1, 2, 3$) where $r$ denotes the number of rules in the fuzzy rule base. Hence it seems reasonable to assume that the adjusted function $f_r^*$ approximates $f = f_i$ when the number of data $r$ increases [3].

## 3 Methodology

From the effective rate laws, the reaction (1) can be given by the following IVP [2]

$$\begin{cases} \dfrac{d[A]}{dt} = -k_1[A], & [A(0)] = [A_0] \\ \dfrac{d[B]}{dt} = k_1[A] - k_2[B], & [B(0)] = [B_0]\,, \\ \dfrac{d[C]}{dt} = k_2[B], & [C(0)] = [C_0] \end{cases} \tag{6}$$

 

where $[X]$ represents the concentration of the reagent $X$. The analytical solution for the system (6) is given by [2]

$$[A(t)] = [A_0]e^{-k_1 t}\,, \quad \big[B(t)\big] = [B_0]e^{-k_2 t} + k_1[A_0]\frac{e^{-k_1 t} - e^{-k_2 t}}{k_2 - k_1} \quad \text{and}$$
$$\big[C(t)\big] = [C_0] + [B_0](1 - e^{-k_2 t}) + [A_0]\left(1 + \frac{k_1 e^{-k_2 t} - k_2 e^{-k_1 t}}{k_2 - k_1}\right).$$

Recall that in a $p$-fuzzy system the vector fields are given by FRBSs (see Section 2). Here, we employ a $p$-fuzzy system in the form of (5) in order to estimate a solution for (6). We use the corresponding $X_1, X_2$ and $X_3$ variables to represent the $[A], [B]$ and $[C]$ chemical concentrations, respectively. The antecedents and consequents of the corresponding fuzzy rules are given by linguistic terms associated respectively with the input and output variables.

The both inputs variables can be classified by 4 linguistic terms expressed as "*low*" ($A_1$ and $B_1$), "*average low*" ($A_2$ and $B_2$), "*average high*" ($A_3$ and $B_3$) and "*high*" ($A_4$ and $B_4$). Moreover, for the output variables (the variations rates) we consider the terms expressed as "*high negative*" ($N_3$), "*average negative*" ($N_2$), "*low negative*" ($N_1$), "*low positive*" ($P_1$), "*average positive*" ($P_2$), and "*high positive*" ($P_3$). Figures 1 and 2 illustrate the form and order in which the antecedents and consequents membership functions are adjusted, respectively.

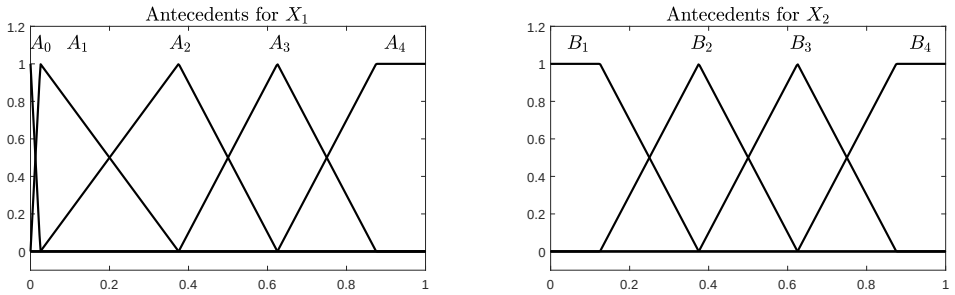


Figure 1: Antecedents (fuzzy numbers as linguistic terms) of inputs variables ($X_1$ and $X_2$) for the consecutive chemical reactions model.

We elaborate a FRBS based on the differential equations for the consecutive chemical reactions model given by (6).

Figure 3 depicts the fuzzy rule-base where the arrows represent the direction and magnitude of the variation rates, that is, the arrow on the right/up (left/down) side indicates positive (negative) variations and the length of the arrow indicates the magnitude of these variations. For this work, one rule-base is established from the graphical interpretation of Figure 3 and we use the notation $\dot{X}_i = \frac{dX_i}{dt}$, with $i = 1, 2, 3$, to represent the variational rates in the fuzzy rules. We construct a rule-base of 20 fuzzy rules of the type:

$r_1$: If $X_1$ is $A_0$ and $X_2$ is $B_1$ then $\dot{X}_1$ is $P_1$ and $\dot{X}_2$ is $N_1$ and $\dot{X}_3$ is $N_1$.

$r_2$: If $X_1$ is $A_1$ and $X_2$ is $B_1$ then $\dot{X}_1$ is $N_1$ and $\dot{X}_2$ is $P_2$ and $\dot{X}_3$ is $N_1$.

$\vdots \qquad \vdots \qquad \vdots$

 

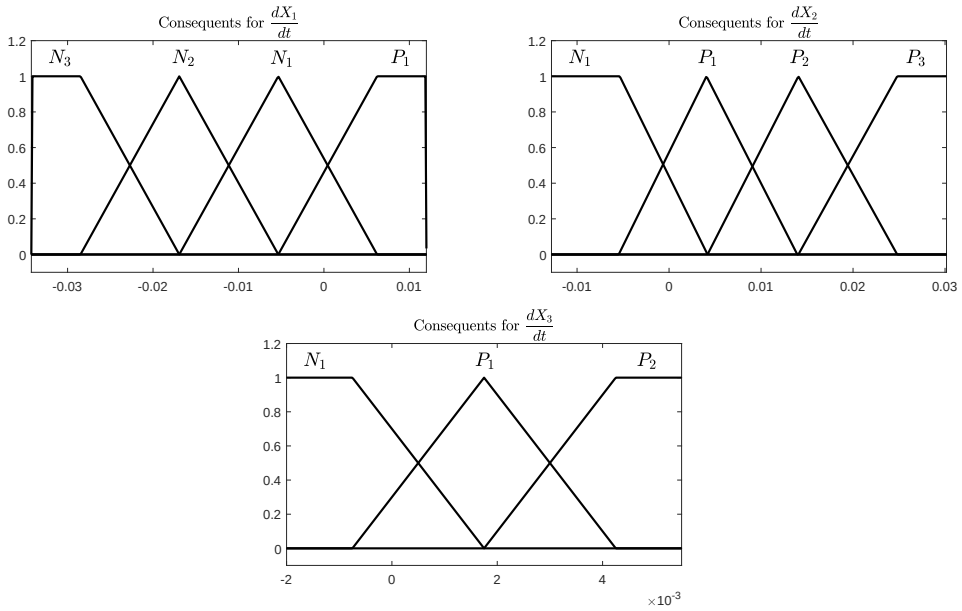


Figure 2: Consequents (fuzzy numbers as linguistic terms) of outputs variables ($\frac{dX_1}{dt}$, $\frac{dX_2}{dt}$ and $\frac{dX_3}{dt}$ ) for the consecutive chemical reactions model.

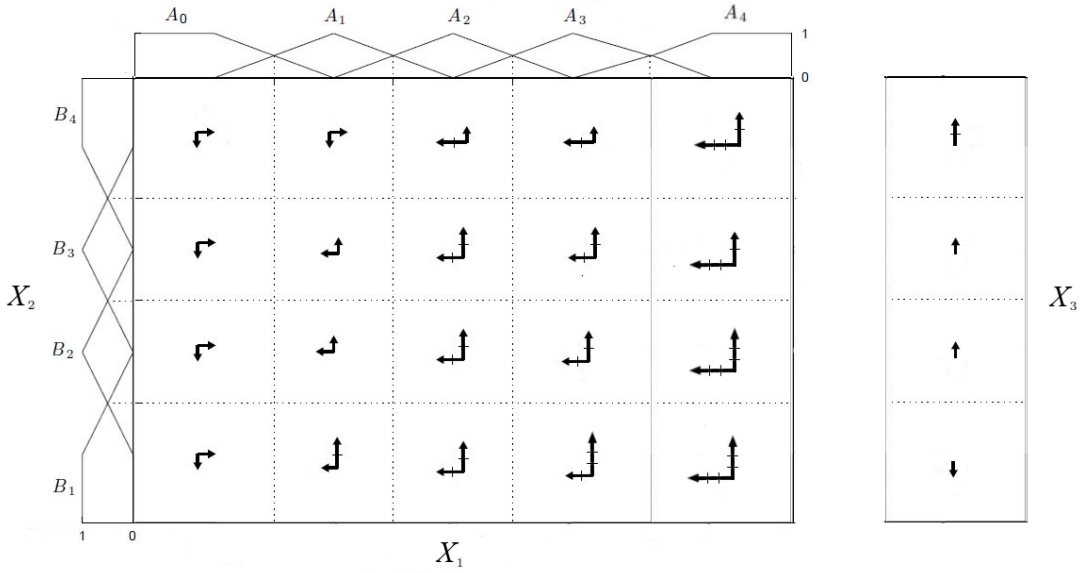


Figure 3: Graphic representation of the fuzzy rules as direction vectors for the consecutive chemical reactions model.

$r_7$: If $X_1$ is $A_1$ and $X_2$ is $B_2$ then $\dot{X}_1$ is $N_1$ and $\dot{X}_2$ is $P_1$ and $\dot{X}_3$ is $P_1$.

$r_8$: If $X_1$ is $A_2$ and $X_2$ is $B_2$ then $\dot{X}_1$ is $N_2$ and $\dot{X}_2$ is $P_2$ and $\dot{X}_3$ is $P_1$.

$\vdots \qquad \vdots \qquad \vdots$

 

$r_{13}$: If $X_1$ is $A_2$ and $X_2$ is $B_3$ then $\dot{X}_1$ is $N_2$ and $\dot{X}_2$ is $P_2$ and $\dot{X}_3$ is $P_1$.
$r_{14}$: If $X_1$ is $A_3$ and $X_2$ is $B_3$ then $\dot{X}_1$ is $N_2$ and $\dot{X}_2$ is $P_2$ and $\dot{X}_3$ is $P_1$.
$\vdots \qquad \vdots \qquad \vdots$
$r_{19}$: If $X_1$ is $A_3$ and $X_2$ is $B_4$ then $\dot{X}_1$ is $N_2$ and $\dot{X}_2$ is $P_1$ and $\dot{X}_3$ is $P_2$.
$r_{20}$: If $X_1$ is $A_4$ and $X_2$ is $B_4$ then $\dot{X}_1$ is $N_3$ and $\dot{X}_2$ is $P_2$ and $\dot{X}_3$ is $P_2$.

Once the rule base is established, we use the Mamdani (in the inference module) and the centroid (in the defuzzification module) methods. Figure 4 illustrates the scheme of the FRBS used in this work.

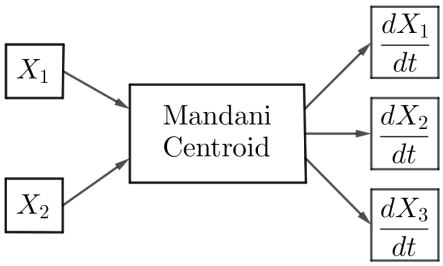


Figure 4: Fuzzy rule-based system for the consecutive chemical reactions model

### 3.1 Results

We use the proposed $p$-fuzzy system to simulate the dynamic behavior of the consecutive chemical reactions for three concentrations $[A], [B]$ and $[C]$. We compare the obtained $p$-fuzzy solution (for $X_1, X_2$ and $X_3$) with the analytical solution given by Equation (7).

Figure 5 presents the three $p$-fuzzy and analytical solutions of system (6) with initial conditions given by $[A_0] = 1, [B_0] = 0$ and $[C_0] = 0$. We can observe that the solutions are qualitative and quantitative similar with the classical solution.

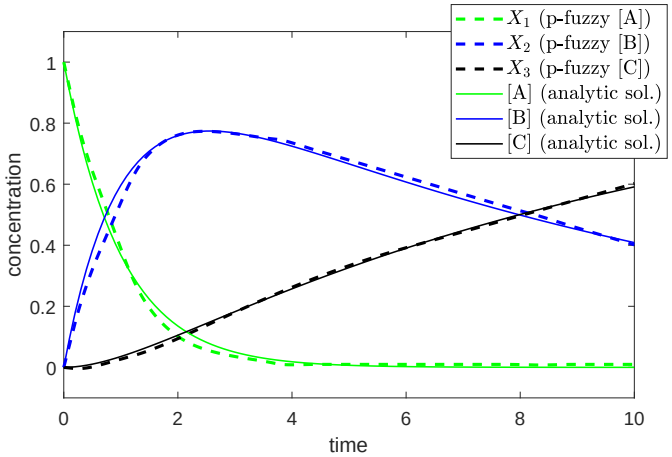


Figure 5: $p$-fuzzy and analytical solutions of IVP (6) with $[A_0] = 1, [B_0] = 0$ and $[C_0] = 0$.

 

## 4 Final Remarks

We present a $p$-fuzzy methodology, based on Fuzzy Rule-Based Systems (FRBS), to produce solutions for consecutive chemical reactions models. The solutions obtained by this approach are (quantitative and qualitative) similar to the ones via differential equations theory (see Figure 5).

Note that the proposed methodology can be used by any chemical researcher and does not require previous experience with differential equations. Finally, it should be noted that the use of the $p$-fuzzy system is based on universal approximation capability, which means that it is a good estimator of theoretical problems.

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