Motion planning for chemical systems: consecutive reactions

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Abstract: Motion planning is widely used for analyzing and controlling nonlinear systems, such as mobile robot navigation and robotic automation. When a mathematical model of the system is available, motion planning allows for system analysis and control without the need for sampling or physical intervention, thereby avoiding any disturbance to the behavior of the system. This study explores the application of motion planning methods to chemical reaction systems. Specifically, it demonstrates how to define desired trajectories for consecutive reactions using the parametrized function class method. The planning assumes isothermal conditions, which are modeled by setting the temperature as a constant time function. Under this assumption, the system describing consecutive reactions becomes linear. Starting from the kinetic model, we derive the time-dependent behavior of the state variables. Based on these results, a controller is designed for a two-step consecutive reaction. The state of the system can be determined at any time from the computed time functions, and the future behavior of the system can be accurately predicted. This approach helps prevent accidents and undesired outcomes by ensuring the reaction proceeds along the planned trajectory.

Keywords: chemical reaction; motion planning; temperature control; strong reachability; controllability

1 Introduction

The purpose of motion planning is to specify the intermediate states of the system when it moves from the initial to the final state. This can be used to estimate the internal variables without explicitly measuring them or to control the system on the desired trajectory. Internal limitations and external obstacles must be considered. The trajectories are specified from the mathematical model during the planning. The time functions of the trajectories can be used to determine where the system is

at any time, and they can help to predict when it is necessary to intervene.

Motion planning is widely used for mechatronic systems [1–5]. In the case of mechatronic systems, the trajectory means the path of the movement. The goal is to drive the robot to the desired place while avoiding obstacles. Often, the task is to determine the shortest path or a route that touches fixed points. For planning the desired trajectories, several methods and algorithms are known (e.g., genetic algorithm, particle swarm optimization algorithm [6]). Sampling-based algorithms are investigated in [7], where new algorithms are introduced and the asymptotic behavior of the cost of the solution is analyzed. The Iterative Structured Orientation is suggested as a coverage path planning strategy in [8]. Motion planning using movement primitives are presented in [9]. Mobile robots represent a special class of mechatronic systems [10–14]. They are controlled mechanical systems designed to change their position autonomously or in response to control inputs. The most commonly used motion planning methods for mobile robots are collected in [15]. A cost function-based algorithm is presented in [16], which allows using combinations of different planning strategies. A Risk-based Dual-Tree Rapidly Exploring Random Tree (DTRRT) algorithm is shown in [17]. The task is to find an optimized trajectory for the robots in dynamic environments with pedestrians. Another method for motion planning in dynamic environments is presented in [18]. Here, a first-order method is used, i.e., it is unnecessary to integrate velocities to determine the positions as time functions.

Motion planning methods can also be applied to chemical systems [19–21]. In this case, the system gets to a final concentration composition from an initial concentration composition; the trajectory means the concentration values that can be measured each time. The motion planning problem is determining the time functions that can specify the instantaneous concentration composition at any time. During the planning, limitations of the system (e.g., in the case of explosive reactions, the system cannot be heated above a specific temperature) and the external "obstacles" (e.g., fixed tank volume, pressure tolerance) must be considered. It is an understudied area; however, chemical aspects appear in the research. A survey on motion planning algorithms applied to molecular modeling is presented in [22]. It gives an overview of extensions to sampling-based motion planning methods. Motion planning for a DOC (Diesel Oxidation Catalyst) outlet temperature is shown in [23]. The method for determining the shortest collision-free path with the help of a chemical processor is investigated in [24]. This method is based on a color change during the formation of a precipitate. Robotic applications in chemical experiments are studied in [25].

We will deal with motion planning for chemical systems. For the planning, the parametrized function class method will be used [38]. The method will be presented in Section 2. The temperature is a well-changeable parameter; therefore, the rate of change of the temperature will be considered as the input of the system [26, 27].

In our work, we will study general structural consecutive reactions. In Subsection 3.1, we will specify the time functions of the state variables and the input function. As parametrized function class, we choose the time function of the temperature in parametrized form. The motion planning results can be applied for modeling. As

an example, we will model a consecutive reaction in Subsection 3.2. Based on the given results, we will design a closed-loop control [31–33] and compare it with the state feedback method.

The temperature dependence of the reaction rate coefficients causes nonlinearity in every chemical reaction. Moreover, the temperature depends on the internal states of the reaction, as well as the environmental temperature. As a result, by controlling the temperature, we can affect the reaction rate coefficient values, e.g., we can ensure that these are constants, making the system linear in Section 3.

2 Models and methods

In the following, we present the general model of chemical reactions and provide the sufficient condition of strong reachability. We interpret the trajectory for chemical systems and show a method for motion planning of chemical reactions.

2.1 General model of chemical reactions

Using conventional notations from chemistry, we present the applied mathematical model and describe the used notations. Consider a chemical system in general form [30], i.e.,

$$\sum_{m=1}^{M} \alpha(m,r)\mathrm{X}_m \xrightarrow{k_r} \sum_{m=1}^{M} \beta(m,r)\mathrm{X}_m, \quad r = 1,2,\ldots,R, \tag{1}$$

where the number of the reaction steps is denoted by $R > 0$, and the number of the species is denoted by $M > 0$. The notation k_r is used for the reaction rate coefficient in rth reaction step, and X_m denotes the mth species. The species on the left-hand side are called reactants, and the species on the right-hand side are called products. The coefficients $\alpha(m,r)$ and $\beta(m,r)$ are the corresponding elements of the reactant complex vector $\alpha(:,r)$ and the product complex vector $\beta(:,r)$, i.e.,

$$\alpha(:,r) = (\alpha(1,r),\alpha(2,r),\ldots,\alpha(m,r))^\top, \tag{2}$$

$$\beta(:,r) = (\beta(1,r),\beta(2,r),\ldots,\beta(m,r))^\top. \tag{3}$$

In order to investigate the dynamics of the system, the differential equations of the system must be known [34–36]. Considering mass action kinetics in the reaction and using the heat balance of (1), the differential equations of the system are described as

$$\dot{x}_m(t) = \sum_{r=1}^{R} \gamma(m,r)k_r(T(t))x(t)^{\alpha(\cdot,r)}, \qquad m = 1,2,\ldots,M, \tag{4}$$

$$\dot{T}(t) = \sum_{r=1}^{R} \frac{1}{\beta_{r,0}} k_r(T(t))x(t)^{\alpha(\cdot,r)} + u(t), \tag{5}$$

where $x_m(t)$ denotes the concentration of $\mathrm{X}(m)$, and $T(t)$ is the temperature at time instant $t \geq 0$. The coefficient $\gamma(m,r)$ is the corresponding element from the stoichiometric matrix γ, whose columns can be calculated as

$$\gamma(:,r) = \beta(:,r) - \alpha(:,r). \tag{6}$$

The reaction rate coefficient $k_r(T(t))$ is specified in the form

$$k_r(T(t)) = k_{r,0} e^{-\frac{E_r}{R_0 T(t)}}, \tag{7}$$

where $k_{r,0}$ is the preexponential factor, E_r is the activation energy and R_0 is the universal gas constant ($k_{r,0}, E_r, R_0 \in \mathbb{R}^+$). The expression $x(t)^{\alpha(\cdot,r)}$ denotes the product of the corresponding concentrations,

$$x(t)^{\alpha(\cdot,r)} = \prod_{p=1}^{M} x_m(t)^{\alpha(m,r)}. \tag{8}$$

The variable $u(t)$ is the single input of the investigated system. In our analysis, it is chosen as the temperature changing $\dot{T}(t)$. In the example in Subsection 3.1 we will also use the inflow of a species as control input after the system is linearized with input $\dot{T}$.

2.2 Controllability and strong reachability

During the reaction process (or the movement), the investigated system achieves from an initial to a final state. For planning the trajectories, the system must be controllable, i.e., a control input $u(t)$ must exist that generates the trajectories $\xi(t)$. More concepts of controllability are known (e.g., strong reachability, small-time local controllability, local controllability, and global controllability). In the following, we present some of them. Throughout the paper, we will give variables and functions at time instant $t \geq 0$ in order to emphasize the dependencies. The only exceptions are at the definitions of functions.

To interpret the controllability, we consider the following nonlinear dynamical system, given by the differential equation

$$\dot{\xi}(t) = f(\xi(t)) + g(\xi(t))u(t), \quad \xi(0) = \xi^* \in \mathbb{R}^n, \tag{9}$$

where $f, g \in \mathbb{C}^\infty(\mathbb{R}^n, \mathbb{R}^n)$ are smooth vector fields and $u(t) \in \mathbb{R}$ is the control input. The vector fields f and g are called drift and control vector fields, respectively. For the sake of completeness, let us now revisit some definitions that are used in the sequel [27–29].

Definition 1 (Reachability sets)**.** *Consider the system given by* (9)*. Define the following sets:*

(i) $\mathscr{R}(\xi^*, t_f) = \{\xi(t_f) |$ *the state of the system at time* t_f *with all allowed control* u *when* $\xi(0) = \xi^*$ *and* $0 < t_f < \infty\}$,

(ii) $\mathscr{R}(\xi^*) = \bigcup_{t\geq 0} \mathscr{R}(\xi^*, t)$.

Definition 2 (Controllability and reachability)**.** *System* (9) *is called*

(i) strongly reachable from the point ξ^**, if the set* $\mathscr{R}(\xi^*, t)$ *has an interior point for all* $t > 0$*,*

(ii) locally controllable from the point ξ^**, if the point* ξ^* *is an interior point of* $\mathscr{R}(\xi^*)$*,*

(iii) globally controllable from the point ξ^**, if* $\mathscr{R}(\xi^*) = \mathbb{R}^n$.

In this work, chemical reactions are investigated. The state vector can be written in form $\xi(t) = (x_1(t), x_2(t), \ldots, x_m(t), T(t))^\top$, and the dynamics of the system are described by (4)–(5). For chemical reactions, the simple sufficient condition is available for strong reachability [27]:

Theorem 1. *Consider a reaction with M species and R reaction steps. Suppose the activation energies* $E_1, E_2, \ldots, E_R$ *of the reaction steps are all different and strictly positive. Then, the reaction dynamics is strongly reachable with temperature change input* $\dot{T}(t)$ *if the concentrations of all reactant species are positive.*

A special characteristic of chemical systems is the positivity [37]. Those compounds whose initial concentration is positive are present in the system during the entire reaction process. Mathematically, their amount cannot decrease to zero at any step. In Theorem 1, we supposed that the concentration of reactant species must be positive. We note that it would be enough to assume that the concentrations of reactant species are initially positive. Then, it already follows that the reactant concentrations cannot decrease to 0 due to the positivity of chemical systems.

2.3 Motion planning

Knowing the trajectories makes it easier to investigate the behavior of a system since they can describe the state of the system at every moment. In the case of chemical reactions, the trajectories mean the concentration and temperature values that can be measured during the reaction. With the help of motion planning, we can determine the trajectories of the investigated system. We can also specify how to choose the values of the input parameters or their time functions to achieve the desired target product [38].

Consider the following nonlinear system,

$$\dot{\xi}(t) = h(\xi(t), u(t)), \tag{10}$$

where $\xi(t) \in X \subseteq \mathbb{R}^n$, $u(t) \in \mathbb{R}^J$ and $t \in \mathbb{R}_0^+$. Suppose we plan a path connecting initial point $\xi_0 = \xi(t_0) \in X$ and final point $\xi_f = \xi(t_f) \in X$ in time $t_f - t_0 > 0$. We are looking for the trajectory $t \mapsto (\xi(t), u(t))$ that satisfies the initial conditions

$$\xi_0 := \xi(t_0), \quad u_0 := u(t_0), \tag{11}$$

in $t_0 \geq 0$, the final conditions

$$\xi_f := \xi(t_f), \quad u_f := u(t_f) \tag{12}$$

in $t_f \geq t_0$, and satisfies (10) for all $t \in [t_0, t_f]$. Solving the motion planning problem is complicated; numerical methods, which are iterative methods, are often used. With numerical methods, the solution is approximated; however, generally, the exact solution cannot be given in a closed form.

An often-used method for trajectory planning of nonlinear systems is to choose a parameterized function class for the time function of a variable and to solve the differential equation of the system based on these functions. This solution method can only be used in some cases because a general method for choosing the appropriate parameterized function class is not known.

3 Motion planning results for consecutive reactions

In the next subsections, we show how the trajectories for chemical reactions can be planned with the help of the interpreted method. We give the trajectories for consecutive reactions and use the results to design a temperature control.

3.1 Motion planning for consecutive reactions

We discuss a motion planning method for consecutive reactions. Consider a consecutive reaction with R reaction steps. The stoichiometric equations in general form are

$$\mathrm{X}_1 \xrightarrow{k_1} \mathrm{X}_2 \xrightarrow{k_2} \ldots \xrightarrow{k_R} \mathrm{X}_{\mathrm{R+1}}. \tag{13}$$

Mathematical analysis requires differential equations describing the dynamics of the process. The system of differential equations for the consecutive reaction considering mass action kinetics reads

$$\dot{x}_1(t) = -k_{1,0} e^{-\frac{E_1}{R_0 T(t)}} x_1(t) \tag{14}$$

$$\dot{x}_2(t) = k_{1,0} e^{-\frac{E_1}{R_0 T(t)}} x_1(t) - k_{2,0} e^{-\frac{E_2}{R_0 T(t)}} x_2(t) \tag{15}$$

$$\vdots$$

$$\dot{x}_R(t) = k_{R-1,0} e^{-\frac{E_{R-1}}{R_0 T(t)}} x_{R-1}(t) - k_{R,0} e^{-\frac{E_R}{R_0 T(t)}} x_R(t) \tag{16}$$

$$\dot{x}_{R+1}(t) = k_{R,0} e^{-\frac{E_R}{R_0 T(t)}} x_R(t) \tag{17}$$

$$\dot{T}(t) = \frac{k_{1,0}e^{-\frac{E_1}{R_0 T(t)}}}{\beta_1}x_1(t) + \frac{k_{2,0}e^{-\frac{E_2}{R_0 T(t)}}}{\beta_2}x_2(t) + \cdots + \frac{k_{R,0}e^{-\frac{E_R}{R_0 T(t)}}}{\beta_R}x_R(t) + u(t). \quad (18)$$

Suppose that the reactant concentrations $x_1(t), x_2(t), \ldots, x_R(t)$ are strictly positive, and the activation energies for each reaction step are all different. Then, according to Theorem 1, (14)–(18) is strongly reachable; i.e., there is a control $u(t)$, which generates the trajectory $\xi(t) = (x_1(t), x_2(t), \ldots, x_{R+1}(t), T(t))$.

For motion planning, we apply the parameterized function class method. Suppose that the desired trajectories satisfy the initial conditions

$$\begin{aligned} &x_r(0) = x_{r,0}, \quad r = 1, 2, \ldots, R+1, \\ &T(0) = T_0, \end{aligned} \quad (19)$$

and the differential equations (14)–(18) for all $t \in \mathbb{R}_0^+$. We consider the reaction isothermal. We choose the constant temperature function as the parametrized function class,

$$T(t) := const., \quad (20)$$

and solve the remaining part of (14)–(18) with the help of it. Since the trajectories must satisfy the initial conditions (19), the time function of the temperature can be given in the form

$$T(t) = T_0. \quad (21)$$

In the case of isothermal reactions, the reaction rate coefficients are time-independent constants; therefore, the system of the differential equations (14)–(18) have a simplified form. It can be written as

$$\dot{x}_1(t) = -k_1 x_1(t) \quad (22)$$

$$\dot{x}_2(t) = k_1 x_1(t) - k_2 x_2(t) \quad (23)$$

$$\vdots$$

$$\dot{x}_R(t) = k_{R-1} x_{R-1}(t) - k_R x_R(t) \quad (24)$$

$$\dot{x}_{R+1}(t) = k_R x_R(t) \quad (25)$$

$$0 = \frac{k_1}{\beta_1}x_1(t) + \frac{k_2}{\beta_2}x_2(t) + \cdots + \frac{k_R}{\beta_R}x_R(t) + u_T(t), \quad (26)$$

where the reaction rate coefficients are $k_r = k_{r,0}e^{-\frac{E_r}{R_0 T_0}}$ for all $r \in \{1, 2, \ldots, R\}$.

The time function $x_1(t)$ is given as the solution of the differential equation (22). It has the form

$$x_1(t) = C_1 e^{-k_1 t}, \quad (27)$$

where C_1 is a constant parameter that can be determined from the initial conditions. Writing this for time $t = 0$ and considering the initial conditions (19), the coefficient

C_1 is given as

$$C_1 = x_{1,0}. \tag{28}$$

Substituting (28) into (27), $x_1(t)$ can be calculated as

$$x_1(t) = x_{1,0}e^{-k_1 t}, \tag{29}$$

To determine the time functions $x_2(t), x_3(t), \ldots, x_{R+1}(t)$ and $u_T(t)$, we solve (22)–(26). For this, we consider that $x_1(t)$ can be calculated according to (27). In the first step, we give the calculation method for the time functions of the concentrations $x_2, x_3, \ldots, x_R$.

Lemma 1. *Consider a consecutive reaction given by* (22)–(26)*. Suppose that the time function of the concentration x_1 is chosen as* (27)*. Then the concentration $x_r(t)$ can be written in the form*

$$\begin{aligned} x_r(t) &= C_r e^{-k_r t} + \sum_{i=1}^{r-1} \left(C_i e^{-k_i t} \cdot \prod_{j=i}^{r-1} \left(\frac{k_j}{k_{j+1} - k_i} \right) \right), \\ C_r &= x_{r,0} - \sum_{i=1}^{r-1} \left(C_i \cdot \prod_{j=i}^{r-1} \left(\frac{k_j}{k_{j+1} - k_i} \right) \right) \end{aligned} \tag{30}$$

for all $r \in \{2, 3, \ldots, R\}$.

We prove the lemma by induction. First, we consider case $r = 2$. The time derivative of $x_2(t)$ can be calculated as

$$\dot{x}_2(t) = k_1 x_1(t) - k_2 x_2(t) \tag{31}$$

according to (23). It is a first-order inhomogeneous linear differential equation whose solution is given as the sum of the homogeneous and the inhomogeneous particular solutions. The corresponding homogeneous equation reads

$$\dot{x}_2(t) = -k_2 x_2(t), \tag{32}$$

whose solution is

$$x_{2,h} = C_2 e^{-k_2 t}, \quad C_2 = const. \tag{33}$$

The particular solution of the inhomogeneous equation can be looked for in the form

$$x_{2,p}(t) = C_2(t) e^{-k_2 t}, \tag{34}$$

where $C_2(t)$ can be determined with the help of the derivative $\dot{x}_2(t)$. We can give the derivative $\dot{x}_2(t)$ in two ways. On the one hand, the time derivative of the concentration $x_2(t)$ can be calculated as

$$\dot{x}_2(t) = \dot{C}_2(t) e^{-k_2 t} - k_2 C_2(t) e^{-k_2 t}, \tag{35}$$

based on (34). On the other hand, substituting (34) and (27) into (23), the time derivative of concentration $x_2(t)$ has the form

$$\dot{x}_2(t) = k_1 C_1 e^{-k_1 t} - k_2 C_2(t) e^{-k_2 t}. \tag{36}$$

Equated (35) and (36), the derivative $\dot{C}_2(t)$ is given as

$$\dot{C}_2(t) = k_1 C_1 e^{(k_2-k_1)t}, \tag{37}$$

and integrating it, the time function $C_2(t)$ reads

$$C_2(t) = \frac{k_1 C_1}{k_2 - k_1} e^{(k_2-k_1)t}. \tag{38}$$

The particular solution of the inhomogeneous equation can be calculated by substituting (38) into (34),

$$x_{2,p}(t) = C_2(t) e^{-k_2 t} = \frac{k_1 C_1}{k_2 - k_1} e^{(k_2-k_1)t} e^{-k_2 t} = \frac{k_1 C_1}{k_2 - k_1} e^{-k_1 t}. \tag{39}$$

The general solution of (23) is given as the sum of the expressions (33) and (39). It can be written in the form

$$x_2(t) = x_{2,h}(t) + x_{2,p}(t) = C_2 e^{-k_2 t} + \frac{k_1 C_1}{k_2 - k_1} e^{-k_1 t}, \tag{40}$$

where the constant C_2 is unknown. We can determine it from the initial conditions. By writing (40) for time $t = 0$ and taking into account (19), the constant C_2 reads

$$C_2 = x_{2,0} - \frac{k_1 C_1}{k_2 - k_1}. \tag{41}$$

Equations (40) and (41) correspond to the form according to the lemma, so the lemma is satisfied for $r = 2$.

Then suppose that the time function $x_{r-1}(t)$ has the form

$$x_{r-1}(t) = C_{r-1} e^{-k_{r-1} t} + \sum_{i=1}^{r-2} \left(C_i e^{-k_i t} \cdot \prod_{j=i}^{r-2} \left(\frac{k_j}{k_{j+1} - k_i} \right) \right), \tag{42}$$

and constant coefficient C_{r-1} can be calculated as

$$C_{r-1} = x_{r-1,0} - \sum_{i=1}^{r-2} \left(C_i \cdot \prod_{j=i}^{r-2} \left(\frac{k_j}{k_{j+1} - k_i} \right) \right), \tag{43}$$

with $x_{r-1,0} = x_{r-1}(0)$ and $r \in \{3, 4, \ldots, R\}$. We prove that the time function $x_r(t)$ has the same form as the expression in the lemma. According to (22)–(26), the time

derivative of the concentration $x_r(t)$ reads

$$\dot{x}_r(t) = k_{r-1}x_{r-1}(t) - k_r x_r(t), \tag{44}$$

and the corresponding homogeneous equation has the form

$$\dot{x}_r(t) = -k_r x_r(t). \tag{45}$$

Then, the homogeneous solution can be written as

$$x_{r,h} = C_r e^{-k_r t}, \quad C_r = const., \tag{46}$$

and the particular solution of the inhomogeneous equation can be looked for in the form

$$x_r(t) = C_r(t)e^{-k_r t}. \tag{47}$$

The time derivative of the concentration $x_r(t)$ can be specified in two ways. The derivative $\dot{x}_r(t)$ by deriving (47) is

$$\dot{x}_r(t) = \dot{C}_r(t)e^{-k_r t} - k_r C_r(t)e^{-k_r t}, \tag{48}$$

and the derivative $\dot{x}_r(t)$ determined based on (44) reads

$$\dot{x}_r(t) = k_{r-1}x_{r-1}(t) - k_r C_r(t)e^{-k_r t}. \tag{49}$$

Equating (48) and (49) and replacing $x_{r-1}(t)$ with the relation according to condition (42) the form of the derivative function $\dot{C}_r(t)$ is

$$\dot{C}_r(t) = k_{r-1}C_{r-1}e^{(k_r-k_{r-1})t} + k_{r-1}\sum_{i=1}^{r-2}\left(C_i e^{(k_r-k_i)t}\cdot\prod_{j=i}^{r-2}\left(\frac{k_j}{k_{j+1}-k_i}\right)\right). \tag{50}$$

Integrating this, the time function $C_r(t)$ reads

$$C_r(t) = \frac{k_{r-1}C_{r-1}}{k_r-k_{r-1}}e^{(k_r-k_{r-1})t} + \sum_{i=1}^{r-2}\left(\frac{k_{r-1}}{k_r-k_i}C_i e^{(k_r-k_i)t}\prod_{j=i}^{r-2}\left(\frac{k_j}{k_{j+1}-k_i}\right)\right). \tag{51}$$

It can be written in a simplified form as

$$C_r(t) = \sum_{i=1}^{r-1}\left(C_i e^{(k_r-k_i)t}\prod_{j=i}^{r-1}\left(\frac{k_j}{k_{j+1}-k_i}\right)\right). \tag{52}$$

Substituting (52) into (47) we get the inhomogeneous particular solution of (44), which reads

$$x_{r,p}(t) = \sum_{i=1}^{r-1}\left(C_i e^{-k_i t}\prod_{j=i}^{r-1}\left(\frac{k_j}{k_{j+1}-k_i}\right)\right). \tag{53}$$

The general solution of (44) is given as the sum of the homogeneous and inhomogeneous solutions (46) and (53) as

$$x_r(t) = C_r e^{-k_r t} + \sum_{i=1}^{r-1} \left(C_i e^{-k_i t} \prod_{j=i}^{r-1} \left(\frac{k_j}{k_{j+1} - k_i} \right) \right), \tag{54}$$

where the constant parameter C_r can be specified from initial conditions (19),

$$C_r = x_{r,0} - \sum_{i=1}^{r-1} \left(C_i \cdot \prod_{j=i}^{r-1} \left(\frac{k_j}{k_{j+1} - k_i} \right) \right). \tag{55}$$

Equations (54) and (55) are the same as the expression of the lemma for all $r \in \{3,4,\ldots,R\}$, so the lemma is fulfilled.

In the second step, we determine how to calculate the time function of the concentration $x_{R+1}(t)$. Based on (25), the derivative of $x_{R+1}(t)$ can be given as

$$\dot{x}_{R+1}(t) = k_R x_R(t), \tag{56}$$

where the time function $x_R(t)$ can be written in the form according to Lemma 1, so

$$\dot{x}_{R+1}(t) = k_R C_R e^{-k_R t} + k_R \cdot \sum_{i=1}^{R-1} \left(C_i e^{-k_i t} \prod_{j=i}^{R-1} \left(\frac{k_j}{k_{j+1} - k_i} \right) \right). \tag{57}$$

The time function $x_{R+1}(t)$ is obtained by integrating (57). It reads

$$x_{R+1}(t) = -C_R e^{-k_R t} - k_R \cdot \sum_{i=1}^{R-1} \left(\frac{C_i}{k_i} \cdot e^{-k_i t} \prod_{j=i}^{R-1} \left(\frac{k_j}{k_{j+1} - k_i} \right) \right) + C_{R+1}, \tag{58}$$

where the parameter C_{R+1} can be specified from the initial conditions (19). It has the form

$$C_{R+1} = x_{R+1,0} + C_R + k_R \cdot \sum_{i=1}^{R-1} \left(\frac{C_i}{k_i} \cdot \prod_{j=i}^{R-1} \left(\frac{k_j}{k_{j+1} - k_i} \right) \right). \tag{59}$$

Substituting (59) into (58), $x_{R+1}(t)$ can be calculated as

$$x_{R+1}(t) = C_R(1 - e^{-k_R t}) + k_R \cdot \sum_{i=1}^{R-1} \left(\frac{C_i}{k_i} \cdot (1 - e^{-k_i t}) \prod_{j=i}^{R-1} \left(\frac{k_j}{k_{j+1} - k_i} \right) \right) + x_{R+1,0} \tag{60}$$

Table 1
Parameter values for the consecutive two-step reaction

	$k_{r,0}\ \left[\frac{\mathrm{dm}^3}{\mathrm{mol}\cdot\mathrm{s}}\right]$	$E_r\ \left[\frac{\mathrm{J}}{\mathrm{mol}}\right]$	$\beta_r\ \left[\frac{\mathrm{mol}}{\mathrm{K}\cdot\mathrm{dm}^3}\right]$
$r=1$	1	100	0.002
$r=2$	0.5	200	0.004

Finally, we provide the calculation method for the input function $u_T(t)$. The time function u_T can be determined based on (26),

$$u_T(t) = -\frac{k_1}{\beta_1}x_1(t) - \frac{k_2}{\beta_2}x_2(t) - \cdots - \frac{k_R}{\beta_R}x_R(t). \tag{61}$$

Thus, the trajectory of the isothermal consecutive reactions can be planned according to the equations (21), (29), (30), (60), and (61).

3.2 Closed-loop control for consecutive reactions

Results obtained during motion planning can be modeled using closed-loop control. The isothermal behavior can be ensured with the help of temperature control. We design closed-loop control for the following two-step consecutive reaction:

$$\mathrm{X}_1 \xrightarrow{k_1} \mathrm{X}_2 \xrightarrow{k_2} \mathrm{X}_3. \tag{62}$$

The dynamics of the investigated system can be described by differential equations

$$\dot{x}_1(t) = -k_1(T(t))x_1(t), \tag{63}$$
$$\dot{x}_2(t) = -k_2(T(t))x_2(t) + k_1(T(t))x_1(t), \tag{64}$$
$$\dot{x}_3(t) = k_2(T(t))x_2(t), \tag{65}$$
$$\dot{T}(t) = \frac{1}{\beta_1}k_1(T(t))x_1(t) + \frac{1}{\beta_2}k_2(T(t))x_2(t) + u_T(t), \tag{66}$$

where $u_T(t)$ is the input of the system. The initial concentrations of the reactant species X_1 and X_2 are $x_{1,0} = 1\ \frac{\mathrm{mol}}{\mathrm{dm}^3}$ and $x_{2,0} = 0\ \frac{\mathrm{mol}}{\mathrm{dm}^3}$, respectively. The parameters for the reaction rate coefficients are chosen to be realistic values from [36] and collected in Table 1.

The structure of the closed-loop control is as follows [39, 40]. The reference values block generates the reference signals for $T(t)$ and $\dot{T}(t)$ and forwards them to the controller. The values are chosen as

$$T_{ref} = 293\,\mathrm{K}, \quad \dot{T}_{ref} = 0\,\frac{\mathrm{K}}{\mathrm{s}}. \tag{67}$$

We demonstrate the utility of motion planning by comparing three control architectures shown in Figures 1– 3. The aim of temperature control is to ensure isothermal behavior.

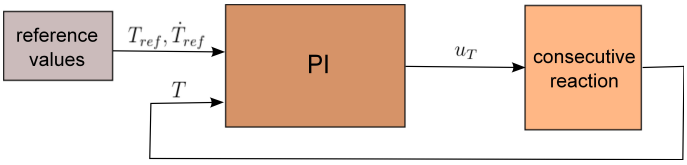

Figure 1
Closed-loop model for the consecutive reaction with PI controller

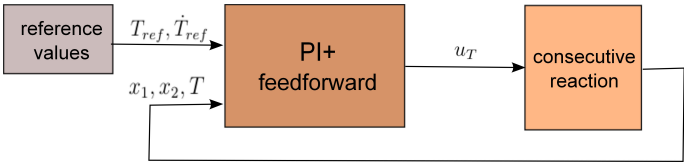

Figure 2
Closed-loop model for the consecutive reaction with PI controller and feedforward term

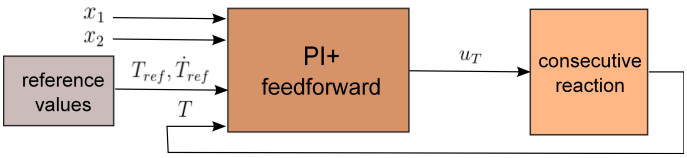

Figure 3
Closed-loop model for the consecutive reaction with PI controller and feedforward term, using the motion planning results

In the first architecture in Figure 1, we apply a PI (Proportional Integral) controller. The chosen control signal is

$$u_T(t) = K_i \int_{\tau=0}^{t} (T(\tau) - T_{ref}) d\tau + K_p (T(t) - T_{ref}), \tag{68}$$

where K_p and K_i are the controller parameters.

A PI controller and a feedforward term are applied in the second architecture, as shown in Figure 2. In the feedforward term, we use measurements of the states $x_1(t)$ and $x_2(t)$.

Table 2
Overshoot values [%] of $T(t)$ for $K_i = -10$ in the case of control architectures shown in Figures 1– 3

	PI controller	PI controller and feedforward term	PI controller and feedforward term using motion planning
$K_p = -25$	5.83	0.23	0.23
$K_p = -20$	7.02	0.34	0.35
$K_p = -15$	8.85	0.57	0.57
$K_p = -10$	12.02	1.08	1.08
$K_p = -5$	18.75	2.80	2.81

In the third architecture, shown in Figure 3, we also use a PI controller and a feedforward term; however, the values of $x_1(t)$ and $x_2(t)$ are calculated with the help of the motion planning results, i.e.,

$$x_1(t) = x_{1,0}e^{-k_1 t}, \tag{69}$$

$$x_2(t) = x_{2,0}e^{-k_2 t} + x_{1,0}\frac{k_1}{k_2 - k_1}\left(e^{-k_1 t} - e^{-k_2 t}\right), \tag{70}$$

In the latter two architectures, we choose the control signal $u_T(t)$ in the form

$$\begin{aligned} u_T(t) = &-\frac{1}{\beta_1}k_1(T(t))x_1(t) - \frac{1}{\beta_2}k_2(T(t))x_2(t) + \\ &K_i \int_{\tau=0}^{t} (T(\tau) - T_{ref})d\tau + K_p(T(t) - T_{ref}), \end{aligned} \tag{71}$$

where K_p and K_i denote the controller parameters. Note that since the error at time t is defined as $T(t) - T_{ref}$, and gains K_p and K_i are negative to ensure negative feedback.

In the consecutive reaction block in Figures 1– 3, the differential equations of the system (63)-(66) are implemented. The inputs of the plant are the control signal $u_T(t)$, and the outputs of the reaction are the state variables.

The overshoot values of the temperature control are listed in Tables 2–3, while the 2% settling times are presented in Tables 4–5 for the control architectures shown in Figures 1–3. When a feedforward term is applied, both the overshoot and the settling time are significantly reduced. Moreover, it can be observed that employing motion planning results for the feedforward term leads to overshoot and settling time values that differ only slightly from those obtained with a conventional feedforward approach. Thus, by utilizing motion planning, similar performance can be achieved without the need to measure the individual state variables.

Table 3
Overshoot values [%] of $T(t)$ for $K_p = -25$ in the case of control architectures shown in Figures 1– 3

	PI controller	PI controller and feedforward term	PI controller and feedforward term using motion planning
$K_i = -25$	5.66	0.51	0.51
$K_i = -20$	5.68	0.42	0.42
$K_i = -15$	5.72	0.33	0.33
$K_i = -10$	5.82	0.23	0.23
$K_i = -5$	6.04	0.11	0.11

Table 4
2% settling times [s] of $T(t)$ for $K_i = -10$ in the case of control architectures shown in Figures 1– 3

	PI controller	PI controller and feedforward term	PI controller and feedforward term using motion planning
$K_p = -25$	1.081	0.083	0.083
$K_p = -20$	1.115	0.101	0.101
$K_p = -15$	1.118	0.128	0.128
$K_p = -10$	2.505	0.175	0.175
$K_p = -5$	2.902	0.995	0.994

Table 5
2% settling times [s] of $T(t)$ for $K_p = -25$ in the case of control architectures shown in Figures 1– 3

	PI controller	PI controller and feedforward term	PI controller and feedforward term using motion planning
$K_i = -25$	0.708	0.079	0.079
$K_i = -20$	0.786	0.080	0.080
$K_i = -15$	0.895	0.081	0.081
$K_i = -10$	1.081	0.083	0.083
$K_i = -5$	1.440	0.084	0.084

The error function of the variable T for the different architectures is presented in Figures 4– 6. The left sides of Figures 4– 6 show the error functions at fixed K_i and different K_p values for the PI controller, the PI controller with feedforward using the measurements of the states, and the PI controller with feedforward term based on motion planning results. Increasing the value of K_p results in a larger overshoot; however, the error function of the temperature reaches zero sooner. The figures show the advantage of the feedforward term since the quality of control is better when feedforward is used, i.e., the transient has lower overshoot and faster settling time. The results with the motion planning (the left side of Figure 6) are similar to the results with the x_1 and x_2 state measurements (the left side of Figure 5), demonstrating that the usage of motion planning can increase the quality of the control without measurements of the states x_1 and x_2, thus using more simple control architecture.

The right sides of Figures 4- 6 show the error functions after fixing $K_p = -25$ (which gave the best results in the left sides of Figures 4– 6) and varying the K_i values. In this case, the error function of the temperature reaches zero sooner at smaller K_i values. The results show that the transient can be further increased by tuning the controller; however, the PI controller with the feedforward term still outperforms the simple PI controller. The right sides of Figures 5– 6 are also similar in this case, demonstrating that the results of the motion planning can be used well instead of state feedback.

Conclusions

We applied a generic motion planning method to the control problem of chemical systems. This is suitable for linearizing chemical reactions with certain structures by guaranteeing isothermal behavior. Thus, it enables simpler control, which can be used to make production processes more efficient and cheaper. Motion planning helped to replace the measurements of some states, which makes the control architecture simpler and the implementation cheaper. Also, there may be practical cases when the concentration of the species can not be directly measured; in such cases, motion planning can be applied to enhance the performance of temperature controllers.

We used the parametrized function class method for consecutive reactions. The presented method can also be applied to other chemical system classes (e.g., the parametrized function class method works for parallel reactions), and the given results can be used for control. Moreover, consecutive reactions are basic components of general chemical reaction architectures; thus, the results can be generalized for general chemical reactions in the future. Furthermore, this can help to make reactions more efficient and, in some cases, reduce emissions of harmful products.

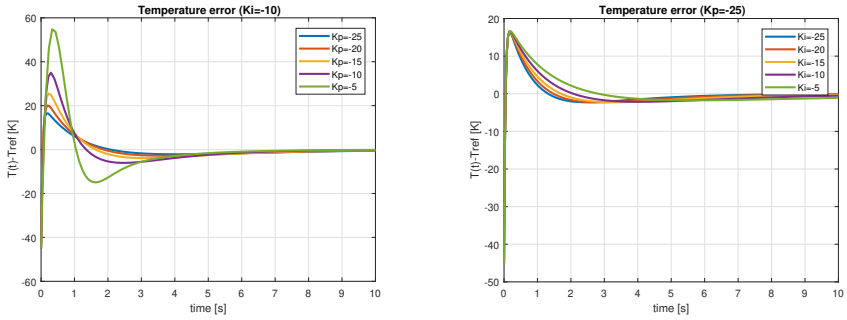

Figure 4
Error functions of $T(t)$ for $K_i = -10$ and $K_p = -25$ in the case of PI controller

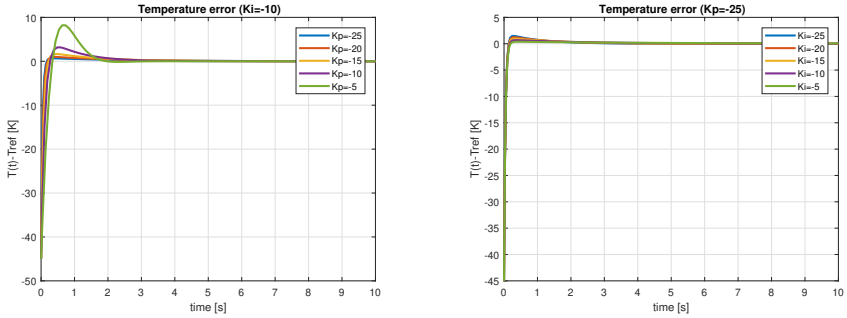

Figure 5
Error function of $T(t)$ for $K_i = -10$ and $K_p = -25$ in the case of PI controller and feedforward term

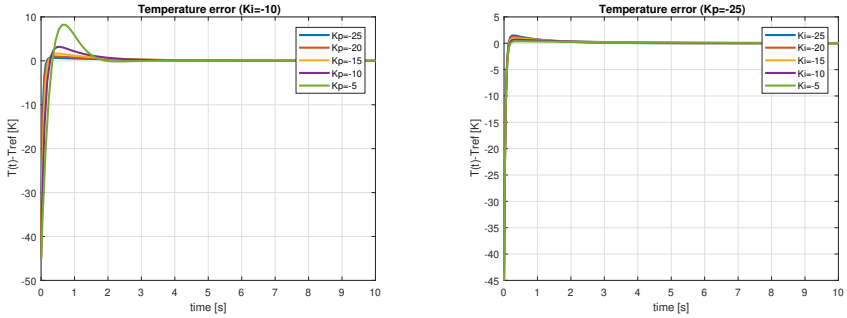

Figure 6
Error function of $T(t)$ for $K_i = -10$ and $K_p = -25$ in the case of PI controller and feedforward term, using the motion planning results

Acknowledgment

Project no. 2019-1.3.1-KK-2019-00007. has been implemented with the support provided from the National Research, Development and Innovation Fund of Hungary, financed under the 2019-1.3.1-KK funding scheme. This project has been supported by the Hungarian National Research, Development and Innovation Fund of Hungary, financed under the TKP2021-NKTA-36 funding scheme. The work of Dániel András Drexler was supported by the Starting Excellence Researcher Program of Obuda University, Budapest, Hungary. This research was partially supported by the European Union (EU HORIZON-MSCA-2023-SE-01-01) and the Hungarian NRDI program (2020-2.1.1-ED-2024-00346) within the DSYREKI: Dynamical Systems and Reaction Kinetics Networks project.

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