

APPLICATION OF VIBRATIONAL CONTROL TO CHEMICAL REACTIONS IN A
CSTR WITH DELAYED RECYCLE STREAM*

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Abstract—Vibrational control is a method of modification of dynamic properties obtained by introducing zero mean oscillations into a system parameters. This paper shows that by introducing oscillations into the flow rates of a continuous stirred tank reactor with delayed recycle stream, it is possible to operate reactions in the vicinity of previously unstable steady states.

1. INTRODUCTION

Vibrational control is a recently developed open loop control technique that, unlike classical methods of feedback and feedforward, does not require measurements. Instead, parametric oscillations are introduced into a system in order to induce a desired dynamic response. Because no state measurements are required, vibrational control is an alternative to feedback and feedforward techniques when measurements are costly or for some reason unavailable.

The theory of vibrational control for ordinary differential equations has been developed in [2,3]. In [1-3], the authors describe a hypothetical application of vibrational control to an irreversible exothermic chemical reaction in a continuous stirred tank reactor (CSTR) and show that by vibrating the flow rates in a CSTR, it is possible to theoretically operate the reactor at (average) conversion rates which were previously unstable.

Operation of a CSTR at or near unstable steady states is an area of important research. Often, these unstable steady states offer optimal yield given technical constraints, such as a maximum operating temperature of a reactor [5,6]. In many cases, a feedback cooling system is used to stabilize previously unstable steady states [4-6]. However, cooling systems require measurements of states which, at times, require large delays to obtain. Additionally, for exothermic reactions, feedback cooling systems have considerable energy expense. Obstacles such as these are why new control techniques for chemical reactors are important to develop.

Vibrational control offers a way to avoid many of these above difficulties. Because it is an open loop control technique, state measurements are not needed and cooling costs are not incurred. In [5] the theoretical postulations of vibrational control of chemical reactions [1-3] were *experimentally* applied to exothermic reactions in a CSTR. It was shown that by appropriately inserting periodic oscillations into the flow rates of a CSTR it is possible to operate at an asymptotically stable periodic orbit in the vicinity of a previously unstable steady state. The results of [5] are significant because they provide experimental verification of benefits of vibrational control which had been only previously hypothesized.

The purpose of this paper is to show that vibrational control is an effective method of stabilizing chemical reactions with delayed recycle stream. A conjecture to this problem is discussed in [8], where preliminary results are given. The results of this paper will show that, for exothermic reactions in a CSTR with delayed recycle stream, it is possible to operate in the vicinity of previously unstable steady states of high conversion. Furthermore, it is possible to give recommendations on the choice of amplitudes and frequencies of vibrations which ensure desired properties of a vibrationally stabilized system.

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Section 2 of this paper develops the theory of vibrational control for differential delay equations. Section 3 gives the model of the chemical reaction under consideration and discusses conditions for stability of steady states. Section 4 describes the vibrational control of the chemical reaction described in Section 3 and provides numerical simulations to support the theory.

2. VIBRATIONAL CONTROL

This section further develops recent advances in vibrational control theory for systems with time delay. Additional discussion of these techniques can be found in [8].

Consider the general class of delay differential equations

$$\begin{aligned} \dot{x}(t) &= \bar{P}_1(x(t), x(t-r)) + \bar{P}_2(\lambda, x(t)) \\ x(t) &= \theta(t) \quad t \in [-r, 0], \end{aligned} \quad (2.1)$$

where $x(t) \in \mathbb{R}^n$, $\bar{P}_1: \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}^n$ and $\bar{P}_2: \mathbb{R}^d \times \mathbb{R}^n \rightarrow \mathbb{R}^n$, are continuously differentiable, $\lambda = [\lambda_1, \lambda_2, \dots, \lambda_d]^T$ are parameters subject to vibrations, r is the constant positive delay, and $\theta(t)$ is the continuous initial function defined on $t \in [-r, 0]$.

Introduce into (2.1) parametric vibrations according to the law $\lambda(t) = \lambda_0 + \frac{1}{\varepsilon_1} f(t/\varepsilon_1)$, where λ_0 is a constant vector, ε_1 is a positive fixed constant, and $f(t)$ is an almost periodic average zero (APAZ) vector so that (2.1) becomes

$$\begin{aligned} \dot{x}(t) &= \bar{P}_1(x(t), x(t-r)) + \bar{P}_2(\lambda_0 + \frac{1}{\varepsilon_1} f(t/\varepsilon_1), x(t)) \\ x(t) &= \theta(t) \quad t \in [-r, 0]. \end{aligned} \quad (2.2)$$

Assume that for a fixed $\lambda = \lambda_0$, equation (2.1) has an equilibrium point $x_s = x_s(\lambda_0) = [x_{1s}(\lambda_0), \dots, x_{ns}(\lambda_0)]^T$.

DEFINITION 1. An equilibrium point $x_s(\lambda_0)$ of (2.1) is said to be *vibrationally δ -stabilizable with respect to component $x_{is}(\lambda_0)$* if for a given fixed $\delta \geq 0$ there exists an APAZ vector $f(t)$ such that (2.2) has asymptotically stable almost periodic solution $x^*(t) = [x_1^*(t), \dots, x_n^*(t)]$, the i th component of which is characterized by

$$\| \bar{x}_i - x_{is}(\lambda_0) \| \leq \delta; \quad \bar{x}_i \equiv \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T x_i^*(t) dt.$$

In order to make analysis simpler, this paper will always assume that $\bar{P}_2(\lambda_0 + \frac{1}{\varepsilon_1} f(t/\varepsilon_1), x(t)) = P(\lambda_0, x(t)) + \frac{1}{\varepsilon_1} P_2(f(t/\varepsilon_1), x(t))$ (where $P_2(\cdot, \cdot)$ is a vector function linear with respect to its first argument).

Then, (2.2) can be rewritten as

$$\dot{x}(t) = P_1(x(t), x(t-r)) + \frac{1}{\varepsilon_1} P_2(f(t/\varepsilon_1), x(t)), \quad (2.3)$$

where $P_1(x(t), x(t-r)) = \bar{P}_1(x(t), x(t-r)) + P(\lambda_0, x(t))$, $P_1(z_1, z_2)$ and $P_2(\cdot, z_1)$ are continuously differentiable in (z_1, z_2) , and the initial function, $\theta(t)$, remains unchanged.

Along with (2.3), consider the "generating equation" given by

$$\dot{x}(t) = P_2(f(t), x(t)). \quad (2.4)$$

Denote the general solution of (2.4) as $h(t, c) = [h_1(t, c), \dots, h_n(t, c)]$, where $c \in \mathbb{R}^n$ is a constant vector. Introduce substitution $x(t) = h(t/\varepsilon_1, y(t))$ into (2.3) to obtain

$$\dot{y}(t) = \left[\frac{\partial h(t/\varepsilon_1, y(t))}{\partial y(t)} \right]^{-1} P_1(h(t/\varepsilon_1, y(t)), h(t/\varepsilon_1 - r, y(t))) \\ \equiv Y(t/\varepsilon_1, y(t), y(t-r), r/\varepsilon_1). \quad (2.5)$$

Now, consider the corresponding "averaged" delay differential equation

$$\dot{z}(t) = P_0(z(t), z(t-r), r/\varepsilon_1) \quad (2.6)$$

where $z(t) = \psi(t)$ for $t \in [-r, 0]$,

$$P_0(c_1, c_2, r/\varepsilon_1) \\ = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \left[\frac{\partial h(t, c_1)}{\partial y(t)} \right]^{-1} P_1(h(t, c_1), h(t-r/\varepsilon_1, c_2)) dt,$$

ε_1 is the positive constant previously given, and initial function $\psi(t)$ is given by the relation $\theta(t) = h(t/\varepsilon_1, \psi(t))$ for $t \in [-r, 0]$, where $\theta(t)$ is the initial function for $x(t)$ defined in (2.1). It is not too difficult to show that $\psi(t)$ exists and is a unique continuous function on $t \in [-r, 0]$.

THEOREM 1. Suppose that, for some fixed positive ε_1 , (2.7) has a uniformly asymptotically stable equilibrium point $z_s \in \Omega \subset \mathbb{R}^n$. Suppose, further, that h , defined in (2.4) is almost periodic in t , and that

$$x_{is}(\lambda_0) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T h_i(t, z_s) dt. \quad (2.7)$$

Then there exists an $\varepsilon_0 > 0$, sufficiently small, such that, if $0 < \varepsilon_1 \leq \varepsilon_0$, equilibrium point $x_s(\lambda)$ of (2.1) is vibrationally δ -stabilizable with respect to component $x_{is}(\lambda_0)$ by vibrations $(1/\varepsilon_1)f(t/\varepsilon_1)$.

Let $x(t; \theta)$, $y(t; \psi)$, and $z(t; \psi)$ denote the solutions to (2.3), (2.5) and (2.6) respectively, where $\theta(t)$ is as given in (2.1) and $\psi(t)$ is uniquely determined by the relationship $\theta(t) = h(t/\varepsilon_1, \psi(t))$ on $t \in [-r, 0]$. By construction, $x(t; \theta) \equiv h(t/\varepsilon_1, y(t; \psi))$.

Introduce

$$\bar{x}_i(y(t; \psi)) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T h_i(\lambda, y(t; \psi)) d\lambda,$$

which represents the i th component of the averaged trajectory of vibrationally controlled system (2.3). If $y(t; \psi)$ and $z(t; \psi)$ are close to each other, $\bar{x}_i(y(t; \psi))$ can be approximated by

$$\bar{x}_i(z(t; \psi)) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T h_i(\lambda, z(t; \psi)) d\lambda,$$

where $\bar{x}_i(z(t; \psi))$ represents the approximate averaged transient behavior of the i th component of the vibrationally controlled system (2.3). Comparison of $x_i(t; \theta)$ with $\bar{x}_i(y(t; \psi))$ and $\bar{x}_i(z(t; \psi))$ reveals the change of global transient behavior of (2.1) due to parametric oscillations.

DEFINITION 2. For any fixed $\sigma > 0$ and any $L > 0$, an APAZ vector $(1/\varepsilon_1)f(t/\varepsilon_1)$ is said to induce a σ -global dynamic equivalence between (2.3) and (2.6) with respect to component i if

$$\|\bar{x}_i(y(t; \psi)) - \bar{x}_i(z(t; \psi))\| < \sigma, \quad t \in [0, L],$$

for all $\psi \in \Omega$, where Ω is an open subset of \mathbb{R}^n .

THEOREM 2. Let Ω be an open subset of \mathbb{R}^n . Assume that

(1) $Y(s, y(t), y(t-r), r/\varepsilon_1)$, defined in (2.6), is continuous in all its arguments and there exists a positive constant $K > 0$ such that for $(s, y_1, y_2) \in \mathbb{R} \times \Omega \times \Omega$

$$\|Y(s, y_1, y_2, r/\varepsilon_1) - Y(s, \bar{y}_1, \bar{y}_2, r/\varepsilon_1)\| \leq K \max_{i=1,2} \|y_i - \bar{y}_i\|;$$

(2) Uniformly with respect to (t, y_1, y_2) in compact sets of $\mathbb{R} \times \Omega \times \Omega$, there exists a limit

$$P_0(y_1, y_2, r/\varepsilon_1) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^{t+T} Y(s, y_1, y_2, r/\varepsilon_1) ds;$$

(3) System (2.6) has an asymptotically stable equilibrium point, $z_s \in \Omega_1$, where $\Omega_1 \subset \Omega$ is the domain of attraction of z_s .

Then for any $\sigma > 0$, there exists an $\varepsilon_0 = \varepsilon_0(\sigma)$ such that, for $0 < \varepsilon_1 \leq \varepsilon_0$, vibrations $(1/\varepsilon_1)f(t/\varepsilon_1)$ induce a σ -global dynamic equivalence with respect to any component i between (2.3) and (2.6) for all $t \geq -r$ provided $z(t; \psi)$ and its ρ vicinity belongs to Ω_1 for $t \geq -r$.

3. IRREVERSIBLE REACTIONS IN A CSTR WITH RECYCLE STREAM

The material and energy balance equations for an irreversible unimolecular reaction with a recycle stream in a CSTR are given as

$$V\dot{c}_A(t) = \lambda Fc_{Af} + (1 - \lambda)Fc_A(t - d) - Fc_A(t) \\ - VK_0c_A(t) \exp\left\{\frac{-E}{RT(t)}\right\} \quad (3.1a)$$

$$V\rho C_p \dot{T}(t) = \rho C_p F[\lambda T_f + (1 - \lambda)T(t - d) - T(t)] \\ - (-\Delta H)VK_0 \exp\left\{\frac{-E}{RT(t)}\right\} - U[T(t) - T_c], \quad (3.1b)$$

where $c_A(t) = \bar{\theta}_1(t)$ and $T(t) = \bar{\theta}_2(t)$ for $t \in [-d, 0]$, $c_A(t)$ is the concentration of chemical A, $T(t)$ is the reactor temperature, λ is the coefficient of recirculation and varies from zero to one, with zero corresponding to total recycle and one corresponding to no recycle. The remaining constants are defined in [1]. Consider the standard change of variables

$$x_1(t) = \frac{c_{Af} - c_A(t)}{c_{Af}}, \quad x_2(t) = \frac{T(t) - T_f}{T_f} \left(\frac{E}{RT_f}\right), \quad \theta_1 = \frac{c_{Af} - \bar{\theta}_1(t)}{c_{Af}}, \\ \theta_2(t) = \frac{\bar{\theta}_2(t) - T_f}{T_f}, \quad t_{new} = \frac{t}{\tau}, \quad \tau = \frac{V}{F\lambda}, \\ D_a = K_0\tau \exp\{-\gamma\}, \quad B = \frac{(-\Delta H)c_{Af}E}{C_p\rho T_f^2 R}, \quad r = \frac{d}{\tau}, \\ \beta = \frac{U\tau}{VC_p\rho}, \quad \gamma = \frac{E}{RT_f}, \quad x_{2c} = \frac{T_c - T_f}{T_f} \left(\frac{E}{RT_f}\right)$$

Then, (3.1) in dimensionless variables becomes

$$\dot{x}_1 = -\frac{1}{\lambda}x_1(t) + \left(\frac{1}{\lambda} - 1\right)x_1(t - r) \\ + D_a \exp\left\{x_2(t)/(1 + \frac{x_2(t)}{\gamma})\right\}(1 - x_1(t)) \quad (3.2a)$$

$$\dot{x}_2(t) = -\left(\frac{1}{\lambda} + \beta\right)x_2(t) + \left(\frac{1}{\lambda} - 1\right)x_2(t - r) \\ + BD_a \exp\left\{x_2(t)/(1 + \frac{x_2(t)}{\gamma})\right\}(1 - x_1(t)) + \beta x_{2c} \quad (3.2b)$$

where $x_i(t) = \theta_i(t)$ for $t \in [-r, 0]$. The state $x_1(t)$ corresponds to the conversion rate of the reaction, $0 \leq x_1(t) \leq 1$, where $x_1(t) = 1$ indicates 100% of chemical A has been turned into product and $x_1(t) = 0$ indicates that no products have been formed. The variable $x_2(t)$ denotes dimensionless temperature. Clearly, (3.3) is valid only when $\lambda \neq 0$. Constants B, β, D_a, γ , and r are all positive.

3.2. Steady State Analysis

For fixed B, β, γ, x_{2c} , the steady state plot of x_{1s} versus D_a , the Damkohler number, can be given by one of two curves, shown in Figure 1. The S shaped curve shows that for fixed D_a , it is possible to have three steady states. The second curve, corresponding to a low

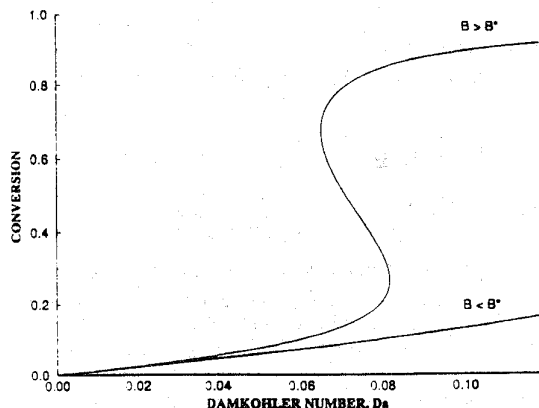


Figure 1. Two possible plots for x_{1s} vs. D_a for (3.2).

conversion rate, gives only one steady state for fixed D_a . Often, it is desired to have an S shaped curve because it allows for possibilities of operating at higher steady state conversion. In order for multiple steady states to appear, the following condition [1,9] must be satisfied:

$$B > \frac{4[1 + \beta + (\beta x_{2c}/\gamma)]^{1/2}}{1 + \beta - (4/\gamma)[1 + \beta + \beta x_{2c}/\gamma]} = B^* \quad (3.3)$$

Due to the special structure of (3.4), the results of [7] show that if a steady state of (3.4) is stable for $r = 0$, then it is stable for all $r \geq 0$. This is a useful result because it permits us to apply the well known stability conditions of [9], which were derived for $r = 0$, to (3.2).

In the special case when $r = 0$, the linearization of (3.2) about x_s is given by $\dot{x}(t) = Ax(t)$. Therefore, by [7], x_s of (3.2) is asymptotically stable provided that $\text{Det}[A] > 0$ and $\text{Tr}[A] < 0$. Using the terminology of [1], define the set $\mathfrak{D} = \{x_{1s} : \text{Det}[A] \leq 0\}$. Similarly, define the set $\mathfrak{T} = \{x_{1s} : \text{tr}[A] \geq 0\}$. In [9], it is shown that the det-instability area coincides with the negative slope part of the steady state characteristic in Figure 1. Hence, in the case of multiple steady states, the middle steady state will always be unstable, since it lies in the set \mathfrak{D} .

Denote $\mathfrak{D} = \{x_{1s} \in [m_1, m_2]\}$, $\mathfrak{T} = \{x_{1s} \in [s_1, s_2]\}$. The relative positions of m_i and s_i depend on the relationship between B and β and is further discussed in [9].

4. VIBRATIONAL CONTROL OF A CSTR WITH RECYCLE

The main contribution of this section, and hence the paper, is that it proposes the first realistic vibrational control application to a true physical system whose model has state delay. Many such examples have been discussed for systems of finite dimension, and in fact, have eventually led to experimental application of the proposed techniques. However, for delay systems, very few examples can be found [12,13].

It is of interest to attempt to vibrationally control the middle steady states of x_{1s} . The upper steady states, which have the best conversion rate for the reaction, often run at too high a temperature for the particular application. In some reactions, high temperatures cause the products (output) to decompose further, creating undesired yield. In other reactions, high temperatures cause reactants and products to become viscous and can cause damage to the reactor or can create inconsistent flow in pipes. More commonly, however, there could be

safety limitations on the operating temperature of the reactor. Any of these cases may make it impossible to operate at any upper steady state. Therefore, there is often a need to operate the reactor at one of the middle steady states, which may give the highest conversion rate (an ultimate control goal) under various temperature constraints.

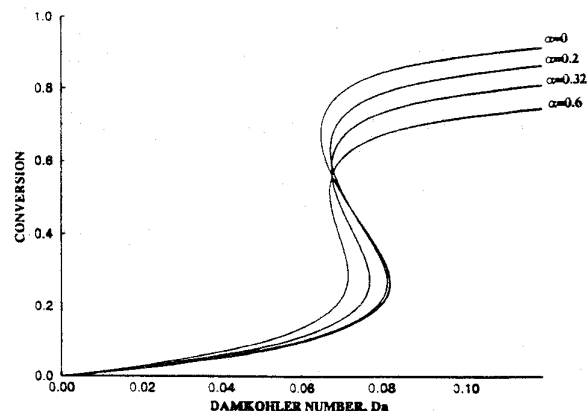


Figure 2. Typical plots of x_{1s} vs. D_a for different values of amplitude of vibration and fixed r/ϵ .

However, as Section 3 discusses, this middle steady state is always unstable.

By properly inserting periodic vibrations into the input and output flow rates of a CSTR, vibrational control allows periodic operation of the reactor in the vicinity of previously unstable steady states. Since the technique is open loop, none of the cooling costs associated with feedback occur, and likewise, the difficulties in obtaining on-line measurements is effectively eliminated.

4.1 Vibrating Input and Output Flow Rates

Introduce vibrations into (3.1) so that the input flow rate and the output flow rate oscillate identically, i.e. consider (3.1) with vibrations as

$$Vc_A(t) = \lambda Fc_{Af}[1 + af(\omega t)] + (1 - \lambda)Fc_A(t - d) - F[1 + \lambda af(\omega t)]c_A(t) - VK_0 c_A(t) \exp\left\{\frac{-E}{RT(t)}\right\} \quad (4.1a)$$

$$V\rho C_p T(t) = \rho C_p F \lambda [T_f + af(\omega t)] + \rho C_p F(1 - \lambda)T(t - d) - \rho C_p F[1 + \lambda af(\omega t)]T(t) + V(-\Delta H)K_0 \exp\left\{\frac{-E}{RT(t)}\right\} - U(T(t) - T_c) \quad (4.1b)$$

where $f(\omega t)$ is an almost periodic zero mean scalar function with frequency ω and "a" is the amplitude of vibration.

Vibrations, $f(\omega t)$ may assume different forms, such as sinusoidal, square wave, etc. For simplicity of calculations, it will always be assumed that the vibrations are symmetric such that $u(t) = \int_t f(\lambda) d\lambda$

has the property that $\overline{u^i(t)u^j(t-r)} = 0$ for $i + j = \text{odd}$ and any $r \geq 0$.

It is now necessary to impose physical constraints on (4.1). In particular, we must require that $\min_{t \geq 0} af(\omega t) \geq -1$. If this were not true, then the first terms in the right-hand side of (4.1a) and (4.1b), respectively, would become negative. This would correspond to the removal of fresh feed from the reactor, which is not possible. This restriction limits the effectiveness of predicting vibrational control; however, the constraint should not be ignored as was originally done in the first postulation of this problem [8].

Suppose that $\omega = \frac{F\lambda}{V\epsilon}$ and $a = \frac{\alpha}{\epsilon}$, where ϵ is a small positive constant. Then, in dimensionless variables, (3.2) with vibrations as in (4.1) becomes

$$\dot{x}_1(t) = -\left[\frac{1}{\lambda} + \frac{\alpha}{\epsilon} f(t/\epsilon)\right]x_1(t) + \left[\frac{1}{\lambda} - 1\right]x_1(t-r) + D_a \exp\left\{x_2(t)/\left(1 + \frac{x_2(t)}{\gamma}\right)\right\}(1 - x_1(t)) \quad (4.2a)$$

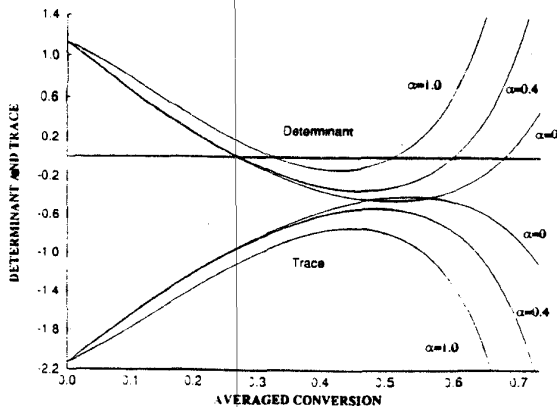


Figure 3. Typical plots of $\text{Det}(A_z)$ and $\text{Tr}(A_z)$ vs. z_{1s} for different values of amplitude of vibrations and fixed r/ϵ .

$$\begin{aligned} \dot{x}_2(t) = & -\left[\frac{1}{\lambda} + \beta + \frac{\alpha}{\epsilon} f(t/\epsilon)\right]x_1(t) + \left[\frac{1}{\lambda} - 1\right]x_1(t-r) \\ & + D_a \exp\{x_2(t)/(1 + \frac{x_2(t)}{\gamma})\}(1 - x_1(t)) + \beta x_{2c} \end{aligned} \quad (4.2b)$$

which is in the form of (2.3), and hence, the techniques of Theorems 1 and 2 can be applied.

Equation (2.4) in this case is $\dot{x}_i(t) = af(t)x_i(t)$ $i = 1, 2$. Let $u(t) = -\int_0^t f(\lambda)d\lambda$. Then using the substitution $x_i(t) = \exp\{au(t/\epsilon)\}y_i(t)$ and performing averaging, the equation corresponding to (2.6) becomes, up to $O(\alpha, \frac{1}{\gamma^2})$,

$$\begin{aligned} \dot{z}_1 = & -\frac{1}{\lambda}z_1(t) + \left(\frac{1}{\lambda} - 1\right)\left[1 + \alpha^2 \frac{u^2(t/\epsilon)}{\epsilon} - \frac{u(t/\epsilon)u(t/\epsilon - r)}{\epsilon}\right]z_1(t-r) \\ & + D_a \exp\{z_2(t)/(1 + z_2(t)/\gamma)\}(1 - z_1(t)) \\ & + \frac{\alpha^2 u^2(t/\epsilon)}{2} \left\{1 - z_2(t) - z_1(t)z_2(t) + z_2^2(t) - z_1(t)z_2^2(t)\right\} \\ & + 2\alpha^2 \frac{u^2(t/\epsilon)}{\epsilon} \left\{z_1(t)z_2^2(t) - z_2^3(t) + z_1(t)z_2^3(t)\right\} \end{aligned} \quad (4.3a)$$

$$\begin{aligned} \dot{z}_2(t) = & -\left(\frac{1}{\lambda} + \beta\right)z_2(t) + \left(\frac{1}{\lambda} - 1\right)\left[1 + \alpha^2 \frac{u^2(t/\epsilon)}{\epsilon} - \frac{u(t/\epsilon)u(t/\epsilon - r)}{\epsilon}\right]z_1(t-r) \\ & + BD_a \exp\{z_2(t)/(1 + z_2(t)/\gamma)\}(1 - z_2(t)) \\ & + \frac{\alpha^2 u^2(t/\epsilon)}{\epsilon} \left\{1 - z_2(t) - z_1(t)z_2(t) + z_2^2(t) - z_1(t)z_2^2(t)\right\} \\ & + 2\alpha^2 \frac{u^2(t/\epsilon)}{\epsilon} \left\{z_1(t)z_2^2(t) - z_2^3(t) + z_1(t)z_2^3(t)\right\} + \left(1 + \frac{\alpha^2 u^2(t/\epsilon)}{2}\right)\beta x_{2c} \\ z_i(t) = & \psi_i(t) \quad t \in [-r, 0], i = 1, 2. \end{aligned} \quad (4.3b)$$

By Section 3 for sufficiently small fixed ϵ , if z_i is asymptotically stable and if $\|\exp\{au(t/\epsilon)\}z_{1s} - x_{1s}\| \leq \delta$, then (3.2) (and hence, (3.1)) is vibrationally δ -stabilizable with respect to conversion. Furthermore, by Theorem 2, if ϵ is sufficiently small, then the average trajectory of conversion, denoted as $\bar{x}_1(y(t; \psi))$, can be approximated by $\exp\{au(t/\epsilon)\}z_{1s}(t) = \bar{x}_1(z(t; \psi))$.

Since (4.2) is in the form of $\dot{z}(t) = f(z(t)) + bz(t-r)$, where $b > 0$, for any $r \geq 0$, the stability properties of the steady state of (4.1) can be analyzed by verifying determinant and trace conditions as discussed in Section 2.

Suppose the linearization of (4.2), when $r = 0$, is given by $\dot{z}(t) = A_z z(t)$. Using the terminology of Section 3, define $\mathfrak{D}_z = \{z_{1s} : \text{Det}[A_z] \leq 0\} = \{z_{1s} \in [n_1, n_2]\}$ and $\mathfrak{F}_z = \{z_{1s} : \text{Tr}[A_z] \geq 0\} = \{z_{1s} \in [q_1, q_2]\}$. Obviously, if z_{1s} lies in \mathfrak{D}_z or \mathfrak{F}_z , z_i is unstable. However, we are attempting to stabilize \bar{x}_1 , not z_{1s} . Therefore, we must use the relationship

$z_{1s} = \overline{\exp\{au(t/\epsilon)\}z_{1s}} \approx \left(1 + \frac{\alpha^2 u^2(t/\epsilon)}{2}\right)z_{1s}$, which represents an estimate of \bar{x}_1 in Definition 1.

Define $\bar{n}_i = \left(1 + \frac{\alpha^2 u^2(t/\epsilon)}{2}\right)n_i$ and

$\bar{q}_i = \left(1 + \frac{\alpha^2 u^2(t/\epsilon)}{2}\right)q_i$, for $i=1, 2$. Denote the sets $\bar{\mathfrak{D}} = \{z_{1s} \in [\bar{n}_1, \bar{n}_2]\}$, $\bar{\mathfrak{F}} = \{z_{1s} \in [\bar{q}_1, \bar{q}_2]\}$. As expected, when $\alpha = 0$, we have $\mathfrak{D} = \bar{\mathfrak{D}}$, $\mathfrak{F} = \bar{\mathfrak{F}}$.

The goal of vibrational stabilization now becomes more clear: attempt to insert vibrations of appropriate amplitude so that $\bar{n}_2 < m_2$ and perhaps $\bar{q}_2 < s_2$. As \bar{n}_2 and \bar{q}_2 decrease, the region of 'high conversion' steady states becomes larger. We are also concerned with the closeness of $\bar{x}_1(z(t; \psi))$ to $\bar{x}_1(y(t; \psi))$ (as given in Definition 2), which requires small ϵ . This is often not feasible, since it is necessary that $\frac{\alpha}{\epsilon} f(t/\epsilon) \geq -1$. In fact, smaller ϵ_0 is usually needed in Theorem 2 than in Theorem 1. Hence, although stabilization is achieved, there may be no σ -global dynamic equivalence, i.e., $\bar{x}_1(z(t; \psi))$ may not accurately predict $\bar{x}_1(y(t; \psi))$.

4.2. Numerical Example

Fix the following parameters: $\rho = 1 \text{ g/cc}$, $C_p = 1 \text{ cal/g}^\circ\text{K}$, $F = 13.33 \text{ cc/sec}$, $T_f = 300^\circ\text{K}$, $V = 2000 \text{ cc}$, $-\Delta H = 10 \text{ Kcal/mole}$, $c_{AF} = .005 \text{ moles/liter}$, $k_0 = 7.86 \times 10^{12}$, $U = 1.356 \text{ cal/}^\circ\text{K} \cdot \text{sec}$, $\lambda = 0.75$, $E/R = 11,320.8^\circ\text{K}$, $T_c = 305^\circ\text{K}$. For these values, we have $B = 6.29$, $\tau = 200 \text{ sec}$, $\beta = 0.1356$, $\gamma = 37.73$, and $x_{2c} = 0.629$. For this example, condition (3.3) is true, which implies that there exist three steady states for some fixed D_a .

For the purposes of illustration, suppose that the vibrations are sinusoidal. That is, introduce vibrations into (3.1) so that (3.1) becomes (4.1) with $af(\omega t) = \frac{\alpha}{\epsilon} \sin\left(\frac{t}{\epsilon}\right)$. In dimensionless variables, (4.1) is given by (4.2) with $\frac{\alpha}{\epsilon} f\left(\frac{t}{\epsilon}\right) = \frac{\alpha}{\epsilon} \sin\left(\frac{t}{\epsilon}\right)$ and with $x(t) = \{0.65, 4.8\}$ for $t \in [-r, 0]$.

An analytic estimate of the average of (4.2) is given as (4.3) with $\frac{u^2(t/\epsilon)}{\epsilon} = 1/2$ and $u(t/\epsilon)u\left(\frac{t-r}{\epsilon}\right) = 0.5 \cos(r/\epsilon)$. Finally,

Figure 3 illustrates the regions of vibrational stabilization with respect to conversion more clearly by plotting the $\text{Det}(A_z)$ and $\text{Tr}(A_z)$ versus z_{1s} for fixed values of r/ϵ . (When $\alpha = 0$, $\text{Det}(A_z) = \text{Det}(A)$ and $\text{Tr}(A_z) = \text{Tr}(A)$.) For the given values simulated, $\text{Tr}(A_z) < 0$ for all non-negative α , and therefore, predicted instability only occurs when $z_{1s} \in \bar{\mathfrak{D}}$, i.e., when $\text{Det}(A_z) < 0$ in Figure 3. As expected, the steady states lying in $z_{1s} \in \bar{\mathfrak{D}}$ correspond to unstable 'middle' steady states in Figure 3. Increasing the amplitude of vibration has the effect of decreasing the size of $\bar{\mathfrak{D}}$, and hence, increasing the possible region of stabilization. It is interesting to note that, for this example, computer simulations show that varying the ratio of r/ϵ has virtually no effect on Figure 2 or 3.

for sinusoidal vibrations, we have $z_{is} = \overline{\exp\{a \cos(t/\epsilon)\}z_{is}} \approx \left(1 + \frac{\alpha^2}{4}\right)z_{is}$ which for sufficiently small ϵ , represents an estimate of \bar{x}_i in Definition 1.

For the parameters given, when $\alpha = 0$ (no vibrations), $\mathfrak{D} = [m_1, m_2] = [0.267, 0.676]$. As α increases, \bar{n}_2 will decrease (< 0.676) and it will be possible to operate the reaction in a regime of a previously unstable steady state provided that $\frac{\alpha}{\epsilon} f\left(\frac{t}{\epsilon}\right) = \frac{\alpha}{\epsilon} \sin\left(\frac{t}{\epsilon}\right) \leq -1$ (which implies that $\alpha \leq \epsilon$). The design trade-off between α and ϵ is as follows. The minimum ϵ allowed under the physical constraints is given by $\epsilon = \alpha$. Therefore, using this minimum value, if α is large, $\epsilon (= \alpha)$ will also be large.

For large $\epsilon (= \alpha)$, the predicted averaged transient behavior of the conversion in system (4.2), given by $\bar{x}_1(z(t; \psi))$, does not accurately

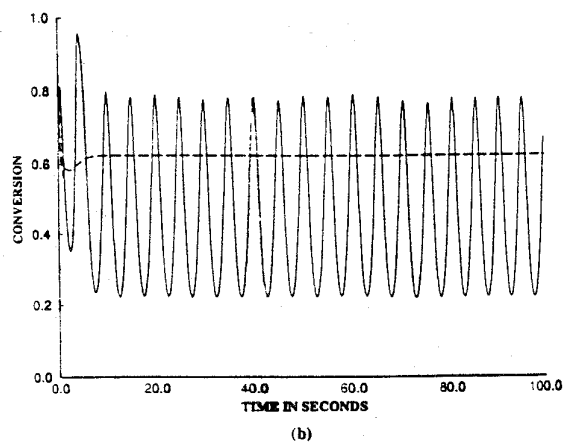
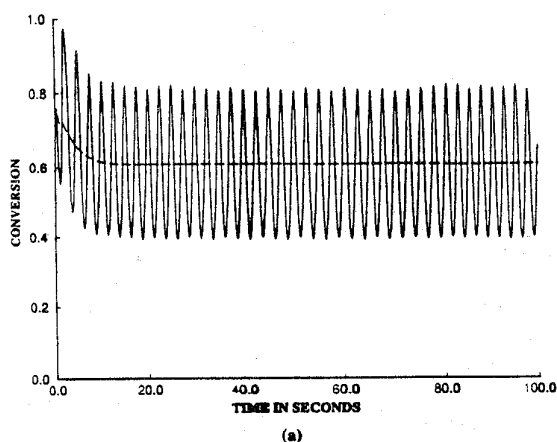


Figure 4a. $\bar{x}_1(y(t, \psi))$, given by the solid curve and $\bar{x}_1(z(t, \psi))$ given by the dashed curve, when $\alpha = \epsilon = 0.4$, $D_a = 0.0685$, $r = 1$, and $x(t) = [0.65, 4.5]$ for $t \in [-1, 0]$; Figure 4b. when $\alpha = \epsilon = 0.8$, $D_a = 0.0705$, $r = 1$, and $x(t) = [0.65, 4.5]$ for $t \in [-1, 0]$.

approximate the actual moving average, $\bar{x}_1(y(t, \psi))$. However, for large α , $\bar{\pi}_2$ decreases and the locus of stabilizable states, \bar{x}_1 , increases. On the other hand, when ϵ is small, α must be small, and the region of vibrational stabilization becomes negligible.

Table 1 shows the effect of vibrational stabilization when $r = 1$. Column 2 of the table gives the theoretical prediction of $\bar{\pi}_2$. Column 3 of Table 1 provides the actual minimum value of \bar{x}_1 that corresponds to a 'high conversion' (high temperature) region of operation, denoted as \bar{m}_2 . This value was found by direct numerical simulation of (4.2) when $\alpha = \epsilon$. All $\bar{x}_1 \geq \bar{m}_2$ represent a stable (averaged) region of operation of (4.2). For example, when $\alpha = \epsilon = 0.56$, if $\bar{x}_1 \geq 0.55$, then the reaction is operating at a 'high conversion' stable almost periodic orbit. This represents a stabilization of average conversion of the region $\bar{x}_1 \in [0.55, 0.676]$.

$\alpha = \epsilon$	$\bar{\pi}_2$	\bar{m}_2
0.24	0.62	0.63
0.32	0.59	0.62
0.40	0.56	0.61
0.48	0.54	0.57
0.56	0.53	0.55
0.64	0.51	0.53
0.72	0.50	0.51
0.80	0.50	0.50
0.88	0.50	0.49
0.96	0.50	0.46

Table 1. Theoretical ($\bar{\pi}_2$) and actual (\bar{m}_2) minimum value of stable averaged high conversion for system (4.2).

Figure 4 shows that for larger values of $\alpha (= \epsilon)$ the accuracy in approximating $\bar{x}_1(y(t, \psi))$ (an average of the actual transient response) by $\bar{x}_1(z(t, \psi))$ becomes poorer. Figure 4a shows the stabilization of \bar{x}_1

$= 0.61$, which occurs when $\alpha = \epsilon = 0.4$, $D_a = 0.0685$, $r = 1$, and with $x(t) = [0.65, 4.5]$ for $t \in [-r, 0]$. As can be seen from the simulation, $\bar{x}_1(z(t, \psi))$ (the dashed curve) accurately predicts $\bar{x}_1(y(t, \psi))$ (the actual response, $\bar{x}_1(y(t, \psi))$), is given by the solid curve) within 3% error. For $\alpha = \epsilon = 0.8$ and $D_a = 0.0705$, Figure 4b shows the stabilization of $\bar{x}_1 = 0.50$ (for $r = 1$ and the same initial function). For these values, there is approximately a 25% error between $\bar{x}_1(z(t, \psi))$ and $\bar{x}_1(y(t, \psi))$.

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