# Slow gas flow passing a solid is a convection/diffusion equation 

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#### Abstract

This paper exposes a formal result showing that a set of two coupled hyperbolic equations governing the thermal exchanges between a gas passing by a solid is actually close, in a detailed mathematical sense, to a single convection/diffusion equation. Exhaust gas passing by a solid catalyst is a typical example of such a situation. This result, the key derivation steps of which are given here, bridges the gap between the two formulations, which have received distinct types of contributions by the control community in the recent years.


Keywords: distributed parameter systems; reduction method; convection and diffusion; thermal exchanges

## 1. INTRODUCTION

With the advent of control methodologies designed for partial differential equations (PDEs), there is a rising interest in addressing numerous classic control systems with new tools. Among these systems are many unit operations in chemical plants that include transport processes and can best be described by PDEs (see Christofides (2012), Dochain (2003), Winkin et al. (2000), Aksikas et al. (2009) and references therein among other sources).

Amid those chemical systems, a class of problems we put a focus on in this article consists on fixed-bed adsorbers. This class is effectively quite large as it ranges from bioreactors to tubular reactors of various sizes and technologies. One of the first works stressing the relevance of hyperbolic PDEs to model these systems is the work by Bastin and Dochain (1991). Generally, their dynamics is well described as follows. In fixed-bed bioreactors, the biomass are entrapped or fixed on a support and other components flow through the reactor (see Dochain et al. (1992)). Interestingly, very similar formulations and physical descriptions can be found in models of automotive after-treatment systems (see Depcik and Assanis (2005) Lepreux et al. (2012)), where exhaust gas travel past a solid catalyst and get partially adsorbed. This last example is closely related to other systems such as tubular reactors treating medium that are not homogeneous, e.g. plug flow reactors using a ion-exchange resin as catalyst (see Weber and Chakravorti (1974)), and other systems found in separation and reaction engineering. These are typical of fixed-bed adsorbers, the interaction of the fluid phase with a distributed adsorption along the absorbent pellets being described in the work by Weber and Chakravorti (1974).

All these systems have in common that their modeling invokes two distinct coupled first-principles equations with very different transport speeds (see Loureiro and Ro-
drigues (1991)). These equations are of hyperbolic type. The ratio of the transport velocities can be zero (as in the case of the bioreactor or the automotive catalyst), or very small as in other instances of tubular reactors ${ }^{1}$. Chemical species travel at very different speeds depending on the strength of the adsorption or their catalyst or support.

The contribution of this paper is to show that such a system of coupled hyperbolic linear partial differential equations with one transport velocity set to 0 can be well represented by a single convection-diffusion equation. Hopefully, this work will help connecting the communities which focus on (diffusion-free) hyperbolic PDEs and diffusion equations, respectively.
The fact that we highlight will not be very surprising to modeling experts who have long had diffusion models in their toolboxes. For example, diffusion is an important factor for mathematical modeling of flow of a fluid transporting reacting species in geometrically complicated media (see e.g. Hornung and Jäger (1991) for porous media used for filtration or phase separation). The resulting models are always of the form of the convection-diffusion reaction. Their coefficients are often determined by experimental identification using empirical parameters which cannot be derived from molecular thermodynamics and dynamics coefficients (see Galarneau et al. (2016) Lee et al. (2016)). However, it is widely acknowledged that there is a general lack of a rigorous bottom up model of adsorption and transport in multi-scale porous materials (see Coasne et al. (2013)). With respect to this lack, some mathematical analysis could be of help.

Our approach here is relatively mathematical. Our result is rather formal, limited to a simple but real example stemming from long periods of experimental tests (see Lep-

[^0]reux et al. (2011, 2012)). As will appear, the elements of derivation are relatively intricate and thus worth detailing.

The paper is organized as follows. We present the coupled hyperbolic PDEs under consideration in Section 2 and detail preliminaries properties of the solution along with a reformulation of the dynamics into slow/fast variables. After approximating the inverse of this transformation in Section 3, we formulate our main result in Section 4 which states in which sense the approximation is valid.

## Notations

Classically, $<., .>$ is the scalar product in $\mathbb{R}^{n}(n \in \mathbb{N})$, $O($.$) and o($.$) are Landau big-O and little-0, respectively.$ $\mathcal{L}_{\infty}$ is the vector space of essentially bounded measurable functions and $\mathcal{H}_{k}$ is the Sobolev space of order $k$.

## 2. PROBLEM STATEMENT AND TRANSFORMATION OF THE DYNAMICS

Consider the following coupled transport PDEs

$$
\begin{align*}
& \frac{\partial T}{\partial t}(z, t)+v \frac{\partial T}{\partial z}(z, t)=k_{1}\left(T_{S}(z, t)-T(z, t)\right)  \tag{1}\\
& \frac{\partial T_{S}}{\partial t}(z, t)=k_{2}\left(T(z, t)-T_{S}(z, t)\right)  \tag{2}\\
& T(0, t)=T_{\text {int }}(t)  \tag{3}\\
& T(z, 0)=g_{1}(z), \quad T_{S}(z, 0)=g_{2}(z) \tag{4}
\end{align*}
$$

over the one-dimensional spatial domain $z \in[0,1]$ with some positive parameters $v, k_{1}, k_{2}$ such that

$$
k_{1} \gg k_{2}, \quad v \ll k_{1}+k_{2}
$$

The initial and boundary conditions are defined by $\left(g_{1}, g_{2}\right) \in \mathcal{L}_{\infty}([0,1], \mathbb{R})^{2}$ and $T_{i n} \in \mathcal{L}_{\infty}(\mathbb{R}, \mathbb{R})$.
In details, this model (1)-(4) embodies the temperature dynamics of a gas flow passing an unmoving medium body, such as a solid, with a low velocity $v$. The two transport equations, with a zero velocity for the solid, involve coupling terms accounting for thermal convection. As exposed in Lepreux (2009), such equations govern the dynamics of a Diesel Oxidation Catalyst (see Figure 1(a)(c)). Experimental tests have clearly demonstrated that a relevant alternative model is the convection/diffusion dynamics $\frac{\partial T}{\partial t}+\frac{k_{2}}{k_{1}} v \frac{\partial T}{\partial z}-\frac{k_{2}}{k_{1}^{2}} v^{2} \frac{\partial^{2} T}{\partial z^{2}}=0$. Indeed, as is reported in Figure 1(b), the response of the system is kindly reproduced by a convection/diffusion model.
Reducing the coupled dynamics above to the soughtafter convection/diffusion model involves several steps of change of variables, using classic linear algebra and the partial derivatives operator, and substitutions to express two equations each bearing on a single unknown, at the exception of additional high orders terms. Here, high order means both small (in terms of ratios of the parameters $v$, $k_{1}, k_{2}$ ) and high derivatives of the variables, which are shown to be well-defined and small (in the usual sense) in the following results.

### 2.1 Existence and boundedness

For sake of determining the approximation of the equations above, we now state some results concerning their solutions. The proofs of these results are omitted for brevity.

They rely on classic elements of functional analysis in relevant functional spaces, namely $\mathcal{L}_{\infty}$, and $\mathcal{H}_{k}$.
Lemma 1. Provided that $T_{i n}, g_{1}$ and $g_{2}$ are $k$ times differentiable and bounded, the $k^{t h}$ order spatial-derivatives of $T$ and $T_{s}$ are well-posed in $\mathcal{L}_{\infty}([0,1], \mathbb{R})$ and satisfy the following equations

$$
\begin{align*}
& \frac{\partial^{k+1} T}{\partial t \partial z^{k}}+v \frac{\partial^{k+1} T}{\partial z^{k+1}}=k_{1}\left(\frac{\partial^{k} T_{S}}{\partial z^{k}}-\frac{\partial^{k} T}{\partial z^{k}}\right)  \tag{5}\\
& \frac{\partial^{k+1} T_{S}}{\partial t \partial z^{k}}=k_{2}\left(\frac{\partial^{k} T}{\partial z^{k}}-\frac{\partial^{k} T_{S}}{\partial z^{k}}\right)  \tag{6}\\
& \frac{\partial^{k} T}{\partial z^{k}}(0, t)=\varphi_{k}\left(t, T_{i n}, \ldots, T_{i n}^{(k)}, g_{2}(0), \ldots, g_{2}^{(k-1)}(0)\right)  \tag{7}\\
& \frac{\partial^{k} T}{\partial z^{k}}(z, 0)=g_{1}^{(k)}(z), \quad \frac{\partial^{k} T_{S}}{\partial z^{k}}(z, 0)=g_{2}^{(k)}(z) \tag{8}
\end{align*}
$$

in which $\varphi_{k}$ is an infinitely continuously differentiable function of its arguments.
Lemma 2. Under the assumptions of Lemma 1, the $k^{\text {th }}$ order spatial-derivatives of $T$ and $T_{s}$ are bounded in the following sense

$$
\begin{equation*}
\left\|\left(T, T_{S}\right)(\cdot, t)\right\|_{\mathcal{H}_{k}} \leq \frac{1}{\sqrt{v}}(O(1)+O(v)), \quad t \geq T_{c} \tag{9}
\end{equation*}
$$

for some $T_{c}=T_{c}\left(v, k_{1}, k_{2},\left\|\left(T, T_{S}\right)(\cdot, 0)\right\|_{\mathcal{H}_{k}}\right)$.

### 2.2 Preliminary reformulation into slow/fast dynamics

We introduce the following variables

$$
\begin{align*}
& W(z, t)=\left[T, \frac{\partial T}{\partial z}, \frac{\partial^{2} T}{\partial z^{2}}, T_{S}, \frac{\partial T_{S}}{\partial z}, \frac{\partial^{2} T_{S}}{\partial z^{2}}\right](z, t) \\
& Y(z, t)=<W(z, t),\left[\alpha_{1}, \beta_{1} v, \gamma_{1} v^{2}, \alpha_{2}, \beta_{2} v, \gamma_{2} v^{2}\right]>  \tag{10}\\
& Z(z, t)=<W(z, t),\left[\tilde{\alpha}_{1}, \tilde{\beta}_{1} v, \tilde{\gamma}_{1} v^{2}, \tilde{\alpha}_{2}, \tilde{\beta}_{2} v, \tilde{\gamma}_{2} v^{2}\right]> \tag{11}
\end{align*}
$$

in which

$$
\begin{array}{ll}
\alpha_{1}=\frac{k_{2}}{k_{1}+k_{2}}, & \tilde{\alpha}_{1}=-\alpha_{1} \\
\beta_{1}=-\frac{\left(k_{1}-k_{2}\right) k_{2}}{\left(k_{1}+k_{2}\right)^{3}}, & \tilde{\beta}_{1}=-\beta_{1} \\
\gamma_{1}=\frac{k_{2}\left(k_{1}-k_{2}\right)^{2}-2 k_{1} k_{2}^{2}}{\left(k_{1}+k_{2}\right)^{5}}, & \tilde{\gamma}_{1}=-\gamma_{1} \\
\alpha_{2}=\frac{k_{1}}{k_{1}+k_{2}}, & \tilde{\alpha}_{2}=\alpha_{1} \\
\beta_{2}=\frac{2 k_{1} k_{2}}{\left(k_{1}+k_{2}\right)^{3}}, & \tilde{\beta}_{2}=-\beta_{2} \\
\gamma_{2}=\frac{3 k_{1} k_{2}\left(k_{2}-k_{1}\right)}{\left(k_{1}+k_{2}\right)^{5}}, & \tilde{\gamma}_{2}=-\gamma_{2}
\end{array}
$$

As will appear in the sequel, $Y$ stands for the slow variable while $Z$ accounts for the fast component of the dynamics. Lemma 3. The variables $Y$ and $Z$ satisfy the following dynamics

$$
\begin{align*}
\frac{\partial Y}{\partial t}= & -\frac{k_{2}}{k_{2}+k_{1}} v \frac{\partial Y}{\partial z}+\frac{k_{1} k_{2}}{\left(k_{1}+k_{2}\right)^{3}} v^{2} \frac{\partial^{2} Y}{\partial z^{2}} \\
& +v^{3} f_{Y}\left(\frac{\partial^{3} T}{\partial z^{3}}, \frac{\partial^{4} T}{\partial z^{4}} \frac{\partial^{3} T_{S}}{\partial z^{3}}, \frac{\partial^{4} T_{S}}{\partial z^{4}}\right)  \tag{18}\\
Y(0, t)= & h_{Y}\left(t, g_{2}(0), g_{2}^{\prime}(0), g_{2}^{\prime \prime}(0), T_{i n}, \dot{T}_{i n}, \ddot{T}_{i n}\right) \tag{19}
\end{align*}
$$



Fig. 1. The Diesel Oxidation Catalyst studied in the works by Lepreux (2009); Petit (2010). (a): multichannel automotive Diesel oxidation catalyst, (b): comparisons of experimental measurements against the convection/diffusion model (after model fitting), (c): schematic view of the slow exhaust gas flow passing the solid catalyst (in one channel). Picture courtesy of IPFen.

$$
\begin{align*}
& \frac{\partial Z}{\partial t}=-\left(k_{1}+k_{2}\right) Z-\frac{k_{1}}{k_{1}+k_{2}} v \frac{\partial Z}{\partial z}-\frac{k_{1} k_{2}}{\left(k_{1}+k_{2}\right)^{3}} v^{2} \frac{\partial^{2} Z}{\partial z^{2}} \\
&+v^{3} f_{Z}\left(\frac{\partial^{3} T}{\partial z^{3}}, \frac{\partial^{4} T}{\partial z^{4}} \frac{\partial^{3} T_{S}}{\partial z^{3}}, \frac{\partial^{4} T_{S}}{\partial z^{4}}\right)  \tag{20}\\
& Z(0, t)=h_{Z}\left(t, g_{2}(0), g_{2}^{\prime}(0), g_{2}^{\prime \prime}(0), T_{i n}, \dot{T}_{i n}, \ddot{T}_{i n}\right) \tag{21}
\end{align*}
$$

in which $\left(f_{Y}, f_{Z}\right) \in O(1)^{2}$ are linear combinations of their arguments and $h_{Y}$ and $h_{Z}$ are infinitely continuously differentiable functions of their arguments.
Remark 1. From (18) and (20), one can infer the reason why we referred to $Y$ and $Z$ respectively as slow and fast variables. Indeed, in a nutshell, as $v \ll k_{1}+k_{2}$, the dynamics of $Y$ is dominated by a transport term, while the one of $Z$ behaves similarly to a weakly coupled asymptotically stable Ordinary Differential Equation (ODE) in time, with a strong contractive factor $k_{1}+k_{2}$.

We now provide the proof of this lemma, which highlights the slow-fast nature of the decomposition of variables.

Proof. We start with the dynamics corresponding to $Y$. Taking a time-derivative of (10) and using (5)-(6) for $k=0,1,2$, one obtains

$$
\begin{align*}
\frac{\partial Y}{\partial t}= & \left(\alpha_{1} k_{1}-\alpha_{2} k_{2}\right)\left(T_{S}-T\right)-\left(\alpha_{1}+\beta_{1} k_{1}-\beta_{2} k_{2}\right) v \frac{\partial T}{\partial z} \\
& -\left(\beta_{1}+\gamma_{1} k_{1}-\gamma_{2} k_{2}\right) v^{2} \frac{\partial^{2} T}{\partial z^{2}}+\left(\beta_{1} k_{1}-\beta_{2} k_{2}\right) v \frac{\partial T_{S}}{\partial z} \\
& +\left(\gamma_{1} k_{1}-\gamma_{2} k_{2}\right) v^{2} \frac{\partial^{2} T_{S}}{\partial z^{2}}-\gamma_{1} v^{3} \frac{\partial^{3} T}{\partial z^{3}} \tag{22}
\end{align*}
$$

Consequently, using

$$
\begin{aligned}
& \alpha_{1} k_{1}-\alpha_{2} k_{2}=0 \\
& \alpha_{1}+\beta_{1} k_{1}-\beta_{2} k_{2}=\alpha_{1}^{2}
\end{aligned}
$$

taking the spatial derivative of (10) and regrouping the common terms in (22) gives

$$
\begin{align*}
\frac{\partial Y}{\partial t}= & -\frac{k_{2}}{k_{2}+k_{1}} v \frac{\partial Y}{\partial z}+\alpha_{1} \frac{k_{1} k_{2}}{\left(k_{1}+k_{2}\right)^{3}} v^{2} \frac{\partial^{2} T}{\partial z^{2}} \\
& +\left(\beta_{1} k_{1}-\beta_{2} k_{2}+\frac{k_{2}}{k_{2}+k_{1}} \alpha_{2}\right) v \frac{\partial T_{S}}{\partial z} \\
& +\left(\gamma_{1} k_{1}-\gamma_{2} k_{2}+\frac{k_{2}}{k_{1}+k_{2}} \beta_{2}\right) v^{2} \frac{\partial^{2} T_{S}}{\partial z^{2}} \\
& +v^{3}\left(-\frac{k_{1}}{k_{1}+k_{2}} \gamma_{1} \frac{\partial^{3} T}{\partial z^{3}}+\frac{k_{2}}{k_{1}+k_{2}} \gamma_{2} \frac{\partial^{3} T_{S}}{\partial z^{3}}\right) \tag{23}
\end{align*}
$$

where we have used the fact that

$$
\beta_{1}+\gamma_{1} k_{1}-\gamma_{2} k_{2}-\frac{k_{2}}{k_{2}+k_{1}} \beta_{1}=-\alpha_{1} \frac{k_{1} k_{2}}{\left(k_{1}+k_{2}\right)^{3}}
$$

Thus, adding and subtracting terms again, and noting that

$$
\begin{aligned}
& \beta_{1} k_{1}-\beta_{2} k_{2}+\frac{k_{2}}{k_{2}+k_{1}} \alpha_{2}=0 \\
& \gamma_{1} k_{1}-\gamma_{2} k_{2}+\frac{k_{2}}{k_{1}+k_{2}} \beta_{2}-\frac{k_{1} k_{2}}{\left(k_{1}+k_{2}\right)^{3}} \alpha_{2}=0
\end{aligned}
$$

one gets

$$
\begin{align*}
\frac{\partial Y}{\partial t} & =-\frac{k_{2}}{k_{2}+k_{1}} v \frac{\partial Y}{\partial z}+\frac{k_{1} k_{2}}{\left(k_{1}+k_{2}\right)^{3}} v^{2} \frac{\partial^{2} Y}{\partial z^{2}} \\
& +v^{3}<\frac{\partial^{2}}{\partial z^{2}} W, w> \tag{24}
\end{align*}
$$

with

$$
\begin{aligned}
w=\left[0,-\alpha_{2} \gamma_{1}-\frac{1}{2} \beta_{1} \beta_{2},-\frac{1}{2} \beta_{2} \gamma_{1} v, \ldots\right. \\
\left.0, \alpha_{1} \gamma_{2}-\frac{1}{2} \beta_{2}^{2},-\frac{1}{2} \beta_{2} \gamma_{2} v\right]
\end{aligned}
$$

which directly gives $f_{Y}$ in (18) as the final term (scalar product) in (24).
The dynamics of $Z$ is obtained following the exact same steps. Taking a time-derivative of (11) and using (5)-(6) for $k=0,1,2$, with

$$
\begin{aligned}
& \tilde{\alpha}_{1}-\left(\tilde{\beta}_{1}+\tilde{\beta}_{2}\right) k_{2}=\frac{k_{1}}{k_{1}+k_{2}} \tilde{\alpha}_{1} \\
& \tilde{\beta}_{1}-\left(\tilde{\gamma}_{1}+\tilde{\gamma}_{2}\right) k_{2}-\frac{k_{1}}{k_{1}+k_{2}} \tilde{\beta}_{1}=\frac{k_{1} k_{2}}{\left(k_{1}+k_{2}\right)^{3}} \tilde{\alpha}_{1} \\
& \frac{k_{1}}{k_{1}+k_{2}} \tilde{\alpha}_{2}+\left(\tilde{\beta}_{1}+\tilde{\beta}_{2}\right) k_{1}=0 \\
& \frac{k_{1}}{k_{1}+k_{2}} \tilde{\beta}_{2}+\left(\tilde{\gamma}_{1}+\tilde{\gamma}_{2}\right) k_{1}+\frac{k_{1} k_{2}}{\left(k_{1}+k_{2}\right)^{3}} \tilde{\alpha}_{2}=0
\end{aligned}
$$

one obtains, after a few steps,

$$
\begin{align*}
\frac{\partial Z}{\partial t}= & -\left(k_{1}+k_{2}\right) Z-\frac{k_{1}}{k_{1}+k_{2}} v \frac{\partial Z}{\partial z}-\frac{k_{1} k_{2}}{\left(k_{1}+k_{2}\right)^{3}} \tilde{v}^{2} \frac{\partial^{2} Z}{\partial z^{2}} \\
& +v^{3}<\frac{\partial^{2}}{\partial z^{2}} W, \omega> \tag{25}
\end{align*}
$$

with

$$
\begin{aligned}
\omega=\left[0, \alpha_{2} \tilde{\gamma}_{1}-\frac{1}{2} \tilde{\beta}_{1} \tilde{\beta}_{2}-\tilde{\gamma}_{1},-\frac{1}{2} \tilde{\beta}_{2} \tilde{\gamma}_{1} v, \ldots\right. \\
\left.0, \alpha_{2} \tilde{\gamma}_{2}-\frac{1}{2} \tilde{\beta}_{2}^{2},-\frac{1}{2} \tilde{\beta}_{2} \tilde{\gamma}_{2} v\right]
\end{aligned}
$$

Thus, this gives (20) and the expression of $f_{Z}$.
The corresponding boundary conditions (19) and (21) are obtained from (10)-(11) using (7) for $k=0,1,2$.

## 3. APPROXIMATION OF THE TRANSFORMED AND INVERSE DYNAMICS

Based on the two time-scales exhibited in (18)-(21), we propose to approximate the fast dynamics in a sense clarified in the sequel. This is a second step of the model reduction, usually known in finite dimension as center manifold reduction (see e.g. Guckenheimer and Holmes (1983); Arnol'd (2013)). In this step, the variables themselves are simplified.

Lemma 4. (Approximation of the fast variable $Z$ ).
There exists $T_{c}^{Z}>0$ depending on $k_{1}, k_{2}, v$ such that

$$
\begin{align*}
\left\|\frac{\partial^{k} Z}{\partial z^{k}}(\cdot, t)\right\|_{\mathcal{L}_{\infty}} \leq \circ\left(v^{2}+\frac{k_{2}}{k_{1}}\right), & t \geq T_{c}^{Z}  \tag{26}\\
\left\|\frac{\partial^{k+1} Z}{\partial t \partial z^{k}}(\cdot, t)\right\|_{\mathcal{L}_{\infty}} \leq \circ\left(v^{2}+\frac{k_{2}}{k_{1}}\right), & t \geq T_{c}^{Z} \tag{27}
\end{align*}
$$

Then, we are looking for an approximation of the mapping $(Y, Z) \mapsto\left(T, T_{S}\right)$ to define the approximate dynamics of $T$ and $T_{S}$ from those of $Y$ and $Z$ given in (18)-(21). From (10)-(17), a few lines of computation yield

$$
\begin{align*}
T= & Y-\frac{k_{1}}{k_{2}} Z+A v \frac{\partial Z}{\partial z}-B v^{2} \frac{\partial^{2} Z}{\partial z^{2}}-C v \frac{\partial Y}{\partial z}+D v^{2} \frac{\partial^{2} Y}{\partial z^{2}} \\
& -v^{3} \tilde{f}_{Y}\left(\frac{\partial^{3} T}{\partial z^{3}}, \frac{\partial^{4} T}{\partial z^{4}}, \frac{\partial^{3} T_{S}}{\partial z^{3}}, \frac{\partial^{4} T_{S}}{\partial z^{4}}\right)  \tag{28}\\
T_{S}= & Y+Z \tag{29}
\end{align*}
$$

in which $\tilde{f}_{Y}$ is a linear function of its arguments and
$A=\left(\beta_{1}-\frac{k_{1}}{k_{2}} \tilde{\beta}_{1}\right) \frac{k_{1}}{k_{2}}-\beta_{2}+\frac{k_{1}}{k_{2}} \tilde{\beta}_{2}$
$B=\left(\beta_{1}-\frac{k_{1}}{k_{2}} \tilde{\beta}_{1}\right)\left(\tilde{\beta}_{1} \frac{k_{1}}{k_{2}}-\tilde{\beta}_{2}\right) \frac{1}{\tilde{\alpha}_{1}}-\left(\gamma_{1}-\frac{k_{1}}{k_{2}} \tilde{\gamma}_{1}\right) \frac{k_{1}}{k_{2}}$

$$
\begin{equation*}
+\gamma_{2}-\frac{k_{1}}{k_{2}} \tilde{\gamma}_{2} \tag{31}
\end{equation*}
$$

$C=\beta_{1}-\frac{k_{1}}{k_{2}} \tilde{\beta}_{1}+\beta_{2}-\frac{k_{1}}{k_{2}} \tilde{\beta}_{2}$
$D=\left(\beta_{1}-\frac{k_{1}}{k_{2}} \tilde{\beta}_{1}\right)\left(\tilde{\beta}_{1}+\tilde{\beta}_{2}\right) \frac{1}{\tilde{\alpha}_{1}}-\gamma_{1}+\frac{k_{1}}{k_{2}} \tilde{\gamma}_{1}-\gamma_{2}+\frac{k_{1}}{k_{2}} \tilde{\gamma}_{2}$

## 4. MAIN RESULT: APPROXIMATION OF THE ORIGINAL DYNAMICS (1)-(4)

We are now ready to formulate the main result of this article, stressing that the convection/diffusion equation $\frac{\partial T}{\partial t}+\frac{k_{2}}{k_{1}} v \frac{\partial T}{\partial z}-\frac{k_{2}}{k_{1}^{2}} v^{2} \frac{\partial^{2} T}{\partial z^{2}}=0$ is a good approximation of the coupled transport PDEs (1)-(2)
Theorem 1. Consider $T, T_{S}$ solution of (1)-(4). Then, there exists $T_{c}^{0}>0$ depending on $k_{1}, k_{2}, v$ such that

$$
\begin{equation*}
\left\|\frac{\partial T}{\partial t}+\frac{k_{2}}{k_{1}} v \frac{\partial T}{\partial z}-\frac{k_{2}}{k_{1}^{2}} v^{2} \frac{\partial^{2} T}{\partial z^{2}}\right\|_{\mathcal{L}_{2}} \leq \circ\left(v^{2}+\frac{k_{2}}{k_{1}}\right) \tag{34}
\end{equation*}
$$

$$
t \geq T_{c}^{0}\left(k_{1}, k_{2}, v\right)
$$

$$
\begin{equation*}
\left\|\frac{\partial T_{S}}{\partial t}+\frac{k_{2}}{k_{1}} v \frac{\partial T_{S}}{\partial z}-\frac{k_{2}}{k_{1}^{2}} v^{2} \frac{\partial^{2} T_{S}}{\partial z^{2}}\right\|_{\mathcal{L}_{2}} \leq \circ\left(v^{2}+\frac{k_{2}}{k_{1}}\right) \tag{35}
\end{equation*}
$$

Proof. Taking the time-derivative (28) and using the linearity of $\tilde{f}_{Y}$, one obtains

$$
\begin{aligned}
\frac{\partial T}{\partial t}= & \frac{\partial Y}{\partial t}-\frac{k_{1}}{k_{2}} \frac{\partial Z}{\partial t}+A v \frac{\partial^{2} Z}{\partial t \partial z}-B v^{2} \frac{\partial^{3} Z}{\partial t \partial z^{2}}-C v \frac{\partial^{2} Y}{\partial t \partial z} \\
& +D v^{2} \frac{\partial^{3} Y}{\partial t \partial z^{2}}+v^{3} \tilde{f}_{Y}\left(\frac{\partial^{4} T}{\partial t \partial z^{3}}, \frac{\partial^{4} T}{\partial t \partial z^{4}}, \frac{\partial^{4} T_{S}}{\partial t \partial z^{3}}, \frac{\partial^{5} T_{S}}{\partial t \partial z^{4}}\right)
\end{aligned}
$$

Using (18) and its space-derivative, it follows that

$$
\begin{align*}
\frac{\partial T}{\partial t}= & -\frac{k_{2}}{k_{1}+k_{2}} v \frac{\partial Y}{\partial z}+\frac{k_{1} k_{2}}{\left(k_{1}+k_{2}\right)^{3}} v^{2} \frac{\partial^{2} Y}{\partial z^{2}} \\
& +v^{3} f_{Y}\left(\frac{\partial^{3} T}{\partial z^{3}}, \frac{\partial^{4} T}{\partial z^{4}}, \frac{\partial^{3} T_{S}}{\partial z^{3}}, \frac{\partial^{4} T_{S}}{\partial z^{4}}\right) \\
& -\frac{k_{1}}{k_{2}} \frac{\partial Z}{\partial t}+A v \frac{\partial^{2} Z}{\partial t \partial z}-B v^{2} \frac{\partial^{3} Z}{\partial t \partial z^{2}} \\
& -C v\left(-\frac{k_{2}}{k_{1}+k_{2}} v \frac{\partial^{2} Y}{\partial z^{2}}+\frac{k_{1} k_{2}}{\left(k_{1}+k_{2}\right)^{3}} v^{2} \frac{\partial^{3} Y}{\partial z^{3}}\right. \\
& \left.+v^{3} \frac{\partial f_{Y}}{\partial z}\left(\frac{\partial^{3} T}{\partial z^{3}}, \frac{\partial^{4} T}{\partial z^{4}}, \frac{\partial^{3} T_{S}}{\partial z^{3}}, \frac{\partial^{4} T_{S}}{\partial z^{4}}\right)\right) \\
& +D v^{2}\left(-\frac{k_{2}}{k_{1}+k_{2}} v \frac{\partial^{3} Y}{\partial z^{3}}+\frac{k_{1} k_{2}}{\left(k_{1}+k_{2}\right)^{3}} v^{2} \frac{\partial^{4} Y}{\partial z^{4}}\right. \\
& \left.+v^{3} \frac{\partial^{2} f_{Y}}{\partial z^{2}}\left(\frac{\partial^{3} T}{\partial z^{3}}, \frac{\partial^{4} T}{\partial z^{4}}, \frac{\partial^{3} T_{S}}{\partial z^{3}}, \frac{\partial^{4} T_{S}}{\partial z^{4}}\right)\right) \\
& +v^{3} \tilde{f}_{Y}\left(\frac{\partial^{3} T}{\partial t \partial z^{3}}, \frac{\partial^{4} T}{\partial t \partial z^{4}}, \frac{\partial^{4} T_{S}}{\partial t \partial z^{3}}, \frac{\partial^{5} T_{S}}{\partial t \partial z^{4}}\right) \tag{37}
\end{align*}
$$

or, equivalently, using (5)-(6) and the space-derivatives of (10),

$$
\begin{align*}
& \frac{\partial T}{\partial t}=-\frac{k_{2}}{k_{1}+k_{2}} v \frac{\partial Y}{\partial z}+\left(\frac{k_{1} k_{2}}{\left(k_{1}+k_{2}\right)^{3}}+C \frac{k_{2}}{k_{1}+k_{2}}\right) v^{2} \frac{\partial^{2} Y}{\partial z^{2}} \\
& +v^{3} \ell_{Y}\left(\frac{\partial^{3} T}{\partial z^{3}}, \frac{\partial^{4} T}{\partial z^{4}}, \frac{\partial^{5} T}{\partial z^{5}}, \frac{\partial^{6} T}{\partial z^{6}}, \frac{\partial^{3} T_{S}}{\partial z^{3}}, \frac{\partial^{4} T_{S}}{\partial z^{4}}, \frac{\partial^{5} T_{S}}{\partial z^{5}}, \frac{\partial^{6} T_{S}}{\partial z^{6}}\right) \\
& +\tilde{\ell}_{Y}\left(\frac{\partial Z}{\partial t}, \frac{\partial^{2} Z}{\partial t \partial z}, \frac{\partial^{3} Z}{\partial t \partial z^{2}}\right) \tag{38}
\end{align*}
$$

in which $\ell_{Y}$ and $\tilde{\ell}_{Y}$ are linear functions. Finally, using (28), it follows that

$$
\begin{align*}
& \frac{\partial T}{\partial t}=-\frac{k_{2}}{k_{1}+k_{2}} v \frac{\partial T}{\partial z}+\frac{k_{1} k_{2}}{\left(k_{1}+k_{2}\right)^{3}} v^{2} \frac{\partial^{2} T}{\partial z^{2}} \\
& +v^{3} \ell_{Y}^{0}\left(\frac{\partial^{3} T}{\partial z^{3}}, \frac{\partial^{4} T}{\partial z^{4}}, \frac{\partial^{5} T}{\partial z^{5}}, \frac{\partial^{6} T}{\partial z^{6}}, \frac{\partial^{3} T_{S}}{\partial z^{3}}, \frac{\partial^{4} T_{S}}{\partial z^{4}}, \frac{\partial^{5} T_{S}}{\partial z^{5}}, \frac{\partial^{6} T_{S}}{\partial z^{6}}\right) \\
& +\tilde{\ell}_{Y}^{0}\left(\frac{\partial Z}{\partial t}, \frac{\partial Z}{\partial z}, \frac{\partial^{2} Z}{\partial t \partial z}, \frac{\partial^{2} Z}{\partial z^{2}}, \frac{\partial^{3} Z}{\partial t \partial z^{2}}, \frac{\partial^{3} Z}{\partial z^{3}}, \frac{\partial^{4} Z}{\partial z^{4}}\right) \tag{39}
\end{align*}
$$

in which $\ell_{Y}^{0}$ and $\tilde{\ell}_{Y}^{0}$ are again linear functions. The desired result follows from there with Lemmas 2 and 4.
Similarly, one obtains

$$
\begin{align*}
& \frac{\partial T_{S}}{\partial t}=-\frac{k_{2}}{k_{2}+k_{1}} v \frac{\partial T_{S}}{\partial z}+\frac{k_{1} k_{2}}{\left(k_{1}+k_{2}\right)^{3}} v^{2} \frac{\partial^{2} T_{S}}{\partial z^{2}} \\
& +v^{3} f_{Y}\left(\frac{\partial^{3} T}{\partial z^{3}}, \frac{\partial^{4} T}{\partial z^{4}} \frac{\partial^{3} T_{S}}{\partial z^{3}}, \frac{\partial^{4} T_{S}}{\partial z^{4}}\right) \\
& +\frac{\partial Z}{\partial t}+\frac{k_{2}}{k_{2}+k_{1}} v \frac{\partial Z}{\partial z}-\frac{k_{1} k_{2}}{\left(k_{1}+k_{2}\right)^{3}} v^{2} \frac{\partial^{2} Z}{\partial z^{2}} \tag{40}
\end{align*}
$$

The desired result follows using again Lemmas 2 and 4, after a further algebraic simplification.

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[^0]:    ${ }^{1}$ It is well documented that inside fixed-bed reactor the reactant waves propagates with a significantly larger speed than the heat wave

