Singularly Perturbed Profiles

V.Bykov\textsuperscript{a}, Y.Cherkinsky, V.Gol’dshtein, N.Krapivnik\textsuperscript{b}, U.Maas\textsuperscript{a}

\textsuperscript{a} Institute of Technical Thermodynamics, Karlsruhe University(TH), Kaiserst.12, 76128 Karlsruhe, Germany
\textsuperscript{b} Department of Mathematics, Ben Gurion University of the Negev, P.O.B. 653, 84105 Beer-Sheva, Israel

Abstract.

In the current paper the so-called REaction-DIffusion Manifold (REDIM) method of model reduction is discussed within the framework of standard singular perturbation theory. According to the REDIM a reduced model for the system describing a reacting flow (accounting for chemical reaction, advection and molecular diffusion) is represented by a low-dimensional manifold, which is embedded in the system state space and approximates the evolution of the system solution profiles in space and in time. This pure geometric construction is reviewed by using Singular Perturbed System (SPS) theory as the only possibility to formalize, to justify and to verify the suggested methodology. The REDIM is studied as a correction by the diffusion of the slow invariant manifold defined for a pure homogeneous system. A main result of the study is an estimation of this correction to the slow invariant manifold. A benchmark model of Michaelis-Menten is extended to the system with the standard diffusion described by the Laplacian and used as an illustration and for validation of analytic results.

1. Introduction

Recently, computational tools of numerical integration have become a prevailing methodology in study of various phenomena in reacting flow systems. For instance, nowadays in combustion theory not only the development of practical devices, which utilize combustion of hydrocarbon fuels, but also theoretical research in the field to a great extent are based on the numerical integration of the mathematical models with detailed kinetics [32, 1]. The problems of pollutant mitigation [14], increase of efficiency, safety, controllability and optimization of combustion facilities and processes cannot be handled without numerical computations using detailed knowledge on the kinetics of combustion [31, 30]. To date there is a number of numerical packages where the detailed reaction mechanisms of oxidation of various hydrocarbon fuels are implemented (see e.g. [13]). There is also a number of very detailed kinetic mechanisms developed specifically to describe the high temperature combustion processes of hydrocarbon oxidation, where all possible reaction paths are accounted for in order to describe combustion processes reliably.

\textsuperscript{1}Corresponding author. E-mail: mordeev@bgu.ac.il
Similar situation in other fields dealing with reacting flows, namely, the kinetic models constantly grow in complexity (non-linearity) and in dimension, e.g. in systems biology, atmospheric chemistry etc.

There are two principal ways to overcome overwhelming growth of mechanisms of chemical kinetics. The first is an accurate modeling focusing on a particular application. Such models can be very accurate, but typically they are valid in very narrow range of the system physical parameters. At this level standard methodologies, as for instance Quasi-Steady State Assumption (QSSA) and Partial Equilibrium Assumption (PEA) (see e.g. [32, 15]), can be applied to obtain very compact descriptions even analytically. However, extrapolation of results obtained by using such models might be in question.

The second more attractive alternative is an automatic model reduction approaches aiming at a compact formulation of a reduced model [26], which is almost completely congruent to the original detailed model. In contrast to conventional methodologies of model reduction, e.g. QSSA and PEA where typically the number of elementary reactions (steps) and species (dimension) is reduced, the methods of automatic model reduction are based on the low-dimensional manifolds (e.g. ILDM, FGM, REDIM etc. [23, 28, 27, 2]) in which though the dimension is reduced no elementary reaction/specie is neglected. In a number of works (e.g. [2, 12, 5, 3, 6, 9]) the progress in the development of this methodology was reported. These methods fully preserve the topological and dynamical structure of chemical reaction networks. They are based on so-called invariant manifolds of low-dimension, which define constrains (relations) between the variables of the detailed model and therefore can be efficiently used to formulate a consistent (with the overall dynamics of the detailed model) reduced model [7, 8, 21].

In the suggested study we focus on one of such methods for the reduced model formulation, namely, on the so-called REaction-Diffusion Manifold (REDIM) approach [2]. In this approach the constrains, which define a manifold such that

- manifolds are slow (i.e. based on the concept of decomposition of motions, which reduces also the stiffness of the reduced model);
- attractive (i.e. guaranties stability with respect to small perturbations);
- invariant (i.e. as itself represents the system solution of the detailed model, which guaranties the accuracy, consistency and congruence of the reduced model);
- low-dimensional (i.e. guarantees dimension reduction).

After the manifold with needed properties has been identified, it can be used to reduce the system by exploiting reformationulation of the system of governing equations for the independent set of system variables (parameters of a manifold) and use them for modelling of reacting flow. As a result we obtain a reduced system – reduced model. The properties above guarantee that not only topology of the original mechanism of chemical kinetics – chemical reaction network will be preserved, but the information on the species concentrations/variables will not be lost by reduction implemented in this way, because the manifold gives us possibility to compute the dependent variables by using independent ones and, therefore, we obtain the information about the whole thermo-chemical state space of reacting systems.

In the next section the theory of slow invariant manifolds for a homogeneous system is briefly outlined for completeness of the exposition. Then, the REDIM method will be discussed as a method to construct the manifold approximating
the evolution of the detailed system solution profiles. Thus, the SPS system with
an additional Laplacian operator is taken to represent mathematically simplest
possible model of the REDIM. Afterwards the standard SPS theory is applied to
analyze the role of the transport (the limit of the slow transport is considered)
with the first and second correction terms to the slow invariant manifold obtained
implicitly. Finally, main results are illustrated by Michaelis-Menten model with
diffusion.

2. Slow invariant manifolds

We start from an intuitive definition of a smooth manifold that belongs to an
open subset $U$ of the Euclidean space $\mathbb{R}^n$, which defines the reacting system state
space. An $d$-dimensional subset $M$ of $U$ is called an $d$-dimensional manifold
if each point $x \in M$ has a neighborhood $V_x \subseteq M$ that is diffeomorphic to the
$d$-dimensional unit ball $B^d$ (i.e., there exist a smooth map \( \varphi : V_x \rightarrow B^d \) with
the smooth inverse map). The tangent space at the point $x \in M$ is a collection
of all vectors (“directions”) tangent to $M$ at $x$. The tangent space is a linear
dimensional subspace of $\mathbb{R}^n$.

Let $F(x)$ be a smooth vector field defined on $U$. A smooth manifold $M$ is an
invariant manifold for $F(x)$ if $F(x)$ is a tangent vector field to $M$, i.e., $F(x) \in M$.
As a result any trajectory $u(t)$ of the system

\[
\frac{du}{dt} = F(u)
\]

that has an initial point $u_0$ in $M$. If $M \subseteq \mathbb{R}^n$ and has not a boundary, then $u(t)$
belongs to $M$ for any $t$. An alternative description that do not use initial data is the
following: A smooth manifold $M$ is an invariant manifold for $F(x)$ if a trajectory
of (2.1) has a common point $u(t_0)$ with $M$ then it belongs to $M$ for $t$ close to $t_0$.

Consider the system of ordinary differential equations in which derivatives of a
number of variables are multiplied by a small parameter i.e. Singularly Perturbed
System (SPS). The conventional form of the SPS is given by

\[
\begin{align*}
\frac{dx}{dt} &= F_s(x, y, \epsilon) \\
\epsilon \frac{dy}{dt} &= F_f(x, y, \epsilon)
\end{align*}
\]

Here $x \in \mathbb{R}^n$, $y \in \mathbb{R}^m$ are vectors in Euclidean spaces, $t \in (t_0, \infty)$ is a variable
with the meaning of time and $0 < \epsilon < \epsilon_0 \ll 1$ is a small positive parameter. In all
cases of interest here, the functions $F_s : \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}^n$, $F_f : \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}^m$
are infinitely differentiable for all $x \in \mathbb{R}^n$, $y \in \mathbb{R}^m$, $0 < \epsilon < \epsilon_0$ (at least,
in the relevant domain). The values $|f_i(x, y, \epsilon)|$ and $|g_j(x, y, \epsilon)|$ ($i = 1, 2, \ldots n$;
$j = 1, 2, \ldots m$) are assumed to be comparable with unity as $\epsilon \rightarrow 0$.

The vector field corresponding to the system (2.2 2.3) is

\[
F_\epsilon(x, y) = (F_s(x, y, \epsilon), \frac{1}{\epsilon} F_f(x, y, \epsilon))
\]

A usual approach for a qualitative study of SPS systems is to consider first the
algebraic differential system (so-called degenerate system)

\[
\frac{dx}{dt} = F_s(x, y, \epsilon)
\]
and then to draw conclusions about the qualitative behavior of the full system for sufficiently small $\epsilon$.

In order to recall a basic notions of the theory of singularly perturbed systems, a system of equations

$$
\frac{dx}{dt} = F_s(x, y, \epsilon)
$$

is called the slow subsystem, $x$ is called the slow variable and the system of equations

$$
\epsilon \frac{dy}{dt} = F_f(x, y, \epsilon)
$$

is called the fast subsystem, $y$ is called the fast variable.

Equation

$$
0 = F_f(x, y, 0)
$$

determines the slow manifold $S$ of the system \((2.2); (2.3)\) [4, 12]. Points of the slow manifold are sub-divided into two types, standard points and turning points. A point $(x, y)$ is a standard point of the slow manifold if in some neighborhood of this point the slow manifold $S$ can be represented as a graph of the function $y = h_0(x)$ such that $F_f(x, h_0(x), 0) = 0$. Practically it means that the condition of the Implicit Function Theorem $\det(D_y F_f(x, h_0(x), 0)) \neq 0$ holds and the slow manifold has the dimension of the slow variable $x$. Points where this condition does not hold are called turning points of the slow manifold.

We are looking for a family $M_\epsilon$ of $n$-dimensional smooth invariant manifolds of the vector field $F_\epsilon(x, y) = (F_s(x, y, \epsilon), \frac{1}{\epsilon} F_f(x, y, \epsilon))$ that can be represented as a graph of the function $y = h(x, \epsilon)$ and satisfy an additional property $\lim_{\epsilon \to 0} h(x, \epsilon) = h_0(x)$. Here $y = h_0(x)$ is an analytic representation of a sheet of $S$. For any fixed $\epsilon$ the invariant manifold $M_\epsilon$ is called the slow invariant manifold or the manifold of slow motions. ||For $\epsilon = 0$ the invariant manifold $M_0$ coincides with slow manifold $S$, in other words, slow manifold $S$ is zero ($\epsilon = 0$) approximation of the slow invariant manifolds $M_\epsilon$. || Under reasonable analytic assumptions was proved existence of $M_\epsilon$ for any comparatively small $\epsilon$.

The motion along the slow manifold is described by the equation:

$$
\frac{dx}{dt} = F_s(x, h_0(x), 0),
$$

and the motion along the slow invariant manifold is described by the equation:

$$
\frac{dx}{dt} = F_s(x, h(x, \epsilon), \epsilon).
$$

In general situations, the determination of the exact form and location of the slow invariant manifold is impossible. Therefore, methods of approximation are necessary. One of them finds the slow invariant manifold as a power series with respect to the small parameter $\epsilon$

$$
h(x, \epsilon) = h_0(x) + \sum_{i=1}^{\infty} \epsilon^i h_i(x).
$$

It is clear that the slow manifold $y = h_0(x)$ is an $O(\epsilon)$ approximation of the slow invariant manifolds. Thus, the general scheme of application of this technique for a singularly perturbed system can be subdivided into the analysis of the fast and
slow motions. The analysis can be considerably simplified by this decomposition and by reducing the dimension of the system to the dimension of the slow variable \(x\) and the dimension of the fast variable \(y\).

Note that the formal substitution of the function \(h(x, \epsilon)\) instead of \(y\) into (2.3) gives the first order PDE, the so-called invariance equation

\[
\frac{\partial h}{\partial x}(x, \epsilon) F_s(x, h(x, \epsilon)), \epsilon) = F_f(x, h(x, \epsilon)), \epsilon).
\]

for \(h(x(t), \epsilon)\), since \(\frac{dy}{dt} = \epsilon \frac{\partial h}{\partial x} \frac{dx}{dt}\).

However, it is generally not possible to find the explicit solution \(y = h_0(x)\) exactly from the equation \(0 = F_f(x, y, 0)\). In this case the slow invariant manifold may be obtained in an implicit form

\[
G(x, y, \epsilon) = 0
\]

(that satisfies the following property: \(G(x, y, 0) = F_f(x, y, 0)\)) or, at least, the function \(G(x, y, \epsilon)\) can be approximated in the implicit form.

The implicit form of the invariance equation is

\[
\frac{\partial G}{\partial y} F_f(x, y, \epsilon) + \epsilon \frac{\partial G}{\partial x} F_s(x, y, \epsilon) = 0.
\]

The verification is based on the Implicit Function Theorem.

To obtain the first order approximation in the implicit form, it is necessary to differentiate the equation \(F_f(x(t), y(t), 0) = 0\) as a function of \(t\) and by virtue of the system (2.2-2.3), the result is

\[
\frac{\partial F_f(x, y, 0)}{\partial y} F_f(x, y, \epsilon) + \epsilon \frac{\partial F_f(x, y, 0)}{\partial x} F_s(x, y, \epsilon) = 0.
\]

If \(\det \frac{\partial F_f}{\partial y} \neq 0\) this equation can be written in the more convenient form

\[
F_f(x, y, \epsilon) + \epsilon \left[ \frac{\partial F_f}{\partial y} \right]^{-1} \frac{\partial F_f}{\partial x} F_s(x, y, \epsilon) = 0.
\]

We recover the zero order approximation, on setting \(\epsilon = 0\). To obtain the second order approximation, it is necessary to differentiate the equation \(F_f(x(t), y(t), 0) = 0\) twice in the respect of \(t\). Suppose \(\det \frac{\partial F_f}{\partial y} \neq 0\). Let us use the short notation

\[
N := \left[ \frac{\partial F_f}{\partial y} \right]^{-1} \frac{\partial F_f}{\partial x} F_s(x, y, \epsilon).
\]

After elementary calculations we have

\[
F_f(x, y, \epsilon) + \epsilon \left[ N + \left[ \frac{\partial F_f}{\partial y} \right]^{-1} \frac{\partial N}{\partial y} F_f(x, y, \epsilon) \right] + \epsilon^2 \left[ \frac{\partial F_f}{\partial y} \right]^{-1} \frac{\partial N}{\partial x} F_s(x, y, \epsilon) = 0.
\]

This is the second approximation of the slow invariant manifold in the implicit form.

2.1. Singularly perturbed systems (SPS) and vector fields (SPVF). A singularly perturbed system (fast-slow system) of ordinary differential equations is considered as the main mathematical construction to handle the multiple time scales [17], [18]. Below the standard SPS is given in the fast time (renormalization of time \(\tau = \epsilon t\) is implemented) formulation to underline the main idea behind the framework of singularly perturbed vector fields (see [4] for more details):

\[
\begin{align*}
\frac{\partial x}{\partial \tau} &= F_f(x, y) \\
\frac{\partial y}{\partial \tau} &= \epsilon F_s(x, y)
\end{align*}
\]
Here \( \varepsilon \ll 1 \) is a small parameter, \( x = (x_1, \ldots, x_m) \) is the fast vector variable, \( y = (y_1, \ldots, y_s) \) is the slow variable, \( n = m_s + m_f \). The time variable is usual for models without renormalization. When the system is considered in the general form and difference in characteristic time scales is assumed, then such system can be treated as the system of ordinary differential equations with a small parameter \( \delta \) where a priori a division on fast and slow sub-systems is not known, but the vector field \( F(u, \delta) \) has a “hidden” fast-slow structure. It means that the vector variable \( u \) has no explicit fast and slow components. Thus, the main idea of SPVF is that after a suitable coordinate transformation \( u \mapsto (x, y) \) the original system (2.1) can be transferred to the standard singularly perturbed system (2.4) with a new small parameter, \( \varepsilon \) that depends on \( \delta \) (see the appendix for more details). After the transformation is , one can apply all powerful technique of singular perturbations approximations fast \( (y = \text{const}) \) and slow manifolds \( (F_f(x, y) = 0) \) etc. Then, by using transformation one can trace the information (decomposition, fast and slow manifolds and their properties etc.) the original variables \( u \).

More details on the concept and the theory of singular perturbed vector fields (SPVF) can be found in [4, 5] . For the implementation, however, two main problems have to be solved:

1) How to check that a vector field under consideration is a singularly perturbed one?

2) How to find a corresponding coordinate transformation that transforms the original system to the standard SPS system?

At the moment, to both questions in the general case , but in the case of a linear transformation of coordinates corresponding algorithm called as a global quasi-linearization (GQL) has been developed (see e.g. [10, 5, 11]).

2.2. GQL and system decomposition. In the case when fast manifolds and the system decomposition have linear structure they can be identified by a gap between the eigenvalues of an appropriate global linear approximation of the Right Hand Side (RHS) - vector function of (2.1) (see [3] for detailed discussion)

\[
Tu \approx F(u).
\]

Note that we did not use a hidden small parameter \( \delta \) in \( F(u) \), because its existence is not known a priori and has to be validated in a course of application of the GQL. Now, if \( T \) has two groups of eigenvalues: the so-called small eigenvalues \( \lambda(\Lambda_s) \) and large eigenvalues \( \lambda(\Lambda_f) \) have sufficiently different order of magnitude, then the vector field \( F(u) \) is regarded as linearly decomposed asymptotic singularly perturbed vector field [4]. Accordingly, fast and slow invariant subspaces given by columns of the matrices \( Z_f,Z_s \) corresponding [22] define the slow and variables . Namely,

\[
(2.5) \quad T \equiv (Z_f \quad Z_s) \cdot \begin{pmatrix} \Lambda_f & 0 \\ 0 & \Lambda_s \end{pmatrix} \cdot \begin{pmatrix} \tilde{Z}_f \\ \tilde{Z}_s \end{pmatrix},
\]

now, if we denote

\[
\tilde{Z} = Z^{-1} = (Z_f \quad Z_s)^{-1} = \begin{pmatrix} (\tilde{Z}_f)_{m_s \times n} \\ (\tilde{Z}_s)_{m_f \times n} \end{pmatrix},
\]
then, new coordinates suitable for an explicit decomposition (and coordinates transformation) are given by $(U, V)$:

$$
U := \tilde{Z}_f u \\
V := \tilde{Z}_s u .
$$

The decomposed form and corresponding fast and slow subsystems becomes

$$
\begin{align*}
\frac{dU}{dt} &= \tilde{Z}_f \cdot F \left( (Z_f Z_s) \left( \begin{array}{c} U \\ V \end{array} \right) \right) \\
\frac{dV}{dt} &= \tilde{Z}_s \cdot F \left( (Z_f Z_s) \left( \begin{array}{c} U \\ V \end{array} \right) \right).
\end{align*}
$$

The small system parameter controlling the characteristic time scales in (2.7) can be estimated by the gap between the smallest eigenvalue of the large group and the largest eigenvalue of the small group of eigenvalues [3]

$$
\varepsilon = \frac{\max |\lambda(\Lambda_s)|}{\min |\lambda(\Lambda_f)|} \ll 1.
$$

In principle, the idea of the linear transformation is not new, see e.g. [26], but the principal point of the developed algorithm concerns evaluation of this transformation. We have developed the efficient and robust method that produces the best possible (to the leading order) decomposition with respect to existing multiple-scales hierarchy (see the attachment and [10, 5, 3] for more details).

3. **Singularly perturbed profiles**

In this section we extend the previous study taking in account transport terms (diffusion and advection in general case). According to the REDIM method the manifold is constructed by implementation of the invariance condition [16, 29, 19, 20] to the system vector field extended by the transport terms [2, 3]. As it was shown in e.g. [2] the advection/convection term does not affect the state space of a reacting system, thus, one needs to account only for the diffusion term. Hence, when an appropriate (with respect to the decomposition of motions defined by the chemical source term) coordinate system $(u,v)$ is defined the simplest mathematical model to the leading order is the following

$$
\begin{align*}
\frac{du(x,t)}{dt} &= F_s (u(x,t), v(x,t)) + L_{1, x}(u(x,t), v(x,t)) \\
\frac{dv(x,t)}{dt} &= \frac{1}{\varepsilon} F_f (u(x,t), v(x,t)) + L_{2, x}(u(x,t), v(x,t))
\end{align*}
$$

Additionally, one can see from [3,1] that our main assumption treats the transport term as slow comparatively with the fast component of the vector field. The slow system evolution is then controlled by

$$
u(x,t) = (u_1(x,t), \ldots, u_{m_s}(x,t)) ,$$

which are assumed to change slowly comparatively to the fast variables

$$v(x,t) = (v_1(x,t), \ldots, v_{m_f}(x,t)) , \quad m_s + m_f = n.$$
The diffusion terms are represented first by very general and smooth differential operators \( L_{1,x}(u(x,t), v(x,t)), L_{2,x}(u(x,t), v(x,t)) \). Suppose that \( u(x,t), v(x,t) \) are smooth functions.

Initial data for the system (3.1) are

\[
(u(x,0), v(x,0)) = (u_0(x), v_0(x)).
\]

Recall that functions \( F_s, F_f \) are of the same order. Then \( \| \frac{dF_f}{dt} \| \sim O(1) \) while \( \| \frac{dF_s}{dt} \| \sim O(\frac{1}{\epsilon}) \). We suppose also that operators \( L_{1,x}(u(x,t), v(x,t)), L_{2,x}(u(x,t), v(x,t)) \) have the same order as \( F_s, F_f \).

The zero approximation \( S \) of the slow invariant manifold in the phase space \((u,v)\) (the space of species) is represented in the implicit form

\[
F_f(u, v) = 0
\]

The initial profile is \( \Gamma_0(x) := (u_0(x), v_0(x)); u_0(x) = u(x,0), v_0(x) = v(x,0). \) Denote \( \Gamma(x, t) \) a profile that is the solution of (3.1) at time \( t \) with the initial profile (initial data) \( \Gamma_0(x) \).

Now, we are going to use the singular perturbed structure of the system (3.1). We will follow formally the classical scheme for singular perturbed systems of ODE. All profiles are surfaces in the phase space \( R^n \). If initial data \( \Gamma_0(x) \) do not belongs to the slow manifold it will be projected to slow manifold along the fast subspaces parallel to the coordinate fast subspace \( R^{m_1} \). As result we obtain the slow initial profile \( \Gamma_{0,s}(x) \) on the slow manifold \( F_f(u, v) = 0 \). For simplicity we can suppose that \( \Gamma_0(x) \) itself belongs to \( S \). In the zero approximation the evolution of the slow initial profile is due to the slow equation

\[
\frac{du(x,t)}{dt} = F_s(u(x,t), v(x,t)) + L_{1,x}(u(x,t), v(x,t))
\]

under additional condition

\[
F_f(u(x,t), v(x,t)) = 0,
\]

i.e. the zero approximation \( \Gamma_0(x,t) \) of \( \Gamma(x, t) \) belongs to \( S \) for all \( t \).

The set \( RM := \cup_{\epsilon \in (0, \infty)} \Gamma_0(x,t) \) is called the reaction-diffusion manifold (REDIM) and \( RM_0 := \cup_{\epsilon \in (0, \infty)} \Gamma_0(x,t) \) is its zero approximation (for \( \epsilon = 0 \)).

If the dimension of the profile is equal to \( s \) \( (\dim \Gamma(x,t) = s) \) then \( \dim RM = \dim RM_0 = s + 1 \).

To obtain the first order approximation of the profile in the implicit form, it is necessary to differentiate the equation \( F_f(x(t), y(t), \epsilon) = 0 \) as a function of \( t \) and by virtue of the system (3.1), the result is

\[
0 = \frac{\partial F_f}{\partial u} \frac{\partial u}{\partial t} + \frac{\partial F_f}{\partial v} \frac{\partial v}{\partial t} = \frac{\partial F_f}{\partial u}(F_s(u(x,t), v(x,t)) + L_{1,x}(u(x,t), v(x,t)) + \frac{1}{\epsilon} F_f(u(x,t), v(x,t)) + L_{2,x}(u(x,t), v(x,t)))
\]

We used the short notation \( \frac{\partial F_f}{\partial u} \) for \( \frac{\partial F_f}{\partial u}(u(x,t), v(x,t)) \) and, correspondingly, for \( \frac{\partial F_f}{\partial v} \). If \( \det \frac{\partial F_f}{\partial v} \neq 0 \), then this equation can be written in the more convenient form

\[
0 = F_f(u(x,t), v(x,t)) + \epsilon \left( \frac{\partial F_f}{\partial u} \right)^{-1} \frac{\partial F_f}{\partial u} F_s(u(x,t), v(x,t)) + \epsilon L_{1,x}(u(x,t), v(x,t)) + \epsilon L_{2,x}(u(x,t), v(x,t)).
\]
We recover the zero order approximation, on setting $\epsilon = 0$. Denote the first approximation coefficient
\[ h_1(u(x, t), v(x, t)) := \left( \frac{\partial F_f}{\partial v} \right)^{-1} \frac{\partial F}{\partial u} F_s(u(x, t), v(x, t)) + \left( \frac{\partial F_f}{\partial v} \right)^{-1} \frac{\partial F}{\partial v} L_{1,x}(u(x, t), v(x, t)) + L_{2,x}(u(x, t), v(x, t)) \]

The first part is the first approximation for ODE, the second part is the transport correction. Thus, the first order approximation is
\[ 0 = F_f(u(x, t), v(x, t)) + \epsilon h_1(u(x, t), v(x, t)). \]

The transport terms $\epsilon L_{1,x}(u(x, t), v(x, t)), L_{2,x}(u(x, t), v(x, t))$ have an influence only on the first approximation.

To shorten formulas we shall drop variable $(x, t)$ when it is clear from the context.

To obtain the second order approximation it is necessary to differentiate the equation $F_f(u(x, t), v(x, t)) = 0$ twice with respect to $t$ and equate it to zero:
\[ 0 = \frac{d^2}{dt^2} F_f(u, v) = \frac{d}{dt} \left( \frac{\partial F_f}{\partial u} \frac{\partial F}{\partial u} + \frac{\partial F_f}{\partial v} \frac{\partial F}{\partial v} \right) = \frac{\partial F_f}{\partial u} \frac{\partial^2 F}{\partial u^2} + \frac{\partial F_f}{\partial u} \frac{\partial^2 F}{\partial v \partial u} + \frac{\partial F_f}{\partial v} \frac{\partial^2 F}{\partial v \partial u} + \frac{\partial F_f}{\partial v} \frac{\partial^2 F}{\partial v^2} + \frac{\partial F_f}{\partial v} \frac{\partial^2 F}{\partial v \partial u} + \frac{\partial F_f}{\partial u} \frac{\partial^2 F}{\partial v \partial u} \]

By using the system (3.1) and linearity of operators $L_{1,x}(u(x, t), v(x, t)), L_{2,x}(u(x, t), v(x, t))$ we obtain
\[ \frac{\partial F_f}{\partial u} \frac{\partial^2 F}{\partial u^2} = \frac{\partial F_f}{\partial u} \frac{\partial F}{\partial u} \left( \frac{1}{\epsilon} F_f(u, v) + L_{2,x}(u(x, t), v(x, t)) \right) = \frac{\partial F_f}{\partial u} \left( \frac{1}{\epsilon} \frac{\partial F_f}{\partial u} \frac{\partial F}{\partial u} + \frac{\partial F_f}{\partial v} \frac{\partial F}{\partial u} \right) + L_{2,x} \left( \frac{\partial F}{\partial u} \frac{\partial F}{\partial u} + \frac{\partial F}{\partial v} \frac{\partial F}{\partial u} \right) = \frac{\partial F_f}{\partial u} \frac{\partial^2 F}{\partial u^2} \]

Equation (3.22) produces $\frac{1}{\epsilon} F_f(u, v) = -h_1(u, v)$, and $\frac{\partial F}{\partial u} = \frac{1}{\epsilon} F_f(u, v) + L_{2,x}(u(x, t), v(x, t))$, thus, equation (3.6) can be rewritten as
\[ \frac{\partial F_f}{\partial u} \frac{\partial^2 F}{\partial u^2} = \frac{\partial F_f}{\partial u} \left( \frac{\partial F}{\partial u} \frac{\partial F}{\partial u} (L_{2,x}(u(x, t), v(x, t)) - h_1(u, v)) + \frac{\partial F_f}{\partial u} \frac{\partial F}{\partial u} \right) = \frac{\partial F_f}{\partial u} \frac{\partial^2 F}{\partial u^2} \]

Similarly, by using equation (3.22) and equations (3.15)
\[ \frac{\partial F_f}{\partial v} (L_{1,x}(u(x, t), v(x, t)) + F_s(u, v))^2 + \frac{\partial F_f}{\partial u} (F_s(u, v) + L_{1,x}(u(x, t), v(x, t))) (L_{2,x}(u(x, t), v(x, t)) - h_1(u, v)), \]
3.1. \textbf{Models} is the case of relatively slow transport processes, namely, 

\[
\frac{\partial^2 F}{\partial u \partial v}(L_{2,x}(u(x,t), v(x,t)) - h_1(u,v))(F_s(u,v) + L_{1,x}(u(x,t), v(x,t))) + \frac{\partial^2 F}{\partial u^2}(L_{1,x}(u(x,t), v(x,t)) - h_1(u,v))^2
\]

Substitution of expressions (3.6), (3.7), (3.8), (3.9) in (3.3) provides

\[
0 = (\frac{1}{2})^2 \left( \frac{\partial F}{\partial u} \right)^2 F_f(u,v) + \frac{1}{2} \left( \frac{\partial F}{\partial v} \right)^2 L_{2,x}(u(x,t), v(x,t)) + \frac{1}{2} \frac{\partial F}{\partial u} \frac{\partial F}{\partial v} (F_s(u,v) + L_{1,x}(u(x,t), v(x,t))) + \frac{\partial^2 F}{\partial u \partial v}(L_{2,x}(u(x,t), v(x,t)) - h_1(u,v)) + \frac{\partial F}{\partial v} \left( \frac{\partial F}{\partial u} \right) (L_{2,x}(u(x,t), v(x,t)) - h_1(u,v))^2 + 2 \frac{\partial^2 F}{\partial u \partial v} (F_s(u,v) + L_{1,x}(u(x,t), v(x,t)))(L_{2,x}(u(x,t), v(x,t)) - h_1(u,v)) + \frac{\partial^2 F}{\partial v^2} (F_s(u,v) + L_{1,x}(u(x,t), v(x,t)))^2.
\]

Multiplication of (3.10) by \(\epsilon^2 \left( \frac{\partial F}{\partial u} \right)^{-2}\) yields

\[
0 = F_f(u,v) + \epsilon L_{2,x}(u(x,t), v(x,t)) + \epsilon \left( \frac{\partial F}{\partial u} \right)^{-1} \frac{\partial F}{\partial u} (F_s(u,v) + L_{1,x}(u(x,t), v(x,t))) + \frac{\partial^2 F}{\partial u \partial v}(L_{2,x}(u(x,t), v(x,t)) - h_1(u,v)) + \frac{\partial F}{\partial v} \left( \frac{\partial F}{\partial u} \right) (L_{2,x}(u(x,t), v(x,t)) - h_1(u,v))^2 + 2 \frac{\partial^2 F}{\partial u \partial v} (F_s(u,v) + L_{1,x}(u(x,t), v(x,t)))(L_{2,x}(u(x,t), v(x,t)) - h_1(u,v)) + \frac{\partial^2 F}{\partial v^2} (F_s(u,v) + L_{1,x}(u(x,t), v(x,t)))^2.
\]

Denote

\[
h_2(u,v) := \left( \frac{\partial F}{\partial u} \right)^{-2} \frac{\partial F}{\partial u} L_{2,x}(u(x,t), v(x,t)) + \frac{\partial F}{\partial u} \left( \frac{\partial F}{\partial u} (L_{2,x}(u(x,t), v(x,t)) - h_1(u,v)) + \frac{\partial F}{\partial v} \left( \frac{\partial F}{\partial u} \right) (L_{2,x}(u(x,t), v(x,t)) - h_1(u,v))^2 + 2 \frac{\partial^2 F}{\partial u \partial v} (F_s(u,v) + L_{1,x}(u(x,t), v(x,t)))(L_{2,x}(u(x,t), v(x,t)) - h_1(u,v)) + \frac{\partial^2 F}{\partial v^2} (F_s(u,v) + L_{1,x}(u(x,t), v(x,t)))^2.
\]

therefore, second order approximation is given by

\[
0 = F_f(u,v) + \epsilon h_1(u,v) + \epsilon^2 h_2(u,v).
\]

3.1. **Slow transport term.** The special case that is typical for chemical kinetics models is the case of relatively slow transport processes, namely,
\[
\begin{align*}
(3.14) \quad \begin{cases}
\frac{du(x,t)}{dt} & = F_s(u(x,t), v(x,t)) + \varepsilon L_{1,x}(u(x,t), v(x,t)) \\
\varepsilon \frac{dv(x,t)}{dt} & = F_f(u(x,t), v(x,t)) + \varepsilon L_{2,x}(u(x,t), v(x,t))
\end{cases}
\end{align*}
\]

For this special case evolution of the slow initial profile for \( \varepsilon = 0 \) is due to the slow equation
\[
\frac{du(x,t)}{dt} = F_s(u(x,t), v(x,t)),
\]
under additional condition
\[
F_f(u(x,t), v(x,t)) = 0,
\]
i.e. on the slow manifold \( F_f(u, v) = 0 \).

The transport term \( \varepsilon L_{1,x}(U(x,t), V(x,t)) \) has an influence only on the first order approximation. In this special case evolution of any point of the initial profile coincides with the evolution of corresponding trajectory on the slow manifold.

### 3.2. First order approximation of the slow invariant manifold for Laplacian.
Consider the following Singularly Perturbed System of equations, where the transport operator is given by the Laplace operator:

\[
\begin{align*}
(3.15) & \quad \frac{\partial u}{\partial t} = \frac{1}{\varepsilon} F(u,v) + \Delta u \\
(3.16) & \quad \frac{\partial v}{\partial t} = G(u,v) + \Delta v
\end{align*}
\]

where \( 0 < \varepsilon << 1 \), \( u = u(x,t), v = v(x,t) \). System (3.15) can be reformulated as

\[
\begin{align*}
(3.17) & \quad \frac{\partial u}{\partial t} = F(u,v) + \varepsilon \Delta u \\
(3.18) & \quad \frac{\partial v}{\partial t} = G(u,v) + \Delta v
\end{align*}
\]

We will find an implicit form of the first approximation of the slow invariant manifold slow manifold

\[
F(u,v) = 0
\]

First approximation is obtained by differentiation of \( F(u,v) = 0 \) with respect to \( t \)

\[
0 = \frac{\partial F}{\partial u} \frac{\partial u}{\partial t} + \frac{\partial F}{\partial v} \frac{\partial v}{\partial t} = \frac{\partial F}{\partial u} \left( \frac{1}{\varepsilon} F(u,v) + \Delta u \right) + \frac{\partial F}{\partial v} (G(u,v) + \Delta v)
\]

Multiplication of (3.19) by \( \varepsilon \left( \frac{\partial F}{\partial v} \right)^{-1} \) yields,

\[
0 = F(u,v) + \varepsilon \left[ \left( \frac{\partial F}{\partial u} \right)^{-1} \frac{\partial F}{\partial v} G(u,v) + \left( \frac{\partial F}{\partial u} \right)^{-1} \frac{\partial F}{\partial v} G(u,v) \Delta v + \Delta u \right]
\]

Denote the first approximation coefficient

\[
(3.21) \quad h_1(u,v) = \left( \frac{\partial F}{\partial u} \right)^{-1} \frac{\partial F}{\partial v} G(u,v) + \left[ \left( \frac{\partial F}{\partial u} \right)^{-1} \frac{\partial F}{\partial v} G(u,v) \Delta v + \Delta u \right]
\]

The first part is the first approximation for ODE, the second part is the transport correction.

Thus, the first order approximation is given by

\[
(3.22) \quad 0 = F(u,v) + \varepsilon h_1(u,v)
\]
The first approximation for slow transport terms [3.14] is

\[ h_1(u, v) = \frac{\partial F}{\partial u} \left( \frac{1}{\epsilon} F(u, v) + \Delta u \right) + \frac{\partial F}{\partial v} \left( \frac{1}{\epsilon} F(u, v) + \Delta v \right) \]

3.3. Second order approximation of the slow manifold for Laplacian. In order to obtain the second order approximation it is necessary to differentiate the equation \( F(u, v) = 0 \) twice with respect to \( t \)

\[
\begin{align*}
0 &= \frac{d^2}{dt^2}(F(u, v)) = \frac{d}{dt} \left( \frac{\partial F}{\partial u} \frac{\partial u}{\partial t} + \frac{\partial F}{\partial v} \frac{\partial v}{\partial t} \right) = \left( \frac{\partial^2 F}{\partial u^2} \frac{\partial u}{\partial t} + \frac{\partial^2 F}{\partial u \partial v} \frac{\partial v}{\partial t} \right) + \\
&\left( \frac{\partial^2 F}{\partial v^2} \frac{\partial v}{\partial t} + \frac{\partial^2 F}{\partial v^2} \frac{\partial u}{\partial t} \right) + \frac{\partial F}{\partial v} \frac{\partial v}{\partial t}^2
\end{align*}
\]

where

\[
\begin{align*}
\frac{\partial F}{\partial u} = \frac{1}{\epsilon} \frac{\partial F}{\partial u} (F(u, v) + \Delta u) + \frac{1}{\epsilon} \frac{\partial F}{\partial v} (G(u, v) + \Delta v) + \Delta \left( \frac{\partial u}{\partial t} \right)
\end{align*}
\]

\[
\frac{\partial F}{\partial v} = \frac{1}{\epsilon} \frac{\partial F}{\partial u} (F(u, v) + \Delta u) + \frac{1}{\epsilon} \frac{\partial F}{\partial v} (G(u, v) + \Delta v) + \Delta \left( \frac{\partial v}{\partial t} \right)
\]

Equation [3.22] produces, \( \frac{1}{\epsilon} F(u, v) = -h_1(u, v) \), and \( \frac{\partial u}{\partial t} = \frac{1}{\epsilon} F(u, v) + \Delta u \), thus, the equation [3.27] can be rewritten as

\[
\frac{\partial F}{\partial v} \left( \frac{\partial G}{\partial u} (\Delta u - h_1(u, v)) + \frac{\partial G}{\partial v} (G(u, v) + \Delta v) + \Delta \left( \frac{\partial v}{\partial t} \right) \right)
\]

Similarly, by using equation [3.22] and equations [3.15]

\[
\begin{align*}
\frac{\partial^2 F}{\partial u^2} \frac{\partial u}{\partial t}^2 + \frac{\partial^2 F}{\partial u \partial v} \frac{\partial v}{\partial t} \frac{\partial u}{\partial t} = \frac{\partial^2 F}{\partial u^2} \left( \frac{\partial u}{\partial t} \right)^2 + \frac{\partial^2 F}{\partial u \partial v} \frac{\partial v}{\partial t} \frac{\partial u}{\partial t} = \\
\frac{\partial^2 F}{\partial u^2} (\Delta u - h_1(u, v))^2 + \frac{\partial^2 F}{\partial u \partial v} (G(u, v) + \Delta v)(\Delta u - h_1(u, v))
\end{align*}
\]

\[
\begin{align*}
\frac{\partial^2 F}{\partial v^2} \left( \frac{\partial G}{\partial u} \frac{\partial u}{\partial t} + \frac{\partial G}{\partial v} \frac{\partial v}{\partial t} \right) = \frac{\partial^2 F}{\partial v^2} \left( \frac{\partial u}{\partial t} \right)^2 + \frac{\partial^2 F}{\partial v^2} \frac{\partial v}{\partial t} \frac{\partial u}{\partial t} = \\
\frac{\partial^2 F}{\partial v^2} (\Delta u - h_1(u, v))(G(u, v) + \Delta v) + \frac{\partial^2 F}{\partial v^2} (G(u, v) + \Delta v)^2
\end{align*}
\]
Substitution of expressions (3.27), (3.28), (3.30), (3.32) in (3.24) provides

\[ 0 = \left( \frac{1}{\epsilon} \right)^2 \left( \frac{\partial F}{\partial u} \right)^2 F(u, v) + \frac{1}{\epsilon} \left( \frac{\partial F}{\partial u} \right)^2 \Delta u + \frac{1}{\epsilon} \frac{\partial F}{\partial u} \frac{\partial F}{\partial v} (G(u, v) + \Delta v) + \frac{\partial F}{\partial u} \Delta (\frac{\partial u}{\partial t}) + \quad (3.33) \]

\[ \frac{\partial F}{\partial v} \left( \frac{\partial G}{\partial u} (\Delta u - h_1(u, v)) + \frac{\partial G}{\partial v} (G(u, v) + \Delta v) + \Delta (\frac{\partial v}{\partial t}) \right) + \quad (3.34) \]

\[ \frac{\partial^2 F}{\partial u \partial v} (\Delta u - h_1(u, v))^2 + \frac{\partial^2 F}{\partial u \partial v} (G(u, v) + \Delta v)(\Delta u - h_1(u, v)) + \quad (3.35) \]

\[ \frac{\partial^2 F}{\partial v^2} (\Delta u - h_1(u, v))(G(u, v) + \Delta v) + \frac{\partial^2 F}{\partial v^2} (G(u, v) + \Delta v)^2 \quad (3.36) \]

Multiplication of (3.36) by \( \epsilon^2 \left( \frac{\partial F}{\partial u} \right)^2 \) yields

\[ 0 = F(u, v) + \epsilon \Delta u + \epsilon \left( \frac{\partial F}{\partial u} \right)^{-1} \frac{\partial F}{\partial v} (G(u, v) + \Delta v) + \quad (3.37) \]

\[ \epsilon^2 \left( \frac{\partial F}{\partial u} \right)^{-2} \left( \frac{\partial F}{\partial u} \Delta (\frac{\partial u}{\partial t}) + \frac{\partial F}{\partial v} \left( \frac{\partial G}{\partial u} (\Delta u - h_1(u, v)) + \frac{\partial G}{\partial v} (G(u, v) + \Delta v) + \Delta (\frac{\partial v}{\partial t}) \right) + \quad (3.38) \]

\[ \frac{\partial^2 F}{\partial u \partial v} (\Delta u - h_1(u, v))^2 + 2 \frac{\partial^2 F}{\partial u \partial v} (G(u, v) + \Delta v)(\Delta u - h_1(u, v)) + \frac{\partial^2 F}{\partial v^2} (G(u, v) + \Delta v)^2 \right). \quad (3.39) \]

Finally, denote

\[ h_2(u, v) = \left( \frac{\partial F}{\partial u} \right)^{-2} \left( \frac{\partial F}{\partial u} \Delta (\frac{\partial u}{\partial t}) + \frac{\partial F}{\partial v} \left( \frac{\partial G}{\partial u} (\Delta u - h_1(u, v)) + \frac{\partial G}{\partial v} (G(u, v) + \Delta v) + \Delta (\frac{\partial v}{\partial t}) \right) + \quad (3.40) \]

\[ \frac{\partial^2 F}{\partial u \partial v} (\Delta u - h_1(u, v))^2 + 2 \frac{\partial^2 F}{\partial u \partial v} (G(u, v) + \Delta v)(\Delta u - h_1(u, v)) + \frac{\partial^2 F}{\partial v^2} (G(u, v) + \Delta v)^2 \right) \]

Therefore, the second order approximation is given by

\[ 0 = F(u, v) + \epsilon h_1(u, v) + \epsilon^2 h_2(u, v). \quad (3.41) \]

4. 3D Michaelis-Menten model with Laplacian

An illustration of the suggested approximation scheme for a system with the diffusion is presented for a benchmark model below. We consider the 3D Michaelis-Menten model. The mathematical model consists of three ODEs

\[ \frac{dX}{dt} = -XZ + L_1(1 - Z - \mu(1 - Y)) \quad (4.1) \]

\[ \frac{dY}{dt} = -L_3 YZ + \frac{L_4}{L_2}(1 - Y) \quad (4.2) \]

\[ \frac{dZ}{dt} = \frac{1}{L_2}((-XZ + 1 - Z - \mu(1 - Y)) + \mu) - L_3 YZ + \frac{L_4}{L_2}(1 - Y)) \quad (4.3) \]
The system parameters are \( L_1 = 0.99, L_2 = 1, L_3 = 0.05, L_4 = 0.1, \mu = 1 \) (see e.g. [24] for details and references). By taking the diffusion into account we obtain the following PDE system with the diffusion constant \( \delta = 0.01 \):

\[
\frac{\partial X}{\partial t} = -XZ + L_1(1 - Z - \mu(1 - Y)) + \delta \Delta X \quad (4.4)
\]
\[
\frac{\partial Y}{\partial t} = -L_3YZ + \frac{L_4}{L_2}(1 - Y) + \delta \Delta Y \quad (4.5)
\]
\[
\frac{\partial Z}{\partial t} = \frac{1}{L_2} \left( (-XZ + 1 - Z - \mu(1 - Y)) + \mu \right) - L_3YZ + \frac{L_4}{L_2}(1 - Y)) + \delta \Delta Z \quad (4.6)
\]

The system (4.4) - (4.6) is considered with the following initial and boundary conditions:
$$\begin{align*}
X(t,0) = X_{eq} \\
Y(t,0) = Y_{eq} \\
Z(t,0) = Z_{eq}
\end{align*}$$\hspace{1cm}(4.7)

$$\begin{align*}
X(t,1) = 2 \\
Y(t,1) = 0 \\
Z(t,1) = 1
\end{align*}$$\hspace{1cm}(4.8)

$$\begin{align*}
X(0,x) = (2 - X_{eq})x + X_{eq} \\
Y(0,x) = (-Y_{eq})x + Y_{eq} \\
Z(0,x) = (1 - Z_{eq})x + Z_{eq}
\end{align*}$$\hspace{1cm}(4.9)

Here \((X_{eq}, Y_{eq}, Z_{eq})\) are coordinates of the equilibrium point that are calculated numerically and \(x\) is spatial variable. Initial conditions are chosen to be straight lines, they satisfy the general assumption - join initial and equilibrium values on boundaries.

As in the previous section the main assumption is the transport term is slow compared with the fast vector field. First, several numerical experiments were performed drawing a 2D slow manifold and stationary solution of the system. Figure 3.1 shows a connection between the zero approximation of the slow manifold and the profile of the stationary system solution to the PDE in the original coordinates \((x, y, z)\). In the Fig. 3.1 the stationary solution can be roughly divided into two parts: the slow part of the stationary solution that is very close to the slow invariant manifold and the second one, which is asymptotically close to the fast sub-field of the system shown by the dashed line. The small third part conjugates the slow and fast parts and can be asymptotically neglected. This simulation demonstrates that the proposed machinery of singularly perturbed profiles is relevant to the problem under consideration. It means that the original system (4.4) - (4.6) can be decomposed into two subsystems: the slow one and the fast one.

In order to implement the scheme described above we apply the GQL method \[5, 8\] to convert the model to a system in the standard SPS form in the new coordinate set \((U,V,W)\). The transformation between \((X,Y,Z)\) and \((U,V,W)\) is

$$\begin{align*}
X &= 0.73U - 0.19V - 0.66W \\
Y &= -0.05U + 0.94V - 0.33W \\
Z &= 0.68U + 0.28V + 0.68W.
\end{align*}$$\hspace{1cm}(4.10-4.12)

Figure 4.1 shows the zero approximation of the slow manifold and trajectory to PDE's solution in the decomposed coordinate system \[12\]. As it has to be in Fig. 4.1 the fast part (which does not belong to the manifold and shown by a dashed line) is approximated by a parallel line to \(U\) coordinate.

At present we concentrate mainly on the slow part, because the fast part is very simple and asymptotically corresponds to one dimensional fast manifold defining a projection of the initial data to the slow manifold in pure homogeneous system. Thus, following the main analytic results we compare the zero and the first order approximation of the slow part of system solution stationary profiles. Figure 4.2 illustrates the stationary solution profiles on the zero order approximation

$$H_0 := F(U(x,t), V(x,t), W(x,t)) = 0$$
and on the first order approximation

\[ H_1 := F(U(x,t), V(x,t), W(x,t)) + \epsilon h_1(U(x,t), V(x,t), W(x,t)) = 0 \]

of the system slow manifold.

Here \( H_0 := F(U, V, W) \) is an implicit form of 2D slow manifold for 3D Michaelis-Menten model given by the left-hand side of the fast part (for variable \( U \)) of the SPS system, namely,

\[ H_0 = F(U, V, W) = 0.007(0.06 - 0.7U^2 + 0.07V^2 + U(-1.03 - 0.12V - 0.06W) + V(0.88 + 0.42W) - 1.4W + 0.63W^2) = 0 \]

Figure 4.2 shows \( H_0(U(x,t), V(x,t), W(x,t)) \) and \( H_1(U(x,t), V(x,t), W(x,t)) \) approximations given in the implicit form. Thus, the error of the approximation can be easily estimated. In this figure we can see that the first order approximation of the profile is more accurate than the zero order approximation.
Figure 4.2. Dashed line matches the solution profile on the zero order approximation and thick line matches the solution profile on the first order approximation with a logarithmically scaled y axis.

The next Fig. 4.3 illustrates the zero order approximation of the slow manifold and the solution profile trajectory of the PDE’s solution in the decomposed coordinate system for the system with boundary condition close to the slow manifold. In Fig. 4.3 the fast part of the system solution profile, which does not belong to the manifold, vanishes.

Similarly to Fig. 4.2, Fig. 4.4 illustrates the stationary solution profiles on the zero order approximation given in the implicit form by the RHS of U, namely, by

$$H_0(U(x, t), V(x, t), W(x, t)) := F(U(x, t), V(x, t), W(x, t))$$

and by the first order correction term correspondingly $$H_1 := (U(x, t), V(x, t), W(x, t)) :$$

$$F(U(x, t), V(x, t), W(x, t)) + c h_1(U(x, t), V(x, t), W(x, t))$$

By comparing of Figs. 4.2 and 4.4 we can see that the approximation error for the system with the boundary condition placed closer to slow manifold is less than for the system with the boundary condition far from slow manifold.

5. Conclusion

The formal functional series for the system in the standard SP form was used to study and approximate the REDIM (as a manifold made of the system solutions profiles). If the transport/diffusion term is considered as a first order correction to the system in the standard SPS form, under assumption we do know the transformation leading to this special form, then the correction terms were estimated until the second order in general form of the transport term. The spatial form of the diffusion described by the Laplacian was used to illustrate and estimate the correction terms explicitly. It was found that the correction terms are spatially dependent and can be evaluated on e.g. system solution profiles (stationary or transient). The results were illustrated and validated by the well known example of Michaelis-Menten enzyme model extended by the Laplace operator. Effects of the system decomposition, influence of the boundary conditions and diffusion transport was studied.
Figure 4.3. System state space (U,V,W) after transformation to the standard SPS form, 2D slow manifold (mesh) and stationary solution profile (black curve) for model with boundary condition which is very close to slow manifold.

Acknowledgments

The financial support by DFG, especially within the GIF (Grant 1162-148.6/2011) project is gratefully acknowledged.

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Figure 4.4. The system with boundary condition close to slow manifold. Dashed line matches the solution profile on the zero order approximation and thick line matches the solution profile on the first order approximation with a logarithmically scaled y axis.

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