Noname manuscript No.
(will be inserted by the editor)

Parameterisations of Slow Invariant Manifolds: Application to a Spray Ignition and Combustion Model

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Received: date / Accepted: date

Abstract A wide range of dynamic models, including those of heating, evaporation and ignition processes in fuel sprays, is characterised by large differences in the rates of change of variables. Invariant manifold theory is an effective technique for investigation of these systems. In constructing the asymptotic expansions of slow invariant manifolds it is commonly assumed that a limiting algebraic equation allows one to find a slow surface explicitly. This is not always possible due to the fact that the degenerate equation for this surface (small parameter equal to zero) is either a high degree polynomial or transcendental. In many problems, however, the slow surface can be described in a parametric form. In this case, the slow invariant manifold can be found in parametric form using asymptotic expansions. If this is not possible, it is necessary to use an implicit presentation of the slow surface and obtain asymptotic representations for the slow invariant manifold in an implicit form. The results of development of the mathematical theory of these approaches and the applications of this theory to some examples related to modelling combustion processes, including those in sprays, are presented.

Keywords Invariant manifold · System order reduction · spray ignition and combustion

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1 Introduction

Modelling of the processes in sprays is a challenging task. It includes the analysis of equations describing coupled fluid dynamics, heat/mass transfer, and ignition/combustion (in the case of fuel sprays) processes in a complex geometry. To take into account the complexity of this geometry, the enclosures (e.g. internal combustion engine chambers) should be split up into millions of cells. The parameters of the continuous phase in each of these cells are constant, but they change over time and from one cell to another. Moreover, the dynamics of the dispersed phase (fuel droplets) and chemical reactions in each cell need to be taken into account. The number of these droplets and chemical reactions in each cell can be many thousands in the general case (e.g. [1,2, 3]). These features of the modelling of spray processes make it impossible to perform their rigorous quantitative analysis. Two main approaches have been developed to deal with this complexity. The first approach is based on the application of rather simplistic physical models of individual processes, but the geometry of the enclosure is approximated as accurately as possible. This approach is incorporated in most commercial Computational Fluid Dynamics (CFD) codes and is most widely used in engineering applications. The second approach is focused on in-depth development of the physical models of individual processes, ignoring the complexities of the geometry and details of interactions between various processes [4]. These two approaches are not contradictory but rather complementary. In a series of our papers, summarised in [4], an attempt was made to develop the third approach to this modelling. This approach is based on establishing a hierarchy of the processes involved (recognising multiple scales in time and space) and finding a compromise between the accuracy of the models and their computer efficiency.

An alternative approach to modelling multi-scale spay processes in individual cells could be based on the theory of invariant manifolds, in which the original system is replaced by another system on an invariant manifold of lower dimension. Despite its obvious attractiveness, this approach is still rarely used in engineering applications (as one of few exceptions we can refer to the old paper [5]). The main reasons for this are: that this approach is still based on a number of assumptions, the applicability of which to engineering systems is far from obvious; the mathematical complexity of the theory; and non-familiarity with this theory by the engineering community at large. The main aim of this paper is to address all three of these factors which will hopefully make this approach more 'friendly' to the engineering community. Further developments of the theory will be performed. Many details of the mathematical analysis, commonly omitted in mathematical publications, will be presented, and the paper is submitted to a journal with mainly engineering readership.

The lowering of the dimensions of the original system describing coupled heat/mass transfer, and ignition/combustion processes in sprays (fluid dynamic processes are not considered) occurs due to decomposition of the original system in the vicinity of the invariant surface into 'slow' and 'fast' subsystems. If the slow invariant manifold is attractive then the analysis of the original system can be replaced with the analysis of the slow subsystem. Asymptotic expansions of slow invariant manifolds in the vicinity of slow surfaces were suggested in [6]-[8]. In terms of perturbation theory slow invariant manifolds are associated with outer (slow) solutions, while fast invariant manifolds are associated with the boundary layer (fast) corrections.

An asymptotic method using slow invariant manifolds in an implicit form was suggested in [9] (see also [10] and [11]). This approach is related to the method of intrinsic low-dimensional manifolds (ILDM) proposed by Maas and Pope [11]. The iterative method was proposed by Fraser [12], and further developed by Fraser and Roussel [13] for autonomous systems that are linear with respect to fast variables in the case of scalar slow and fast variables. This method was extended to the nonautonomous systems with vector variables in [11].

All these methods are related to the invariant manifold method. The links between these methods were demonstrated in [14], where an overview of reduction methods in chemical kinetics was presented (see [11] for further details).

A slow invariant manifold of a singularly perturbed system can be presented as an explicit, implicit or parametric function. To illustrate this, let us consider the following system:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = y, \quad \varepsilon\frac{\mathrm{d}y}{\mathrm{d}t} = x - y^2, \tag{1}$$

the exact slow invariant manifold of which could be presented in an explicit form. A possible parametric presentation of this manifold is as follows

$$x = v^2 + \varepsilon/2, \quad y = v, \quad \frac{\mathrm{d}v}{\mathrm{d}t} = \frac{1}{2}.$$

It is well known that any curve or surface can be parameterised in an infinite number of ways. The method chosen above has the advantage that one of the variables of the system under consideration plays the role of a parameter.

In the case shown in Fig. 1, the slow invariant manifold consists of two leaves; the explicit form of the stable (attractive) leaf is $y = \sqrt{x - \varepsilon/2}$, $\frac{\mathrm{d}x}{\mathrm{d}t} = \sqrt{x - \varepsilon/2}$, and the explicit form of the unstable (repelling) leaf is $y = -\sqrt{x - \varepsilon/2}$, $\frac{\mathrm{d}x}{\mathrm{d}t} = -\sqrt{x - \varepsilon/2}$.

In constructing asymptotic expansions of slow invariant manifolds, it is commonly assumed that the degenerate (limiting) equation allows one to find a slow surface (invariant manifold in the limit $\varepsilon \to 0$) explicitly, as in the case of the abovementioned example. In many problems, however, this is not possible due to the fact that the degenerate equation is either a high degree polynomial or transcendental. An alternative approach is based on the observation that the slow surface can be described implicitly and even in a parametric form. The approaches based on the presentation of slow surfaces in parametric or implicit forms have never been applied to the analysis of equations describing fuel spray ignition and combustion, to the best of our knowledge.

The theoretical background of these approaches is discussed in Section 2. In Section 3, the application of one of these approaches is illustrated for examples taken from the theory of heating, evaporation, ignition and combustion of fuel

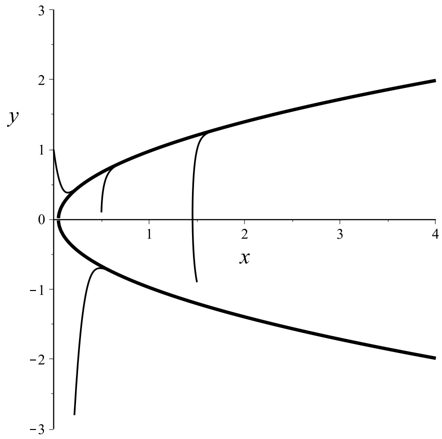

Fig. 1 The slow invariant manifold (thick curve) and four representative trajectories (thin curves) of System (1) for $\varepsilon = 0.1$

sprays in Diesel engine-like conditions (see [15] and [16]). The main results of the paper are summarised in Section 4.

The preliminary results of our analysis were presented in [17]. The approach described in this paper is complementary to the one suggested in [18].

2 Theoretical background

In constructing asymptotic expansions of slow invariant manifolds it is commonly assumed that the degenerate equation (with small parameter $\varepsilon = 0$) allows one to find an explicit expression for the slow surface. As mentioned in Section 1, on many occasions this is not possible, but the slow invariant manifold can be found in a parametric form using asymptotic expansions [11]. Alternatively, one might need to obtain asymptotic representations for the slow invariant manifold in implicit forms. In what follows, basic principles of constructing manifolds in both cases are described, and characteristic examples illustrating this, including those taken from spray combustion theory, are presented and analysed.

2.1 Explicit and Implicit Slow Invariant Manifolds

Let us consider the following autonomous system:

$$\left.\begin{aligned} \dot{x} &= f(x,y) \\ \varepsilon\dot{y} &= g(x,y) \end{aligned}\right\}, \tag{2}$$

where $0 < \varepsilon \ll 1$, $x \in \mathcal{R}^m$, $y \in \mathcal{R}^n$, $\mathcal{R}^{m+n} = \mathcal{R}^m \times \mathcal{R}^n$. A surface $y = \aleph(x, \varepsilon)$ is called a slow invariant manifold of System (2) if any trajectory $x = x(t, \varepsilon)$, $y = y(t, \varepsilon)$ of System (2) that has at least one common point $x = x_0$, $y = y_0$ with the surface $y = \aleph(x, \varepsilon)$, i.e. $y_0 = \aleph(x_0, \varepsilon)$, lies entirely on this surface, i.e. $y(t, \varepsilon) = \aleph(x(t, \varepsilon), \varepsilon)$.

This definition is based on the explicit representation $y = \aleph(x, \varepsilon)$ of the manifold. Let the degenerate equation

$$g(x, y) = 0 \tag{3}$$

has solution $y = \phi(x)$. A surface described as $y = \phi(x)$ is called a slow surface or slow manifold (e.g. [11]). If functions f, g, and ϕ are sufficiently smooth and the eigenvalues $\lambda_i = \lambda_i(x)$ $(i = 1, \ldots, n)$ of the matrix $g_y(x, \phi(x))$ satisfy the conditions

$$|\mathrm{Re}\,\lambda_\mathrm{i}| \geq \gamma > 0, \quad \mathrm{i} = 1, \ldots, \mathrm{n}, \tag{4}$$

then the approximation to $\aleph(x, \varepsilon)$ can be obtained as an asymptotic expansion in powers of ε [6]. Note that Condition (4) guarantees that matrix $g_y^{-1}(x, \phi(x))$ exists and its norm is bounded in the corresponding domain in $\mathcal{R}^m$ [11]. Moreover, if (4) takes the form of

$$\mathrm{Re}\,\lambda_\mathrm{i} \leq -\gamma < 0, \quad \mathrm{i} = 1, \ldots, \mathrm{n},$$

then the invariant manifold $\aleph(x, \varepsilon)$ is attractive and can be used for order reduction of System (2).

It is not always possible to find function $y = \phi(x) = \aleph(x, 0)$ from the degenerate equation (Equation (3)). In this case the slow invariant manifold can be obtained in an implicit form

$$G(x, y, \varepsilon) = 0, \tag{5}$$

and the flow on this manifold is described by the first equation in System (2), in which x and y satisfy (5). In this case function G can be found from the invariance equation [11]:

$$G_y(x, y, \varepsilon) g(x, y) + \varepsilon G_x(x, y, \varepsilon) f(x, y) = 0. \tag{6}$$

This equation is the result of differentiation of (5) remembering (2).

Let us now calculate partial derivatives of function $\aleph(x, \varepsilon)$, which describes the slow invariant manifold $y = \aleph(x, \varepsilon)$. Remembering (5) we find

$$G_x + G_y \aleph_x = 0,$$

i.e. $\aleph_x = -G_y^{-1} G_x$.

Having substituted this expression for the partial derivative of $\aleph$ into the invariance equation in the form $\varepsilon \aleph_x f = g$ we obtain

$$-\varepsilon G_y^{-1} G_x f = g,$$

which is identical to Equation (6) under the condition that $\det G_y \neq 0$.

The zeroth approximation to the flow on the slow invariant manifold (slow surface) is described by the differential-algebraic system:

$$\dot{x} = f(x, y), \tag{7}$$

$$0 = g(x, y) \equiv G(x, y, 0). \tag{8}$$

To obtain the first order approximation, one needs to find the full derivative of $g \equiv g(x, y)$ with respect to time:

$$\frac{\mathrm{d}}{\mathrm{d}t} g = \frac{1}{\varepsilon} g_y g + g_x f. \tag{9}$$

When calculating the right hand side of this equation, (2) was used. Remembering (7)–(9), the slow invariant manifold is described by the following system of differential-algebraic equations:

$$\dot{x} = f(x, y), \tag{10}$$

$$g_y g + \varepsilon g_x f = 0. \tag{11}$$

Equation (11) may be rewritten in a more convenient form when $\det g_y \neq 0$:

$$g + \varepsilon g_y^{-1} g_x f = 0. \tag{12}$$

or

$$g + \varepsilon N = 0, \tag{13}$$

where $N = g_y^{-1} g_x f$. We recover (8) (the zeroth approximation) by setting $\varepsilon = 0$.

To obtain the second order approximation, we need to set the second derivative of $g(x, y)$ to zero, using (2). In this case, after differentiating $\varepsilon(g + \varepsilon N) = 0$ with respect to t, and remembering that $g_t = 0$ and $N_t = 0$, we obtain:

$$\varepsilon \frac{\mathrm{d}}{\mathrm{d}t}(g + \varepsilon N) = g + \varepsilon N + \varepsilon g_y^{-1} N_y g + \varepsilon^2 g_y^{-1} N_x f.$$

Setting the right hand side of this equation to zero we find:

$$g + \varepsilon \left[N + g_y^{-1} N_y g \right] + \varepsilon^2 g_y^{-1} N_x f = 0. \tag{14}$$

Since the second order approximation differs from the first one by the terms of order $O(\varepsilon^2)$, we expect $\varepsilon g_y^{-1} N_y g = O(\varepsilon^2)$. This can be proven remembering that $g = -\varepsilon N$ (see Expression (13)). In this case, $\varepsilon g_y^{-1} N_y g = -\varepsilon^2 g_y^{-1} N_y N$. Hence, Equation (14) can be rewritten as:

$$g + \varepsilon N + \varepsilon^2 g_y^{-1} (N_x f - N_y N) = 0. \tag{15}$$

This is the second order approximation to the slow invariant manifold, the flow on which is described by Equation (10).

A stability analysis of slow invariant manifolds is presented in Section 2.2 of [11] in the general case. In the case of scalar y the condition for attractivity of these manifolds is simplified to the statement:

$$\frac{\partial g(x,y)}{\partial y} < 0 \tag{16}$$

on the slow manifold $g(x,y) = 0$.

Note that if functions $f = f(x,y,\varepsilon)$ and $g = g(x,y,\varepsilon)$ in (2) are sufficiently smooth, then the above formulae for the approximations to the slow invariant manifold are still valid. There is no need to take into account terms of order $O(\varepsilon)$ in the zero order approximation, and terms of order $O(\varepsilon^2)$ in the first order approximation. In the general case, in the k–order approximation all higher order terms in the expansions can be ignored.

As an illustration, we consider the following system describing the classical heat explosion model with reactant consumption [21,22,23]:

$$\frac{\mathrm{d}\eta}{\mathrm{d}\tau} = -\eta e^{\theta} = f(\eta,\theta), \tag{17}$$

$$\varepsilon\frac{\mathrm{d}\theta}{\mathrm{d}\tau} = \eta e^{\theta} - \alpha\theta = g(\eta,\theta), \tag{18}$$

where θ, η and τ are dimensionless temperature, fuel concentration, and time, respectively. This system is autonomous and the theory described above can be applied to it.

The zero-order approximation to the slow invariant manifold is:

$$g = \eta e^{\theta} - \alpha\theta = 0, \tag{19}$$

which implies that $\eta(\theta) = \alpha\theta e^{-\theta}$. This manifold is stable when $\eta e^{\theta} - \alpha < 0$ (see Condition (16)). As Equation (19) cannot be explicitly solved with respect to the fast variable θ, its implicit solution is used to obtain approximations to the slow invariant manifold.

The first order approximation $g + \varepsilon g_\eta f/g_\theta = 0$ can be rewritten as:

$$\eta e^{\theta} - \alpha\theta - \varepsilon\eta e^{2\theta}/g_\theta = 0,$$

where $g_\theta = \eta e^{\theta} - \alpha$. The equation for the second order approximation $g + \varepsilon N + \varepsilon^2 g_\theta^{-1}(N_\eta f - N_\theta N) = 0$ can be presented as:

$$\eta e^{\theta} - \alpha\theta - \varepsilon\eta e^{2\theta}/g_\theta - \varepsilon^2\left(\alpha\eta e^{3\theta}/g_\theta^3 + \eta^2 e^{4\theta}(\eta e^{\theta} - 2\alpha)/g_\theta^4\right) = 0,$$

since $N = g_\eta f/g_\theta = -\eta e^{2\theta}/g_\theta, N_\eta = \alpha e^{2\theta}/g_\theta^2, N_\theta = -\left(\eta^2 e^{\theta} - 2\alpha\eta\right) e^{2\theta}/g_\theta^2$. These approximations are compared in Fig. 2. As can be seen from this figure, none of the approximations are really good near the critical point $\theta = 1$, where $g_\theta = 0$. Except in the vicinity of this point, the difference between the slow invariant manifold and its first- and second-order approximation is small and can be ignored in most engineering applications.

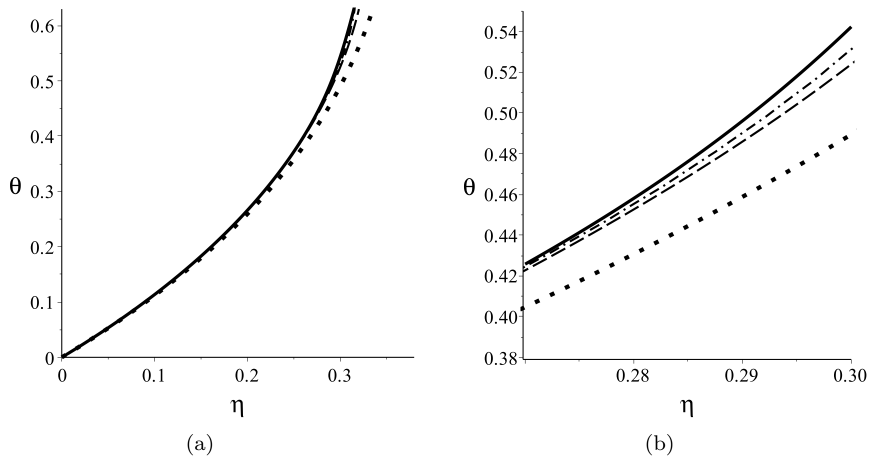

Fig. 2 (a) The slow invariant manifold (solid thick curve), the slow curve (dotted), the first-order approximation (dashed), the second-order approximation (dash–dotted) to the slow invariant manifold of (17); $\varepsilon = 0.01$, $\alpha = 1$. (b) Zoomed part of the plots for $0.27 < \eta < 0.3$.

2.2 Parametric Representation of Invariant Manifolds

As mentioned earlier, in many problems, the analysis of which is based on invariant manifolds, it is not possible to find an explicit solution to equation $g(x, y, 0) = 0$, but this solution can be found in a parametric form:

$$x = \chi_0(v), \qquad y = \varphi_0(v),$$

where $v \in \mathcal{R}^m$, and the following identity holds

$$g(\chi_0(v), \varphi_0(v), 0) \equiv 0.$$

In this case, the slow invariant manifold may also be found in a parametric form:

$$x = \chi(v, \varepsilon), \qquad y = \varphi(v, \varepsilon),$$

where $\chi(v, 0) = \chi_0(v)$, $\varphi(v, 0) = \varphi_0(v)$. The flow on the invariant manifold is described by the following equation:

$$\dot{v} = F(v, \varepsilon), \tag{20}$$

where function $F(v, \varepsilon)$ is determined later. Functions χ, φ, and F can be presented as the following asymptotic expansions:

$$\begin{aligned} \chi(v, \varepsilon) &= \chi_0(v) + \varepsilon\chi_1(v) + \ldots + \varepsilon^k\chi_k(v) + \ldots, \\ \varphi(v, \varepsilon) &= \varphi_0(v) + \varepsilon\varphi_1(v) + \ldots + \varepsilon^k\varphi_k(v) + \ldots, \\ F(v, \varepsilon) &= F_0(v) + \varepsilon F_1(v) + \ldots + \varepsilon^k F_k(v) + \ldots . \end{aligned} \tag{21}$$

Remembering (2) and (20), we obtain:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{\mathrm{d}\chi(v,\varepsilon)}{\mathrm{d}t} = \frac{\partial\chi}{\partial v}F = f(\chi,\varphi,\varepsilon), \tag{22}$$

$$\varepsilon\frac{\mathrm{d}y}{\mathrm{d}t} = \varepsilon\frac{\mathrm{d}\varphi(v,\varepsilon)}{\mathrm{d}t} = \varepsilon\frac{\partial\varphi}{\partial v}F = g(\chi,\varphi,t,\varepsilon). \tag{23}$$

Equating coefficients before powers of small parameter ε we obtain equations:

$$\frac{\partial\chi_0}{\partial v}F_0 = f(\chi_0,\varphi_0,0), \qquad g(\chi_0,\varphi_0,0) = 0,$$

(zero order approximation) and

$$\frac{\partial\chi_1}{\partial v}F_0 + \frac{\partial\chi_0}{\partial v}F_1 = f_x(\chi_0,\varphi_0,0)\chi_1 + f_y(\chi_0,\varphi_0,0)\varphi_1 + f_1,$$

$$\frac{\partial\varphi_0}{\partial v}F_0 = g_x(\chi_0,\varphi_0,0)\chi_1 + g_y(\chi_0,\varphi_0,0)\varphi_1 + g_1,$$

(first order approximation), where

$$f_1 = \left.\frac{\partial f}{\partial\varepsilon}\right|_{\chi_0,\varphi_0,0}, \quad g_1 = \left.\frac{\partial g}{\partial\varepsilon}\right|_{\chi_0,\varphi_0,0}.$$

This process can continue to obtain higher order approximations.

Two vector equations, describing the zero order approximation, contain three unknown vector functions χ_0, φ_0 and F_0. This is equivalent to $m+n$ scalar equations containing $m+n+m$ unknown scalar functions. The number of free unknown functions coincides with the dimension of vector v (dimensionality of vector x or function χ). The same statement applies to the equations describing the first order approximation.

In the general case, Equations (22) and (23) contain unknown functions χ, φ, F. In some specific problems it is possible to consider one of these functions, or any scalar components of χ, φ and F, as known functions. The remaining functions may be found from (22) and (23). Moreover, it is possible at any step of the calculation of the coefficients in (21) to choose any m components of these coefficients as given functions. In the case when F is a given or known function, Equations (22) and (23) can be used to calculate the coefficients in the asymptotic expansions of χ and φ. If it is possible to predetermine function χ, these equations allow us to calculate F and φ. To clarify this we consider several examples.

If y on the manifold can be presented in the explicit form $y = \aleph(x,\varepsilon)$, we can assume that $x = v$ and write

$$\chi = v, \quad \varphi = \aleph(v,\varepsilon), \quad F = f(v,\aleph(v,\varepsilon),\varepsilon),$$

since $\dot{v} = \dot{x} = f$. Then Equation (23) takes the form

$$\varepsilon\frac{\partial\aleph}{\partial v}f(v,\aleph,\varepsilon) = g(v,\aleph,\varepsilon).$$

Let us now assume that $y = v$, provided that dim $x =$ dim y (dimensions of x and y are the same). In this case, $\varphi = v$ and

$$\frac{\partial \chi}{\partial v} F = f(\chi, v, \varepsilon), \quad g(\chi, v, \varepsilon) = \varepsilon F. \tag{24}$$

When deriving this equation, (20) and the second equation in System (2) (see also (22)) were used. The equation for χ follows directly from Equation (24):

$$\frac{\partial \chi}{\partial v} g(\chi, v, \varepsilon) = \varepsilon f(\chi, v, \varepsilon).$$

Assuming that $\det(\frac{\partial \chi_0}{\partial v}) \neq 0$, it is possible to calculate χ using its asymptotic expansion with respect to ε. Note that the condition $g(\chi_0, \varphi_0, 0) = 0$ implies that Equation (20) is regularly perturbed with respect to ε. This follows from the fact that $F = O(1)$ as $\varepsilon \to 0$ (see the second equation in (24)).

Three cases of effective parameterization for System (2) with slow variable x ($\dim x = m$) and fast variable y ($\dim y = n$) are considered in the Appendix.

3 Spray ignition and combustion model

In this section some of the mathematical tools described above are applied to the analysis of the system of equations for spray ignition and combustion.

The analysis is based on the model developed in [16], where spray ignition and combustion are considered as an explosion process. The endothermic (droplet evaporation) versus exothermic (combustion in the gaseous phase) competition determines explosion regimes. The analysis is focused on a spatially homogeneous mixture of an optically thin, combustible gas with a monodispersed spray of evaporating fuel droplets. Both convective and radiative heating of droplets are taken into account. The effect of droplets on the incident radiation and the effects of droplet movement are ignored. It is assumed that the incident radiation is absorbed inside semi-transparent droplets. The system is assumed to be adiabatic and gas pressure is assumed to be constant. The thermal conductivity of the liquid phase is assumed to be infinitely large. The effects of the Stefan flow on droplet heating and evaporation are ignored (Nu=Sh=2). The heat transfer coefficient of the mixture is assumed to be controlled by the thermal properties of the gaseous component. The ignition and combustion processes are described by the first order exothermic reaction, taking place in the gaseous phase. See [4] and [20] for further discussion of these assumptions.

Given these assumptions the spray ignition and combustion process is described by the following equations [16]:

$$c_{pg}\rho_g\varphi_g \frac{\mathrm{d}T_g}{\mathrm{d}t} = \dot{\omega} M_f Q_f \varphi_g - 4\pi R_d^2 n_d q_c, \tag{25}$$

$$\frac{\mathrm{d}C_f}{\mathrm{d}t} = -\nu_f \dot{\omega} + 4\pi R_d^2 n_d \frac{(q_c + q_r)}{L M_f \varphi_g} \left(1 - \zeta(T_d)\right), \tag{26}$$

$$\frac{dC_{ox}}{dt} = -\nu_{ox}\dot{\omega}, \tag{27}$$

$$c_f m_d \frac{\mathrm{d}T_d}{\mathrm{d}t} = 4\pi R_d^2 (q_c + q_r)\zeta(T_d), \tag{28}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{4}{3}\pi R_d^3 \rho_f\right) = -4\pi R_d^2 \frac{(q_c + q_r)}{L} \left(1 - \zeta(T_d)\right), \tag{29}$$

with the initial conditions

$$T_d(0) = T_{d0}, \quad T_g(0) = T_{g0}, \quad R_d(0) = R_{d0}, \quad C_f(0) = C_{f0}, \quad C_{ox}(0) = C_{ox0},$$

where

$$\dot{\omega} = C_f^{af} C_{ox}^{bx} A \exp\left(-\frac{E}{RT_g}\right), \quad \zeta(T_d) = \frac{T_b - T_d}{T_b - T_{d0}}, \quad q_c = h_c(T_g - T_d),$$

$$h_c = \frac{\lambda_g}{R_d}, \quad q_r = k_1 \sigma T_{\mathrm{ext}}^4, \quad k_1 = a R_d^b,$$

$$a = a_0 + a_1 \left(\frac{T_{\mathrm{ext}}}{10^3}\right) + a_2 \left(\frac{T_{\mathrm{ext}}}{10^3}\right)^2, \tag{30}$$

$$b = b_0 + b_1 \left(\frac{T_{\mathrm{ext}}}{10^3}\right) + b_2 \left(\frac{T_{\mathrm{ext}}}{10^3}\right)^2. \tag{31}$$

Gas is assumed to be optically thin (radiative temperature is equal to the external temperature T_{ext}). We assume that $\rho_g \varphi_g = \mathrm{const}$ and the process takes place at constant pressure (approximation of Diesel engine-like conditions).

Introducing the dimensionless variables:

$$\theta_g = \frac{E}{RT_{d0}} \frac{T_g - T_{d0}}{T_{d0}}, \quad \theta_d = \frac{E}{RT_{d0}} \frac{T_d - T_{d0}}{T_{d0}}, \quad r = \frac{R_d}{R_{d0}}, \quad \eta = \frac{C_f}{C_{ff}}, \quad \xi = \frac{C_{ox}}{C_{ox0}},$$

$$\tau = \frac{t}{t_{\mathrm{react}}}, \quad t_{\mathrm{react}} = \frac{1}{A C_{ff}^{af-0.5} C_{ox0}^{bx-0.5}} \exp\left(\frac{1}{\beta}\right), \quad \beta = \frac{RT_{d0}}{E},$$

$$\gamma = \frac{c_{pg} T_{d0} \rho_g \beta}{(C_{ox0} C_{ff})^{0.5} Q_f M_f}, \quad C_{ff} = \frac{4\pi}{3} R_{d0}^3 \rho_f n_d \frac{1}{M_f}(1 + \omega_f), \quad \omega_f \ll 1,$$

$$\varepsilon_1 = \frac{4\pi R_{d0} n_d \lambda_{g0} T_{d0} \beta}{C_{ff}^{af} C_{ox0}^{bx} A Q_f \varphi_g M_f} \exp\left(\frac{1}{\beta}\right), \quad \varepsilon_2 = \frac{(C_{ox0} C_{ff})^{0.5} Q_f \varphi_g M_f}{\rho_f L \varphi_f},$$

$$\varepsilon_3 = \frac{4 T_{d0}^3 \sigma R_{d0} k_{10}}{\lambda_{g0}}, \quad \varepsilon_4 = \frac{c_f T_{d0} \beta}{L},$$

$$\tilde{\nu}_f = \frac{1}{\nu_f} \sqrt{\frac{C_{ff}}{C_{ox0}}}, \quad \tilde{\nu}_{ox} = \frac{1}{\nu_{ox}} \sqrt{\frac{C_{ox0}}{C_{ff}}},$$

we can rewrite Equations (25)–(29) as

$$\frac{\mathrm{d}\theta_g}{\mathrm{d}\tau} = \frac{1}{\gamma}\big(P_1(\theta_g, \eta, \xi) - P_2(\theta_g, \theta_d, r)\big), \tag{32}$$

$$\frac{\mathrm{d}\eta}{\mathrm{d}\tau} = \frac{1}{\tilde{\nu}_f}\left[-P_1(\theta_g, \eta, \xi) + \frac{\psi}{\nu_f} P_{23}(\theta_g, \theta_d, r)\big(1 - \zeta(\theta_d)\big)\right], \tag{33}$$

$$\frac{\mathrm{d}\xi}{\mathrm{d}t} = -\frac{1}{\tilde{\nu}_{ox}} P_1(\theta_g, \eta, \xi), \tag{34}$$

$$\frac{\mathrm{d}\theta_d}{\mathrm{d}\tau} = \frac{\varepsilon_2}{\varepsilon_4 r^3} P_{23}(\theta_g, \theta_d, r)\zeta(\theta_d), \tag{35}$$

$$\frac{\mathrm{d}\left(r^3\right)}{\mathrm{d}\tau} = -\varepsilon_2 P_{23}(\theta_g, \theta_d, r)\big(1 - \zeta(\theta_d)\big), \tag{36}$$

with the initial conditions:

$$\theta_g(0) = \theta_{g0} \neq 0, \quad \theta_d(0) = \theta_{d0} = 0,$$

$$r(0) = r_0 = 1, \quad \eta(0) = \eta_0, \quad \xi(0) = \xi_0 = 1,$$

where

$$P_1(\theta_g, \eta, \xi) = \eta^a \xi^b \exp\left(\frac{\theta_g}{1 + \beta\theta_g}\right), \quad P_2(\theta_g, \theta_d, r) = \varepsilon_1 r \sqrt{\frac{T_{d0}(1 + \beta\theta_g)}{T_{g0}}}(\theta_g - \theta_d),$$

$$P_3(r) = \frac{\varepsilon_1\varepsilon_3}{4\beta} r^{2+b}\left(1 + \beta\theta_g^{\mathrm{ext}}\right)^4, \quad P_{23}(\theta_g, \theta_d, r) = P_2(\theta_g, \theta_d, r) + P_3(r),$$

$$\theta_g^{\mathrm{ext}} = \frac{1}{\beta}\frac{T_{\mathrm{ext}} - T_{d0}}{T_{d0}}, \quad \zeta(\theta_d) = \frac{T_b - T_{d0}\left(1 + \beta\theta_d\right)}{T_b - T_{d0}}.$$

We assume that System (32)–(36) is singularly perturbed with gas temperature (θ_g) being the fast variable ($\gamma \to 0$), while η, ξ, θ_d, r are slow variables. Although we appreciate that this is a rather artificial (but not unrealistic) case from the point of view of applications to modelling the processes in Diesel engines, it allows us to illustrate the application of mathematical tools described earlier in this paper.

Although it is not possible to explicitly solve the degenerate equation

$$P_1(\theta_g, \eta, \xi) - P_2(\theta_g, \theta_d, r) = 0 \tag{37}$$

with respect to the fast variable θ_g, we can use the implicit or parametric forms to obtain an approximation to the slow invariant manifold.

Before focusing on the formal analysis of this equation let us rewrite it in the form:

$$\eta^a \xi^b = \varepsilon_1 r \sqrt{\frac{T_{d0}(1 + \beta\theta_g)}{T_{g0}}}(\theta_g - \theta_d)\exp\left(-\frac{\theta_g}{1 + \beta\theta_g}\right).$$

Using the original dimensional variables this equation can be rewritten as:

$$C_f^a C_{ox}^b = \mu R_d T_g^{0.5} \left(T_g - T_d\right) \exp\left(\frac{E}{RT_g}\right), \tag{38}$$

where

$$\mu = \frac{4\pi n_d \lambda_{g0} C_{ff}^a C_{ox0}^b}{C_{ff}^{af} C_{ox0}^{bx} A Q_f \varphi_g M_f T_{g0}^{0.5}} = \frac{4\pi n_d \lambda_{g0} C_{ff}^{a-af} C_{ox0}^{b-bx}}{A Q_f \varphi_g M_f T_{g0}^{0.5}}.$$

Formula (38) gives us an explicit expression for fuel vapour and oxidiser concentrations as a function of gas and droplet temperatures, and droplet radius. The approximations of higher order to the slow invariant manifold can be considered as an improvement of this formula.

An implicit form of the first order approximation of (37) can be presented as:

$$\begin{aligned}
&\left[P_1(\theta_g,\eta,\xi)\tfrac{1}{(1+\beta\theta_g)^2} - P_2(\theta_g,\theta_d,r)\left(\tfrac{\beta}{2(1+\beta\theta_g)} - \tfrac{1}{\theta_g-\theta_d}\right)\right]\left(P_1(\theta_g,\eta,\xi) - P_2(\theta_g,\theta_d,r)\right)\\
&+\gamma\left[-\tfrac{a}{\tilde\nu_f\eta}P_1^2(\theta_g,\eta,\xi) + \tfrac{a\psi}{\tilde\nu_f\nu_f\eta}P_1(\theta_g,\eta,\xi)P_{23}(\theta_g,\theta_d,r)\big(1-\zeta(\theta_d)\big) - \tfrac{b}{\tilde\nu_{ox}\xi}P_1^2(\theta_g,\eta,\xi)\right.\\
&\qquad\left. + \tfrac{\varepsilon_2}{r^3}P_2(\theta_g,\theta_d,r)P_{23}(\theta_g,\theta_d,r)\left(\tfrac{\zeta(\theta_d)}{\varepsilon_4(\theta_g-\theta_d)} + \tfrac{1-\zeta(\theta_d)}{3}\right)\right] = 0.
\end{aligned} \tag{39}$$

The process described by this equation is stable when

$$\eta^a\xi^b \exp\left(\frac{\theta_g}{1+\beta\theta_g}\right)\frac{1}{(1+\beta\theta_g)^2} - \varepsilon_1 r\sqrt{\frac{T_{d0}(1+\beta\theta_g)}{T_{g0}}}\left(1+\frac{\beta(\theta_g-\theta_d)}{(1+\beta\theta_g)}\right) < 0.$$

The flow on the manifold is described by System (33)–(36) where the terms of order $o(\gamma)$ $(\gamma \to 0)$ are ignored.

To construct the slow invariant manifold in the parametric form, it is convenient to use η, ξ, θ_d, and θ_g as parameters:

$$r = \chi(\eta,\xi,\theta_d,\theta_g,\gamma) = \chi_0(\eta,\xi,\theta_d,\theta_g) + \gamma\chi_1(\eta,\xi,\theta_d,\theta_g) + \dots\ , \tag{40}$$

where

$$\chi_0(\eta,\xi,\theta_d,\theta_g) = \frac{\eta^a\xi^b}{\varepsilon_1(\theta_g-\theta_d)}\sqrt{\frac{T_{g0}}{T_{d0}(1+\beta\theta_g)}}\exp\left(\frac{\theta_g}{1+\beta\theta_g}\right). \tag{41}$$

Having substituted Expression (40) into the invariance equation

$$\begin{aligned}
&\frac{\partial\chi}{\partial\eta}\frac{1}{\tilde\nu_f}\left[-P_1(\theta_g,\eta,\xi) + \frac{\psi}{\nu_f}P_{23}(\theta_g,\theta_d,\chi)\big(1-\zeta(\theta_d)\big)\right] - \frac{\partial\chi}{\partial\xi}\frac{1}{\tilde\nu_{ox}}P_1(\theta_g,\eta,\xi)\\
&\quad + \frac{\partial\chi}{\partial\theta_d}\frac{\varepsilon_2}{\varepsilon_4\chi^3}P_{23}(\theta_g,\theta_d,\chi)\zeta(\theta_d) + \frac{\partial\chi}{\partial\theta_g}\frac{1}{\gamma}\big(P_1(\theta_g,\eta,\xi) - P_2(\theta_g,\theta_d,\chi)\big)\\
&\qquad = -\frac{\varepsilon_2\big(1-\zeta(\theta_d)\big)}{3\chi^2}P_{23}(\theta_g,\theta_d,\chi),
\end{aligned}$$

and equating the coefficients before the powers of γ, we obtain the expressions for coefficients in asymptotic expansion (40). Indeed, equating the coefficients before γ^0, we find

$$\chi_1(\eta,\xi,\theta_d,\theta_g)=\left\{\frac{\partial\chi_0}{\partial\eta}\frac{1}{\tilde\nu_f}\left[-P_1(\theta_g,\eta,\xi)+\frac{\psi}{\nu_f}P_{23}(\theta_g,\theta_d,\chi_0)\big(1-\zeta(\theta_d)\big)\right]\right.$$
$$\left.-\frac{\partial\chi_0}{\partial\xi}\frac{1}{\tilde\nu_{ox}}P_1(\theta_g,\eta,\xi)+P_{23}(\theta_g,\theta_d,\chi_0)\left[\frac{\varepsilon_2\zeta(\theta_d)}{\varepsilon_4\chi_0^3}\frac{\partial\chi_0}{\partial\theta_d}+\frac{\varepsilon_2\big(1-\zeta(\theta_d)\big)}{3\chi_0^2}\right]\right\}$$
$$\times\left[\sqrt{\frac{T_{d0}(1+\beta\theta_g)}{T_{g0}}}(\theta_g-\theta_d)\frac{\partial\chi_0}{\partial\theta_g}\right]^{-1}, \tag{42}$$

where

$$\frac{\partial\chi_0}{\partial\eta}=\frac{a\eta^{a-1}\xi^b}{\varepsilon_1(\theta_g-\theta_d)}\sqrt{\frac{T_{g0}}{T_{d0}(1+\beta\theta_g)}}\exp\left(\frac{\theta_g}{1+\beta\theta_g}\right),$$

$$\frac{\partial\chi_0}{\partial\xi}=\frac{b\eta^{a}\xi^{b-1}}{\varepsilon_1(\theta_g-\theta_d)}\sqrt{\frac{T_{g0}}{T_{d0}(1+\beta\theta_g)}}\exp\left(\frac{\theta_g}{1+\beta\theta_g}\right),$$

$$\frac{\partial\chi_0}{\partial\theta_d}=\frac{\eta^{a}\xi^{b}}{\varepsilon_1(\theta_g-\theta_d)^2}\sqrt{\frac{T_{g0}}{T_{d0}(1+\beta\theta_g)}}\exp\left(\frac{\theta_g}{1+\beta\theta_g}\right),$$

$$\frac{\partial\chi_0}{\partial\theta_g}=\chi_0\left[\frac{1}{(1+\beta\theta_g)^2}-\frac{1}{\theta_g-\theta_d}-\frac{\beta}{2(1+\beta\theta_g)}\right].$$

Hence, Expressions (40)–(42) give us the first-order approximation to the slow invariant manifold in the parametric form in the case $r\neq 0$. The flow on this manifold is determined by the system

$$\frac{\mathrm{d}\theta_g}{\mathrm{d}\tau}=-\varepsilon_1\chi_1(\eta,\xi,\theta_d,\theta_g)\sqrt{\frac{T_{d0}(1+\beta\theta_g)}{T_{g0}}}(\theta_g-\theta_d)+O(\gamma), \tag{43}$$

$$\frac{\mathrm{d}\eta}{\mathrm{d}\tau}=\frac{1}{\tilde\nu_f}\left[-P_1(\theta_g,\eta,\xi)+\frac{\psi}{\nu_f}P_{23}(\theta_g,\theta_d,\chi(\eta,\xi,\theta_d,\theta_g))\big(1-\zeta(\theta_d)\big)\right], \tag{44}$$

$$\frac{\mathrm{d}\xi}{\mathrm{d}t}=-\frac{1}{\tilde\nu_{ox}}P_1(\theta_g,\eta,\xi), \tag{45}$$

$$\frac{\mathrm{d}\theta_d}{\mathrm{d}\tau}=\frac{\varepsilon_2}{\varepsilon_4\chi^3(\eta,\xi,\theta_d,\theta_g)}P_{23}(\theta_g,\theta_d,\chi(\eta,\xi,\theta_d,\theta_g))\zeta(\theta_d). \tag{46}$$

System (43)-(46) has at least three advantages compared with the original model described by Equations (32)–(36). Firstly, System (43)-(46) contains four equations instead of five variables in the original system, i.e. its dimension is lower than that of the original system. Secondly, System (43)-(46) makes it possible to eliminate the stiffness of the original system due to the presence of singular perturbations.[1] Thirdly, the analytic expression (38) for the slow invariant manifold gives a relationship between the original dimensional variables of the system of differential equations. This relationship can be regarded as a first integral for this system and a kinetic law, analogous to the Michaelis-Menten kinetic law [26], applied to the spray combustion model.

4 Conclusions

New effective techniques for investigation of singularly perturbed differential systems based on the application of the invariant manifolds theory are described. It is shown that in some cases the slow invariant manifold can be found in parametric form as a result of asymptotic expansions. If this is not possible, one needs to use an implicit presentation of the slow surface and obtain asymptotic representations for the slow invariant manifold in an implicit form. The results of the development of the mathematical theory of these approaches and the application of this theory to the analysis of the system of equations describing heating, evaporation, ignition and combustion of fuel sprays are presented. It is shown that the application of this new mathematical technique can allow one to reduce the number of equations describing these processes in sprays and eliminate the stiffness of the original system of equations.

Acknowledgements

E. Shchepakina was supported by the Ministry of Education and Science of the Russian Federation (Project RFMEFI58716X0033). S. Sazhin was supported by EPSRC (UK) (grant EP/M002608/1).

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[1] Since the slow invariant manifold is attractive and $0 < \gamma \ll 1$, the trajectory approaches the manifold very quickly after the initial instant of time and then follows it. Thus, the effect of the initial perturbations is expected to be lost in the long term. Note that an analytical solution, uniformly valid for $t \geq 0$, could be found based on the matched asymptotic expansion [24] or multiple-scale expansion [25].

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Appendix

Effective methods of parameterisation

Case $m = n$

Let us assume that the degenerate equation (3) can be solved with respect to x in the form $x = \chi_0(y)$ and matrices $A(y) = \frac{\partial \chi_0(y)}{\partial y}$ and $B(y) = g_x(\chi_0(y), y)$ are invertible with bounded norms of inverse matrices. In this case, the fast variable y can be chosen as a parameter and the slow invariant manifold of System (2) can be found in the parametric form

$$x = \chi(y, \varepsilon) = \chi_0(y) + \varepsilon\chi_1(y) + ... + \varepsilon^k \chi_k(y) + ... \, . \tag{47}$$

From (2) and (47) we obtain the invariance equation

$$\frac{\partial \chi}{\partial y} g(\chi, y) = \varepsilon f(\chi, y). \tag{48}$$

Using the asymptotic representations

$$f(\chi_0 + \varepsilon\chi_1 + \varepsilon^2 ..., y) = f(\chi_0, y) + \varepsilon ...,$$

$$g(\chi_0 + \varepsilon\chi_1 + \varepsilon^2 ..., y) = g(\chi_0, y) + \varepsilon g_x(\chi_0, y)\chi_1 + \varepsilon^2 ... = \varepsilon g_x(\chi_0, y)\chi_1 + \varepsilon^2 ... ,$$

and the assumption that $g(\chi_0, y) = 0$, Equation (48) allows us to obtain the following equation:

$$A(y)B(y)\chi_1 = f(\chi_0, y).$$

Hence

$$\chi_1 = B^{-1}(y)A^{-1}(y)f(\chi_0, y).$$

Thus, we obtain the first order approximation to the slow invariant manifold in the form:

$$x = \chi(y, \varepsilon) = \chi_0(y) + \varepsilon\chi_1(y) = \chi_0(y) + \varepsilon\chi_1 = B^{-1}(y)A^{-1}(y)f(\chi_0, y).$$

The higher order approximations can be obtained in a similar way.

Returning to the classical combustion problem, described by Equations (17) and (18), consider the degenerate equation (19) which implies that

$$\eta = \chi_0(\theta) = \alpha\theta \mathrm{e}^{-\theta}.$$

Fast variable θ is used as parameterising variable v, see Subsection 2.2.

In the general case when

$$\eta = \chi(\theta) = \chi_0(\theta) + \varepsilon\chi_1(\theta) + \varepsilon^2\chi_2(\theta) + \ldots,$$

we can rewrite Equation (18) as:

$$\varepsilon \frac{\mathrm{d}\theta}{\mathrm{d}\tau} = \varepsilon(\chi_1(\theta) + \varepsilon\chi_2(\theta) + \ldots)\mathrm{e}^{\theta} \equiv \varepsilon F. \tag{49}$$

Remembering that $\eta = \chi(\theta)$ does not explicitly depend on time, we have $\frac{\partial \chi}{\partial t} = 0$. This allows us to simplify Equation (24) to:

$$\frac{\partial \chi}{\partial \theta} F = -\chi(\theta, \varepsilon) \mathrm{e}^{\theta}. \tag{50}$$

Remembering the definition of F in (49), we can rewrite Equation (50) as:

$$\left(\frac{\partial \chi_0}{\partial \theta} + \varepsilon \frac{\partial \chi_1}{\partial \theta} + \varepsilon^2 \frac{\partial \chi_2}{\partial \theta} + \dots \right) (\chi_1(\theta) + \varepsilon \chi_2(\theta) + \dots) \, \mathrm{e}^{\theta}$$
$$= - \left(\chi_0(\theta) + \varepsilon \chi_1(\theta) + \varepsilon^2 \chi_2(\theta) + \dots \right) \mathrm{e}^{\theta}.$$

Equating the coefficients before powers of ε, we find

$$\frac{\partial \chi_0}{\partial \theta} \chi_1 = -\chi_0, \quad \frac{\partial \chi_0}{\partial \theta} \chi_2 + \frac{\partial \chi_1}{\partial \theta} \chi_1 = -\chi_1, \quad \frac{\partial \chi_0}{\partial \theta} = \alpha(1-\theta) \mathrm{e}^{-\theta}.$$

Hence, explicit formulae for χ_1 and χ_2 can be presented as:

$$\chi_1 = \frac{\theta}{\theta - 1}, \quad \chi_2 = \mathrm{e}^{\theta} \frac{\theta^2(\theta-2)}{\alpha(\theta-1)^4}.$$

This allows us to obtain the following expression for η:

$$\eta = \chi(\theta, \varepsilon) = \alpha \theta \mathrm{e}^{-\theta} + \varepsilon \frac{\theta}{\theta - 1} + \varepsilon^2 \mathrm{e}^{\theta} \frac{\theta^2(\theta-2)}{\alpha(\theta-1)^4} + O(\varepsilon^3).$$

This representation is correct outside a certain neighbourhood of $\theta = 1$. It gives us an approximation of the attractive (repulsive) one-dimensional slow invariant manifold if $0 \le \theta < 1$ ($\theta > 1$).

Case $m < n$

Let us present vector y in the form $y = (y_1, y_2)^T$, where $\dim y_1 = n - m$ and $\dim y_2 = m$, and vector g in the form $g = (g_1, g_2)^T$, where $\dim g_1 = n - m$ and $\dim g_2 = m$. In this case, System (2) can be rewritten as

$$\begin{aligned} \dot{x} &= f(x, y_1, y_2), \\ \varepsilon \dot{y}_1 &= g_1(x, y_1, y_2), \\ \varepsilon \dot{y}_2 &= g_2(x, y_1, y_2). \end{aligned} \tag{51}$$

Let us assume that the solution to the degenerate equation $g(x, y) = 0$ can be presented as:

$$x = \chi_0(y_2), \;\; y_1 = \psi_0(y_2).$$

In this case, the slow invariant manifold can be found in the following parametric form

$$x = \chi(y_2, \varepsilon), \;\; y_1 = \psi(y_2, \varepsilon). \tag{52}$$

From (52) and (51) we have the invariance equations

$$\frac{\partial \chi}{\partial y_2} g_2(\chi, \psi, y_2) = \varepsilon f(\chi, \psi, y_2),$$

$$\frac{\partial \psi}{\partial y_2} g_2(\chi, \psi, y_2) = g_1(\chi, \psi, y_2).$$

These equations can be rewritten as:

$$A_1(y_2)(K_3(y_2)\chi_1(y_2) + K_4(y_2)\psi_1(y_2)) = f(\chi_0(y_2), \psi_0(y_2), y_2), \tag{53}$$

$$A_2(y_2)(K_3(y_2)\chi_1(y_2) + K_4(y_2)\psi_1(y_2)) = K_1(y_2)\chi_1(y_2) + K_2(y_2)\psi_1(y_2), \tag{54}$$

where $A_1(y_2) = \frac{\partial \chi_0(y_2)}{\partial y_2}$, $A_2(y_2) = \frac{\partial \psi_0(y_2)}{\partial y_2}$.

When deriving (53) and (54) the following asymptotic representations for $\chi(y_2, \varepsilon)$, $\psi(y_2, \varepsilon)$, $f(\chi, \psi, y_2)$, $g_1(\chi, \psi, y_2)$, and $g_2(\chi, \psi, y_2)$ were used:

$$\chi(y_2, \varepsilon) = \chi_0(y_2) + \varepsilon\chi_1(y_2) + ...,$$

$$\psi(y_2, \varepsilon) = \psi_0(y_2) + \varepsilon\psi_1(y_2) + ...,$$

$$f(\chi_0(y_2) + \varepsilon\chi_1(y_2) + ..., \psi_0(y_2) + \varepsilon\psi_1(y_2) + ..., y_2) = f(\chi_0(y_2), \psi_0(y_2), y_2) + \varepsilon ...,$$

$$\begin{aligned} &g_1(\chi_0(y_2) + \varepsilon\chi_1(y_2) + ..., \psi_0(y_2) + \varepsilon\psi_1(y_2) + ..., y_2) \\ &= g_1(\chi_0(y_2), \psi_0(y_2), y_2)) + \varepsilon K_1(y_2)\chi_1(y_2) + \varepsilon K_2(y_2)\psi_1(y_2) + \varepsilon^2 ..., \end{aligned}$$

$$\begin{aligned} &g_2(\chi_0(y_2) + \varepsilon\chi_1(y_2) + ..., \psi_0(y_2) + \varepsilon\psi_1(y_2) + ..., y_2) \\ &= g_2(\chi_0(y_2), \psi_0(y_2), y_2)) + \varepsilon K_3(y_2)\chi_1(y_2) + \varepsilon K_4(y_2)\psi_1(y_2) + \varepsilon^2 ..., \end{aligned}$$

where

$$K_1(y_2) = \frac{\partial g_1}{\partial x}(\chi_0, \psi_0, y_2), \quad K_2(y_2) = \frac{\partial g_2}{\partial x}(\varphi_0, \psi_0, y_2),$$

$$K_3(y_2) = \frac{\partial g_1}{\partial y_1}(\varphi_0, \psi_0, y_2), \quad K_4(y_2) = \frac{\partial g_2}{\partial y_1}(\varphi_0, \psi_0, y_2).$$

System (53) and (54) is a linear algebraic system for $\chi_1(y_2)$ and $\psi_1(y_2)$. If the determinant of this system is not equal to zero, we can find the first approximation to the slow invariant manifold in the form:

$$x = \chi_0(y_2) + \varepsilon\chi_1(y_2), \; y_1 = \psi_0(y_2) + \varepsilon\psi_1(y_2).$$

The higher order approximations can be obtained in a similar way.

Case $m > n$

Let us present vector x in the form $x = (x_1, x_2)^T$, where $\dim x_1 = n$ and $\dim x_2 = m - n$, and vector f in the form $f = (f_1, f_2)^T$, where $\dim f_1 = n$ and $\dim f_2 = m - n$. In this case, System (2) can be rewritten as

$$\begin{aligned}\dot{x}_1 &= f_1(x_1, x_2, y),\\ \dot{x}_2 &= f_2(x_1, x_2, y),\\ \varepsilon\dot{y} &= g(x_1, x_2, y).\end{aligned} \tag{55}$$

Let us assume that the solution to the degenerate equation $g(x, y) = 0$ can be presented as: $x_1 = \chi_0(x_2, y)$. In this case, the slow invariant manifold can be found in the following parametric form

$$x_1 = \chi(x_2, y, \varepsilon). \tag{56}$$

From (56) and (55) we obtain the invariance equation

$$\varepsilon\frac{\partial\chi}{\partial x_2}f_2(\chi, x_2, y, \varepsilon) + \frac{\partial\chi}{\partial y}g(\chi, x_2, y) = \varepsilon f_1(\chi, x_2, y). \tag{57}$$

From (57) we obtain

$$\frac{\partial\chi_0}{\partial x_2}f_2(\chi_0(x_2, y), x_2, y) + L(x_2, y)M(x_2, y)\chi_1(x_2, y) = f_1(\chi_0(x_2, y), x_2, y). \tag{58}$$

When deriving (58) the following asymptotic representations for χ, f_1, f_2, and g were used:

$$\chi(x_2, y, \varepsilon) = \chi_0(x_2, y) + \varepsilon\chi_1(x_2, y) + \varepsilon^2...,$$

$$f_1(\chi_0(x_2, y) + \varepsilon\chi_1(x_2, y) + \varepsilon^2..., x_2, y) = f_1(\chi_0(x_2, y), x_2, y) + \varepsilon...,$$

$$f_2(\chi_0(x_2, y) + \varepsilon\chi_1(x_2, y) + \varepsilon^2..., x_2, y) = f_2(\chi_0(x_2, y), x_2, y) + \varepsilon...,$$

$$g(\chi_0(x_2, y) + \varepsilon\chi_1(x_2, y) + \varepsilon^2..., x_2, y), x_2, y) = \varepsilon M(x_2, y)\chi_1(x_2, y) + \varepsilon^2...,$$

where $L(x_2, y) = \frac{\partial\chi_0}{\partial y}$, $M(x_2, y) = g_{x_1}(\chi_0, x_2, y)$. Assuming that matrices L and M are invertible, function $\chi_1 = \chi_1(x_2, y)$ can be found in the form:

$$\chi_1(x_2, y) = M^{-1}(x_2, y)L^{-1}(x_2, y)\left(f_1(\chi_0(x_2, y), x_2, y) - \frac{\partial\chi_0}{\partial x_2}f_2(\chi_0(x_2, y), x_2, y)\right).$$

The higher order approximations can be obtained in a similar way.

Let us illustrate this approach in the case of a system of three differential equations, which can be considered as a simplified version of the system describing spray combustion analysed in Section 3:

$$\dot{x}_1 = x_2, \quad \dot{x}_2 = y, \quad \varepsilon\dot{y} = -y - \mathrm{e}^y - x_1 - x_2.$$

This system has an attractive slow invariant manifold since (see Condition (16))

$$\frac{\partial}{\partial y}(-y - \mathrm{e}^y - x_1 - x_2) = -1 - \mathrm{e}^y < 0.$$

The degenerate equation

$$0 = -y - \mathrm{e}^y - x_1 - x_2$$

cannot be solved with respect to the fast variable y, but it can be solved with respect to one of the slow variables x_1 or x_2. Thus, the fast variable y and the slow variable x_2 can be chosen as parameters and the slow invariant manifold can be represented in the form

$$x_1 = \chi(x_2, y, \varepsilon) = \chi_0(x_2, y) + \varepsilon\chi_1(x_2, y) + \varepsilon^2\chi_2(x_2, y) + O(\varepsilon^3),$$

where $\chi_0(x_2, y) = -y - \mathrm{e}^y - x_2$. The flow on this manifold is described by the equations

$$\dot{x}_2 = y, \quad \varepsilon\dot{y} = -\chi_1(x_2, y) - \varepsilon\chi_2(x_2, y) + O(\varepsilon^2).$$

The invariance equation

$$\frac{\mathrm{d}\chi}{\mathrm{d}t} = \frac{\partial\chi}{\partial x_2}\frac{dx_2}{dt} + \frac{\partial\chi}{\partial y}\frac{dy}{dt}$$

in this case can be presented as

$$\frac{\partial\chi}{\partial x_2}y + \frac{\partial\chi}{\partial y}\frac{1}{\varepsilon}\left(-y - \mathrm{e}^y - \chi - x_2\right) = x_2.$$

This equation can be rewritten as:

$$\left(\frac{\partial\chi_0}{\partial x_2} + \varepsilon\frac{\partial\chi_1}{\partial x_2} + \dots\right)y + \left(\frac{\partial\chi_0}{\partial y} + \varepsilon\frac{\partial\chi_1}{\partial y} + \dots\right)(-\chi_1 - \varepsilon\chi_2 - \dots) = x_2.$$

Equating the coefficients before the powers of ε we obtain

$$\chi_1 = \frac{x_2 + y}{1 + \mathrm{e}^y}, \quad \chi_2 = \left(-\frac{\partial\chi_1}{\partial x_2}y + \frac{\partial\chi_1}{\partial y}\chi_1\right)/(1 + \mathrm{e}^y).$$

When deriving these equations we took into account that $\frac{\partial\chi_0}{\partial y} = -1 - \mathrm{e}^y$.

Note that in all cases considered so far, some systems variables are used for the parameterisation of slow invariant manifolds. In some cases, however, this approach turned out to be impossible or ineffective. This is illustrated for the following system of equations:

$$\dot{x} = y, \quad \varepsilon\dot{y} = 4x^2 + y^2 - 9, \tag{59}$$

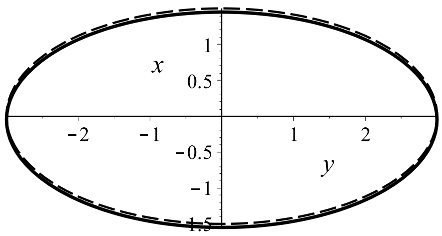

Fig. 3 The slow curve (dashed) and the exact slow invariant manifold (solid) of (59); $\varepsilon = 0.1$.

The parametric form of the slow invariant manifold for this system can be presented as:

$$x = \frac{r}{2}\cos\theta - \frac{\varepsilon}{2}, \quad y = r\sin\theta,$$

where $r = \sqrt{9-\varepsilon^2}$, θ is the polar angle. The flow on this slow invariant manifold is described by the equation $\dot{\theta} = -2$.

The implicit form of this slow invariant manifold can be described by the following equation:

$$4\left(x + \frac{\varepsilon}{2}\right)^2 + y^2 = 9 - \varepsilon^2.$$

The part of this ellipse, shown in Fig. 3, with $y < 0$ is attractive and the part with $y > 0$ is repulsive.