Order Reduction in Models of Spray Ignition and Combustion

Sergei S. Sazhin*

Sir Harry Ricardo Laboratories, Advanced Engineering Centre, School of Computing, Engineering and Mathematics, University of Brighton, Brighton, BN2 4GJ, UK

Elena Shchepakina

Samara National Research University, 34, Moskovskoye Shosse, Samara 443086, Russia

Vladimir Sobolev

Samara National Research University, 34, Moskovskoye Shosse, Samara 443086, Russia

Abstract

In most papers focused on the system order reduction models, describing processes of heating, evaporation and ignition in fuel sprays, it is assumed that all functions in corresponding differential equations are sufficiently smooth and consequently Lipschitzian. In many cases, however, these functions are non-Lipschitzian. This means that the conventional approach to system order reduction, based on the theory of integral manifolds, cannot be applied. It is pointed out that the order reduction of systems with non-Lipschitzian nonlinearities can be performed, using a concept of positively invariant manifolds. This concept is discussed and applied to the analysis of spray ignition based on five ODEs (for gas temperature, fuel vapour and oxygen concentrations, and droplet temperatures and radii). This system is reduced to single ordinary differential equations for the gas temperature or fuel concentrations. It is shown that the equation for gas temperature predicts an increase in gas temperature

*Corresponding author
Email addresses: S.Sazhin@brighton.ac.uk (Sergei S. Sazhin)

up to its limiting value during finite time. The reaching of this temperature is accompanied by the complete depletion of either fuel vapour or oxygen depending on their initial concentrations, as follows from the analysis of the equations for gas temperature and fuel concentration.

Key words:
spray ignition, Diesel fuel, combustion, thermal explosion, thermal radiation, order reduction, non-Lipschitzian nonlinearities
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Nomenclature

a	coefficient introduced in Equation (16) [m^{-b}]
a_i	(i = 0, 1, 2) coefficients introduced in Equation (16) [$\mathrm{m}^{-b}\mathrm{K}^{-i}$]
af, bx	powers used in the definition of $\dot{\omega}$
A	pre-exponential factor [$\mathrm{kmol}^{1-(af+bx)}\mathrm{m}^{3-3(af+bx)}\mathrm{s}^{-1}$]
$\mathcal{A}, \mathcal{B}$	parameters introduced in Equation (5)
b	coefficient introduced in Equation (17)
b_i	(i = 0, 1, 2) coefficients introduced in Equation (17) [K^{-i}]
c	specific heat capacity [J kg^{-1} K^{-1}]
C	molar concentration [kmol m^{-3}]
E	activation energy [J kmol^{-1}]
g	function introduced in Equation (8)
h	convection heat transfer coefficient [W m^{-2} K^{-1}]
k_1	efficiency factor of absorption
L	specific heat of evaporation [J kg^{-1}]
$\mathcal{L}$	positive parameter introduced in Equation (2)
m_d	droplet mass [kg]
M	molar mass [kg kmol^{-1}]
n_d	number of droplets per unit volume [m^{-3}]
Nu	Nusselt number
$P_i,\ P_{23}$	(i = 0, 1, 2, 3) dimensionless components in the RHS of Equations (18)-(22)

q_c (q_r)	convective (radiative) heat flux [W m^{-2}]
q	r^3
Q	specific combustion energy [J kg^{-1}]
r	dimensionless droplet radius
R_d	droplet radius [m]
R	universal gas constant [J kmol^{-1} K^{-1}]
Sh	Sherwood number
t	time [s]
T	temperature [K]
$\mathcal{T}$	finite interval of time [s]
V	Lyapunov function
$x,\ y$	vectors in $\mathcal{R}^m$ and $\mathcal{R}^n$ spaces or scalars
z	$\bar{y} - y$

Greek and miscellaneous symbols

$\aleph$	slow invariant manifold
α	parameter in the definition of $f(y)$
β	RT_{d0}/E
γ	dimensionless parameter introduced in Equations (18)-(22)
ε_i	(i= 1, 2, 3, 4) dimensionless parameters introduced in Equations (18)-(22)
ε	small positive parameter
η	dimensionless fuel concentration
θ	dimensionless temperature
ζ	parameter introduced in Eqs. (12) and (15)
λ	thermal conductivity [W m^{-1} K^{-1}]
ν	stoichiometric coefficient
ξ	dimensionless oxidiser concentration
ρ	density [kg m^{-3}]
σ	Stefan–Boltzmann constant [W m^{-2} K^{-4}]
τ	dimensionless time

φ	dimensionless volumetric phase content
ω_f	small dimensionless parameter introduced in the definition of C_{ff}
$\dot{\omega}$	chemical reaction rate [kmol s^{-1}]
ψ	function introduced in Equation (8)
$\wp$	parameter introduced in Equation (3)

Subscripts

b	boiling point
c	convection
d	droplet
ext	external (also superscript)
f	fuel
g	gas
ox	oxidiser
p	constant pressure
r	thermal radiation
react	reaction
0	initial state

1. Introduction

The importance of modelling spray ignition and combustion processes in various engineering, including automotive, applications is well recognised [1]. In most cases this modelling has been based on the application of Computational Fluid Dynamics (CFD) codes [2], although the limitations of this approach have been widely discussed in the literature [3, 4]. An alternative approach to modelling these processes was based on the observation that they are characterised by large differences in the rates of change of variables which allows one to apply asymptotic methods for their analysis [5]. These methods cannot replace

the conventional approach to the problem based on CFD modelling but can effectively complement it by highlighting the physical background of individual processes [5]. One of the most efficient methods for the analysis of these processes has been based on the theory of integral manifolds for singularly perturbed systems [6, 7, 8, 9]. In the case of autonomous systems this theory is known as the theory of invariant manifolds and is focused on the following equations:

$$\left.\begin{array}{rcl} \dot{x} & = & f(x,y,\varepsilon) \\ \varepsilon\dot{y} & = & g(x,y,\varepsilon) \end{array}\right\}, \tag{1}$$

where $0 < \varepsilon \ll 1$, $x \in \mathcal{R}^m$, $y \in \mathcal{R}^n$, in $\mathcal{R}^{m+n} = \mathcal{R}^m \times \mathcal{R}^n$. A surface $y = \aleph(x,\varepsilon)$ is called a slow invariant manifold of System (1) if any trajectory $x = x(t,\varepsilon)$, $y = y(t,\varepsilon)$ of System (1) 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. $y(t,\varepsilon) = \aleph(x(t,\varepsilon),\varepsilon)$. Finding this manifold is based on the requirement that functions $f(x,y,\varepsilon)$ and $g(x,y,\varepsilon)$ are sufficiently smooth and therefore satisfy the Lipschitzian condition [10]:

$$\|g(x_1,y_1) - g(x_2,y_2)\| \le \mathcal{L}(\|x_1 - x_2\| + \|y_1 - y_2\|), \tag{2}$$

where (x_1,y_1), (x_2,y_2) are arbitrary arguments from the domain and $\mathcal{L} > 0$. Note that the Lipschitzian condition is usually used in ODE theory to guarantee the uniqueness of the initial value problem (e.g. [10]).

The application of this theory to the modelling of spray ignition and combustion processes is described in numerous papers including [5, 11]. In these papers the analysis of both these processes is based on the same simple Arrhenius chemical model and these processes are indistinguishable from the point of view of modelling. The authors of [12] paid attention to the fact that in the model described in [5], Condition (2) is not satisfied which brought the validity of the results presented in [5] into question. In [12] an alternative approach to the analysis of the problem described in [5], using the new concept of positively (negatively) invariant manifolds, is performed. It is shown that a manifold similar to the one inferred from the analysis of the Lipschitzian systems can be

obtained for the singularly perturbed systems with non-Lipschitzian nonlinearities, if the five assumptions of the Tikhonov theorem are satisfied [12] (also see [3]). This provided rigorous justification of the results earlier reported in [5].

As in [12], the analysis of this paper will be focused on the investigation of *positively invariant manifolds* for non-Lipschitzian systems, describing the processes of spray ignition and combustion. In contrast to [12] the focus will be, not on the model originally described in [5], but on a more advanced model of these processes, taking into account the volumetric absorption of the thermal radiation in droplets, described in [14]. Our analysis will not be restricted to the case of small ε and will be based on the application of positively invariant manifolds and Lyapunov functions. The preliminary results of the analysis were presented in [13].

The underlying physical phenomenon related to the case when the Lipschitzian condition is not satisfied is described in Section 2. A concept of positively invariant manifolds is discussed in detail in Section 3. In the same section, the predictions of the model based on this manifold are compared with the rigorous numerical solution to the system of ODEs using a relatively simple example. The spray ignition and combustion model, described in [14], is briefly reviewed in Section 4. A new approach to the reduction of this model, based on the analysis of a positively invariant manifold and the Lyapunov function, is described in Section 5. The main results of the paper are summarised in Section 6.

2. Smoothness and Finite Time Processes

It is well known that a wide class of dynamic processes is described by ODE systems with sufficiently smooth functions. If these systems are asymptotically stable it is necessary to use an infinite time interval to attain a steady state. At the same time, some physical processes are characterised by a finite period of existence. For example, the time taken for a droplet to evaporate is usually finite. This means that it is necessary to use non-smooth ODEs to describe such processes.

This can be illustrated by considering a physical process described by the scalar ODE:

$$dy/dt = f(y), \quad f(0) = 0, \quad y(0) = y_0 > 0.$$

Let us assume that after finite time $\mathcal{T}$ variable y vanishes, i.e. $y(\mathcal{T}) = 0$. After the integration of this differential equation we obtain

$$\int_{y_0}^{0} \frac{dy}{f(y)} = \mathcal{T}, \quad y(\mathcal{T}) = 0.$$

For $f(y) = -y^\alpha$ the integral in the left hand side of this equation

$$\int_{y_0}^{0} \frac{dy}{f(y)} = \frac{y_0^{1-\alpha}}{1-\alpha} = \mathcal{T}, \quad y(\mathcal{T}) = 0$$

converges if and only if $\alpha < 1$; this means that in the case of a finite $\mathcal{T}$, function $f(y) = -y^\alpha$ does not satisfy the Lipschitzian condition.

The same appears to be true in a more general case

$$f(y) = -y^\alpha(\wp + f_1(y)), \quad 0 < \wp < \infty, \tag{3}$$

where $|f_1(y)| \leq \mu < \wp$. To prove this, it is sufficient to note that $\wp - \mu \leq \wp + f_1(y) \leq \wp + \mu$ and, therefore, $\mathcal{T}_- < \mathcal{T} < \mathcal{T}_+$ where

$$\mathcal{T} = \int_{y_0}^{0} \frac{dy}{f(y)}, \quad y(\mathcal{T}) = 0,$$

and

$$\mathcal{T}_+ = \int_{y_0}^{0} \frac{dy}{-y^\alpha(\wp - \mu)} = \frac{y_0^{1-\alpha}}{(1-\alpha)(\wp - \mu)}, \; \mathcal{T}_- = \int_{y_0}^{0} \frac{dy}{-y^\alpha(\wp + \mu)} = \frac{y_0^{1-\alpha}}{(1-\alpha)(\wp + \mu)}.$$

This will be used in the following sections to justify the existence of a positively invariant manifold in the model of spray ignition and combustion and to describe the behaviour of solutions of the reduced equations.

To illustrate the concepts of positively invariant manifolds consider function $f(y) = -y^\alpha$, introduced earlier, for $\alpha = 1/2$. For the system

$$dx/dt = 1, \quad dy/dt = -y^{1/2}; \quad x(0) = x_0, \quad y(0) = y_0 \tag{4}$$

the trajectory $y = 0$ plays the role of a positively invariant manifold. Indeed, the trajectory for any solution to (4) with $y_0 = 0$ lies on this manifold for all

$t > 0$. On the other hand, the trajectory of any solution to (4) with $y_0 > 0$,

$$y = \left(y_0^{1/2} + (x_0/2) - (x/2)\right)^2,$$

reaches this manifold at the point $x = 2y_0^{1/2} + x_0$ and then it lies on this manifold when t increases. This means that $y = 0$ is positively invariant but it is not invariant since trajectories can leave this manifold when t decreases. This follows from the fundamental property of differential equations with non-Lipschitzian nonlinearities: for them, the solution of an initial value problem is not unique. Hence, an infinite number of trajectories with $y_0 > 0$ pass through any point on $y = 0$.

Let us consider one more example of the process described by the differential equation

$$dy/dx = -\mathcal{A}y^{1/3} - \mathcal{B}y^{2/3}, \tag{5}$$

where constants $\mathcal{A}$ and $\mathcal{B}$ are positive parameters. This equation describes the ignition and combustion of a monodisperse spray when $y^{1/3}$ is a dimensionless droplet radius [12].

The right hand side of Equation (5) can be considered as a particular example of (3) when $\alpha = 1/3$, $\wp = \mathcal{A}$, and hence does not satisfy the Lipschitzian condition. Let us rewrite Equation (5) in the form of a differential system of equations on the plane:

$$dx/dt = 1, \quad dy/dt = -\mathcal{A}y^{1/3} - \mathcal{B}y^{2/3}. \tag{6}$$

The right hand side of the second equation of this system is not Lipschitzian, as in the case of the previous example, but it has a positively invariant manifold $y = 0$. To check the attractivity of this manifold, we use the Lyapunov theory which allows us to establish whether or not this manifold is stable without finding the trajectories (i.e. without solving the above system). This theory is based on finding the Lyapunov function $V(y)$ such that $V(y) = 0$ if and only if $y = 0$ and $V(y) > 0$ if and only if $y \neq 0$. If this function exists and its derivative $\dot{V} < 0$ then the positively invariant manifold $y = 0$ is asymptotically stable. Taking function $V(y) = y^2/2$, one can see that it is equal to zero if and only if

$y = 0$ and $V(y) > 0$ if and only if $y \neq 0$ (hence, this is the Lyapunov function). Also, $\dot{V} = -\mathcal{A}y^{4/3} - \mathcal{B}y^{5/3} < 0, \;\; y \geq 0$. Hence, the positively invariant manifold $y = 0$ is asymptotically stable. All trajectories with $y(x_0) > 0$ approach this manifold as t increases, and reach it at a finite time interval, as shown in Fig. 1.

3. Positively invariant manifolds

Recall now the notions of an invariant manifold and a positively invariant manifold for a differential system

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

In contrast to the previously introduced System (1), System (7) is not singularly perturbed.

Definition 1. *A surface $y = \aleph(x)$ ($x \in R^m$, $y \in R^n$) is an invariant manifold of System (7) if any trajectory $x = x(t)$, $y = y(t)$ predicted by this system that has at least one point (x_0, y_0) in common with the surface $y = \aleph(x)$, i.e., $y_0 = \aleph(x_0)$ at $t = 0$, lies entirely on this surface for all $t \in (-\infty, \infty)$.*

Definition 2. *A surface $y = \aleph(x)$ ($x \in R^m$, $y \in R^n$) is a positively invariant manifold of System (7) if any trajectory $x = x(t)$, $y = y(t)$ predicted by this system that has at least one point (x_0, y_0) in common with the surface $y = \aleph(x)$, i.e., $y_0 = \aleph(x_0)$ at $t = 0$, lies entirely on this surface for all $t > 0$.*

Attractive positively invariant manifolds can be used for non-Lipschitzian system reduction. However, the justification of this reduction is beyond the scope of traditional invariant manifold theory and requires other mathematical tools. In our analysis of non-Lipschitzian systems we use the Lyapunov function theory. The reduction of non-Lipschitzian systems is justified by the attractivity of positively invariant manifolds.

Let us now focus our analysis on the following system:

$$\dot{x} = f(x, y), \quad \dot{y} = \psi(y)g(x, y), \tag{8}$$

where x and y are a vector and scalar, respectively; scalar function $\psi(y)$ is non-Lipschitzian. We assume that $0 < \wp_1 \leq g(x,y) \leq \wp_2$ for sufficiently small non-negative values of y, $f(x,y)$ and $g(x,y)$ are continuous functions.

Firstly, we consider a simple case: $\psi = -y^\alpha$ $(0 < \alpha < 1)$. Since the right hand side of the equation for y in (8) is zero at $y = 0$, any trajectory, described by (8), with initial point $(x_0, 0)$ on the surface $y = 0$ lies on this surface for all $t \geq 0$. This surface, however, is not invariant since not all trajectories of System (8) which have at least one point in common with this surface lie entirely on it, as trajectories can leave this manifold when t decreases. This surface, however, is positively invariant and any solution to System (8) with initial point (x_0, y_0) with sufficiently small positive y_0 reaches this surface during a finite time interval. Moreover, it is attractive. To prove this we use the approach suggested in [15]. This approach is based on considering the Lyapunov function $V(y) = y^2/2$ with the derivative

$$\dot{V}(x,y) = -y^{1+\alpha} g(x,y).$$

This derivative is negative for $y > 0$ for all values of x under consideration. This implies the asymptotic stability of $y = 0$ with respect to variable y, i.e. $y \to 0$ as t increases.

The same analysis can be applied to the case when $\psi = (\bar{y} - y)^\alpha$, where $\bar{y}$ is a positive constant since the change of variable $z = \bar{y} - y$ leads to the equation $\dot{z} = -z^\alpha g(x, \bar{y} - z)$.

In what follows the usefulness of the concept of positively invariant manifolds and the accuracy of the predicted results will be illustrated for one specific example.

Example 1. Consider the system

$$\dot{x} = \nu(-x^a y^b - \mu - \lambda z^c),\ \dot{y} = -x^a y^b e^x,\ \dot{z} = -z^c \left(1 + z(x - y)\right), \qquad (9)$$

where $0 < a < 1$, $0 < b < 1$, $0 < c < 1$. System (9) can be considered as a specific example of System (8). It has the positively invariant manifold $z = 0$.

The reduced system on this manifold has the form

$$\dot{x} = \nu(-x^a y^b - \mu),\ \dot{y} = -x^a y^b e^x. \tag{10}$$

In Figure 2 the solutions $x = x(t)$ and $y = y(t)$ of (9) and (10) are compared for the following set of parameters: $a = 0.2$, $b = 0.7$, $c = 1/3$, $\nu = 0.5$, $\mu = 0.2$, $\lambda = 0.125$.

As follows from Figure 2, the values of $x = x(t)$ and $y = y(t)$ predicted by the full and reduced systems are reasonably close (the values of $y = y(t)$ are almost indistinguishable). This illustrates the usefulness of the concept of positively invariant manifolds discussed in this paper for the analysis of System (9) and the accuracy of the predictions made by the model based on this concept.

4. Spray ignition and combustion model

Following [14], spray ignition and combustion are considered as an explosion problem, where droplets are regarded as the source of endothermicity. The endothermic versus exothermic competition determines explosion regimes and their dependence on the physical and chemical parameters of the system. The medium is modelled as a spatially homogeneous mixture of an optically thin, combustible gas with a monodispersed spray of evaporating spherical fuel droplets (the effects of non-sphericity of droplets on their heating and evaporation were investigated in [16]). Both convective and radiative heating of droplets are taken into account. The distortion of the incident radiation by surrounding droplets and the effects of droplet movement are ignored (the Nusselt (Nu) and Sherwood (Sh) numbers are taken equal to 2). It is assumed that the incident radiation has a black-body spectrum and is absorbed inside the droplets (this assumption is different from the one used in [5], where the absorption of thermal radiation was considered as a surface phenomenon; the limitations of the latter approach are discussed in detail in Section 3.2 of [3]). The system is assumed to be adiabatic. With a view to the application of the results to Diesel engines,

we assume that gas pressure is constant. The thermal conductivity of the liquid phase is assumed to be infinitely large. The volume fraction of the liquid phase is assumed to be much less than that of the gaseous phase. Thus, the heat transfer coefficient of the mixture is controlled by the thermal properties of the gaseous component. It is assumed that the burning process, described by the first order exothermic reaction, takes place in the gaseous phase only. The effects of the Stefan flow on droplet heating and evaporation are ignored (Spalding heat and mass transfer numbers are assumed to be much less than 1). The range of applicability of these assumptions has been discussed in numerous papers and monographs (e.g. [3]).

Under these assumptions the process is described by the following equations [14]:

$$c_{pg}\rho_g\varphi_g\frac{dT_g}{dt} = \dot{\omega}M_f Q_f\varphi_g - 4\pi R_d^2 n_d q_c, \tag{11}$$

$$\frac{dC_f}{dt} = -\nu_f\dot{\omega} + 4\pi R_d^2 n_d \frac{(q_c+q_r)}{LM_f\varphi_g}\left(1-\zeta(T_d)\right), \tag{12}$$

$$\frac{dC_{ox}}{dt} = -\nu_{ox}\dot{\omega}, \tag{13}$$

$$c_f m_d\frac{dT_d}{dt} = 4\pi R_d^2(q_c+q_r)\zeta(T_d), \tag{14}$$

$$\frac{d}{dt}\left(\frac{4}{3}\pi R_d^3\rho_f\right) = -4\pi R_d^2\frac{(q_c+q_r)}{L}\left(1-\zeta(T_d)\right), \tag{15}$$

where

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

$$q_c = h_c(T_g-T_d), \quad h_c = \frac{\lambda_g}{R_d}, \quad q_r = k_1\sigma T_{\rm ext}^4, \quad k_1 = aR_d^b,$$

$$a = a_0 + a_1\left(\frac{T_{\rm ext}}{10^3}\right) + a_2\left(\frac{T_{\rm ext}}{10^3}\right)^2, \tag{16}$$

$$b = b_0 + b_1\left(\frac{T_{\rm ext}}{10^3}\right) + b_2\left(\frac{T_{\rm ext}}{10^3}\right)^2. \tag{17}$$

The initial conditions are the following:

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

155 Gas is assumed to be optically thin and the radiation absorption in droplets is controlled by the external temperature T_{ext}. We assume that $\rho_g \varphi_g = \text{const}$ (the process takes place at constant pressure; approximation of Diesel engine-like conditions).

Introducing the following dimensionless variables:

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

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

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

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

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

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

we can rewrite Eqs. (11)–(15) as

$$\frac{d\theta_g}{d\tau} = \frac{1}{\gamma} \big(P_1(\theta_g, \eta, \xi) - P_2(\theta_g, \theta_d, r) \big), \tag{18}$$

$$\frac{d\eta}{d\tau} = \frac{1}{\tilde{\nu}_f} \left[-P_1(\theta_g, \eta, \xi) + \frac{\psi}{\nu_f} P_{23}(\theta_g, \theta_d, r) \big(1 - \zeta(\theta_d)\big) \right], \tag{19}$$

$$\frac{d\xi}{dt} = -\frac{1}{\tilde{\nu}_{ox}} P_1(\theta_g, \eta, \xi), \tag{20}$$

$$\frac{d\theta_d}{d\tau} = \frac{\varepsilon_2}{\varepsilon_4 r^3} P_{23}(\theta_g, \theta_d, r) \zeta(\theta_d), \tag{21}$$

$$\frac{d\left(r^3\right)}{d\tau} = -\varepsilon_2 P_{23}(\theta_g, \theta_d, r) \big(1 - \zeta(\theta_d)\big), \tag{22}$$

where

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

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

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

with the initial conditions:

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

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

5. Reduction of the model

In our previous paper [12], a system of equations similar to the one presented in the previous section, was considered. The main difference in the physical models considered is that in the previous paper the radiative heating of droplets was considered as a surface phenomenon, while in the current paper this heating is considered as a volumetric phenomenon. Also, the analysis of [12] was based on the assumption that the droplet radius is the fastest variable in the model, which allowed the authors of [12] to base their analysis on the Tikhonov theorem (this is one of the tools for the analysis of singularly perturbed systems). In contrast to [12], our present analysis is not based on this assumption and we do not use the Tikhonov theorem (we do not assume that the system is singularly perturbed). Instead, our approach is based on the concept of positively invariant manifolds and the analysis of the Lyapunov functions.

Let us introduce a new variable $q=r^3$ and rewrite (18)–(22) as:

$$\frac{d\theta_g}{d\tau}=\frac{1}{\gamma}\big(P_1(\theta_g,\eta,\xi)-P_2(\theta_g,\theta_d,q^{1/3})\big),\tag{23}$$

$$\frac{d\eta}{d\tau}=\frac{1}{\tilde{\nu}_f}\left[-P_1(\theta_g,\eta,\xi)+\frac{\psi}{\nu_f}P_{23}(\theta_g,\theta_d,q^{1/3})\big(1-\zeta(\theta_d)\big)\right],\tag{24}$$

$$\frac{d\xi}{dt} = -\frac{1}{\tilde{\nu}_{ox}} P_1(\theta_g, \eta, \xi), \tag{25}$$

$$\frac{d\theta_d}{d\tau} = \frac{\varepsilon_2}{\varepsilon_4 q} P_{23}(\theta_g, \theta_d, q^{1/3}) \zeta(\theta_d), \tag{26}$$

$$\frac{dq}{d\tau} = -\varepsilon_2 P_{23}(\theta_g, \theta_d, q^{1/3}) \big(1 - \zeta(\theta_d)\big). \tag{27}$$

System (23)-(27) is identical to the one derived in [14]. The analysis of this system, performed by its authors, was correct except they referred to invariant manifolds instead of positively invariant manifolds. In what follows this part of their analysis will be corrected and some assumptions made in [14] will be relaxed.

System (23)–(27) has the positively invariant manifold $q \equiv 0$. To prove this it is sufficient to note that this system can be represented in the form of (8) when q plays the role of y and the vector with coordinates $\theta_g, \eta, \xi, \theta_d$ plays the role of vector x. Moreover, the right hand side of (27) can be presented as $-q^{1/3} g(x, q)$ for

$$g(x,q) = \varepsilon_2 \left(\varepsilon_1 \sqrt{\frac{T_{d0}(1+\beta\theta_g)}{T_{g0}}} (\theta_g - \theta_d) + \frac{\varepsilon_1 \varepsilon_3}{4\beta} q^{(1+\beta)/3} \left(1 + \beta\theta_g^{\text{ext}}\right)^4 \right) \big(1 - \zeta(\theta_d)\big).$$

To prove the attractivity of this manifold we use the same approach as in Section 2. We consider Lyapunov function $V(q) = q^2/2$ with derivative

$$\dot{V}(q) = -q\varepsilon_2 P_{23}(\theta_g, \theta_d, q^{1/3}) \big(1 - \zeta(\theta_d)\big).$$

$\dot{V}(q)$ is negative for all values of θ_g, θ_d under consideration. This implies the asymptotic stability of $q = 0$ with respect to q, i.e. $q \to 0$ as $t \to +\infty$.

System (23)–(27) has the partial integral (see [14]):

$$q = \left(e^{\theta_d} (\zeta(\theta_d))^{\theta_{db}} \right)^{\varepsilon_4}.$$

As follows from this expression, $\zeta(\theta_d) \to 0$ as $q \to 0$, i.e. the droplet surface temperature approaches the boiling temperature ($\theta_d \to \theta_{db}$) when $q \to 0$. Hav-

ing substituted $q = 0$ and $\theta_d = \theta_{db}$[1] into System (23)–(27), the latter can be simplified to

$$\frac{d\theta_g}{d\tau} = \frac{1}{\gamma} P_1(\theta_g, \eta, \xi), \tag{28}$$

$$\frac{d\eta}{d\tau} = -\frac{1}{\tilde{\nu}_f} P_1(\theta_g, \eta, \xi), \tag{29}$$

$$\frac{d\xi}{dt} = -\frac{1}{\tilde{\nu}_{ox}} P_1(\theta_g, \eta, \xi). \tag{30}$$

Two integrals

$$\gamma\theta_g + \tilde{\nu}_f\eta = \gamma\theta_{g0} + \tilde{\nu}_f\eta_0 \tag{31}$$

and

$$\gamma\theta_g + \tilde{\nu}_{ox}\xi = \gamma\theta_{g0} + \tilde{\nu}_{ox} \tag{32}$$

of System (28)–(30) allow us to exclude equations for η and ξ from the following investigation and to obtain the final equation for θ_g in the form

$$\frac{d\theta_g}{d\tau} = \frac{1}{\gamma} P_1 \left(\theta_g, \eta_0 - \frac{\gamma}{\tilde{\nu}_f}(\theta_g - \theta_{g0}), 1 - \frac{\gamma}{\tilde{\nu}_{ox}}(\theta_g - \theta_{g0}) \right). \tag{33}$$

Thus, using positively invariant manifold $q = 0$ for System (23)–(27) we performed the order reduction of the original non-Lipschitzian system (18)–(22) and obtained scalar equation (33) for θ_g. A reduced equation for η is considered in the next section.

6. Analysis of the reduced equations

Remembering the definition of P_1 and Equations (31), (32) we rewrite Equation (33) in the form:

$$\frac{d\theta_g}{d\tau} = \frac{1}{\gamma} \left(\eta_0 - \frac{\gamma}{\tilde{\nu}_f}(\theta_g - \theta_{g0}) \right)^a \left(1 - \frac{\gamma}{\tilde{\nu}_{ox}}(\theta_g - \theta_{g0}) \right)^b \exp\left(\frac{\theta_g}{1 + \beta\theta_g} \right). \tag{34}$$

[1] From the point of view of the physical background of the problem this implies that the droplets are assumed to have evaporated; note that, in contrast to [12], we did not assume that q is the fastest variable in our analysis.

Equation (34) has two steady states

$$\bar{\theta_g} = \theta_{g0} + \eta_0 \tilde{\nu}_f/\gamma \text{ and } \bar{\bar{\theta}}_g = \theta_{g0} + \tilde{\nu}_{ox}/\gamma.$$

Remembering that positive parameters a and b are less than 1 for most applications relevant to Diesel engines, the right hand side of Equation (34) is non-Lipschitzian in the neighbourhoods of these steady states. For $0 < a < 1$ and $0 < b < 1$, expressions

$$\left(\eta_0 - \frac{\gamma}{\tilde{\nu}_f}(\theta_g - \theta_{g0})\right)^a, \quad \left(1 - \frac{\gamma}{\tilde{\nu}_{ox}}(\theta_g - \theta_{g0})\right)^b$$

have physical meaning only when:

$$\eta_0 - \frac{\gamma}{\tilde{\nu}_f}(\theta_g - \theta_{g0}) \geq 0, \quad 1 - \frac{\gamma}{\tilde{\nu}_{ox}}(\theta_g - \theta_{g0}) \geq 0.$$

This means that dimensionless gas temperature θ_g increases and attains the steady state value

$$\min\{\bar{\theta_g}, \bar{\bar{\theta}}_g\}.$$

For

$$C_{f0}/C_{ox0} < \nu_f/\nu_{ox} \tag{35}$$

we have:

$$\min\{\bar{\theta_g}, \bar{\bar{\theta}}_g\} = \bar{\theta_g}.$$

This implies that θ_g reaches $\bar{\theta_g}$ during a finite time interval. Once this has happened, it remains constant $\theta_g = \bar{\theta_g}$. Also, Equation (31) implies that

$$\eta = \eta_0 - \frac{\gamma}{\tilde{\nu}_f}(\theta_g - \theta_{g0}).$$

This means that all fuel is completely burned away ($\eta = 0$) when $\theta_g = \bar{\theta_g}$ if (35) is valid.

If

$$C_{f0}/C_{ox0} > \nu_f/\nu_{ox} \tag{36}$$

θ_g reaches $\bar{\bar{\theta}}_g$ during a finite time interval. Once this has happened, $\theta_g = \theta_{g0} + \tilde{\nu}_{ox}/\gamma$. In this case, remembering (32), we have

$$\xi = 1 - \frac{\gamma}{\tilde{\nu}_{ox}}(\theta_g - \theta_{g0}).$$

This means that the oxidiser is completely spent on combustion ($\xi = 0$) when $\theta_g = \bar{\bar{\theta}}_g$ if (36) is valid.

The plots of θ_g, η ξ versus time, inferred from (34), (31) and (32), for lean and rich mixtures (Condition (35) or (36) is valid) are shown in Figure 3. The
190 following parameter values were used: $\eta_0 = 1$, $\beta = 0.0328202363$, $a = 0.0182$, $b = 0.68843625$, $\gamma = 1$, $\theta_{g0} = 0.3$ for both mixtures; $\tilde{\nu}_f = 0.3$, $\tilde{\nu}_{ox} = 0.32$ for the lean mixture and $\tilde{\nu}_f = 0.32$, $\tilde{\nu}_{ox} = 0.3$ for the rich mixture. As follows from this figure, $\theta_g = \theta_g(t)$ reaches $\bar{\theta}_g$ and $\bar{\bar{\theta}}_g$, for lean and rich mixtures, respectively, at finite times. This agrees with the analysis presented above.

To describe the fuel consumption process it is convenient to use the reduced equation for variable η instead of θ_g. This equation is inferred from (31) after the change of variable in (34):

$$\frac{d\eta}{d\tau} = -\frac{1}{\tilde{\nu}_f}\eta^a \left(1 - \frac{\tilde{\nu}_f}{\tilde{\nu}_{ox}}(\eta_0 - \eta)\right)^b \exp\left(\frac{\Psi(\eta)}{1 + \beta\Psi(\eta)}\right). \tag{37}$$

where

$$\theta_g - \theta_{g0} = -\frac{\tilde{\nu}_f}{\gamma}(\eta - \eta_0),$$

$\Psi(\eta) = \theta_g = \theta_{g0} - \frac{\tilde{\nu}_f}{\gamma}(\eta - \eta_0)$. Equation (37) has two steady states: $\bar{\eta} = 0$ (lean mixtures; (35) is valid) and $\bar{\eta} = \eta_0 - \frac{\tilde{\nu}_{ox}}{\tilde{\nu}_f}$ (rich mixtures; (36) is valid). In the dimensional form the latter can be presented as:

$$\bar{C}_f = C_{f0}\left(1 - \frac{\nu_f}{\nu_{ox}}\frac{C_{ox0}}{C_{f0}}\right).$$

Note that integrals (31) and (32) imply:

$$\eta - \eta_0 = \frac{\tilde{\nu}_{ox}}{\tilde{\nu}_f}(\xi - 1)$$

and (in the dimensional form)

$$C_{f0} - C_f = \frac{\nu_f}{\nu_{ox}}(C_{ox0} - C_{ox}).$$

In the case of rich mixtures we can expect that the oxidiser is completely spent on combustion and the latter equation can be simplified to:

$$\tilde{C}_f = C_{f0} - \mathrm{FAR}\, C_{ox0},$$

where FAR $= \frac{\nu_f}{\nu_{ox}}$ is the fuel-air ratio. In the case of lean mixtures a similar formula can be obtained for the molar oxidiser concentration.

7. Conclusions

A concept of a positively invariant manifold for non-linear systems with non-Lipschitzian nonlinearities has been used to reduce the order of the system of ODEs describing Diesel fuel spray heating/evaporation and ignition/combustion. The dynamics of thermal explosion in a fuel droplet/hot air mixture are investigated using this approach. Effects of the thermal radiation, semi-transparency of droplets and oxidiser are taken into account. The system of ordinary differential equations for gas temperature, fuel vapour and oxygen concentrations, and droplet temperatures and radii is reduced to single ordinary differential equations for gas temperature or fuel concentrations. It is shown that the equation for gas temperature predicts an increase in gas temperature up to its limiting value during finite time. The reaching of this temperature is accompanied by the complete depletion of either fuel vapour or oxygen depending on their initial concentrations, as follows from the analysis of the equations for gas temperature and fuel concentration.

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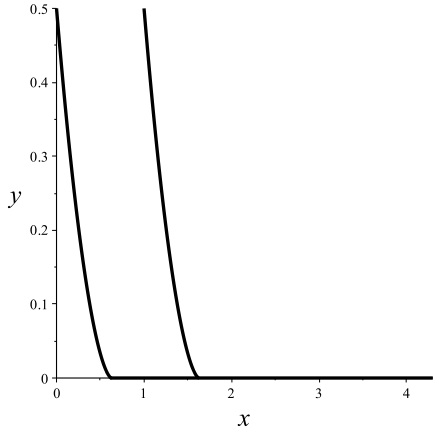
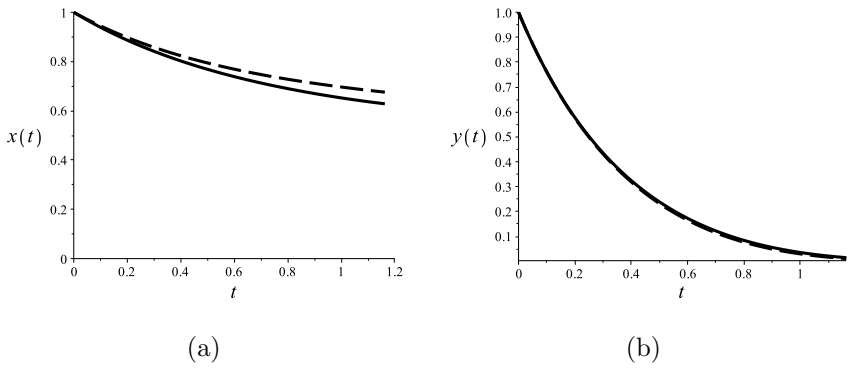


Figure 1: Typical trajectories described by Equation (5) for $\mathcal{A} = 1, \mathcal{B} = 1$.



(a) (b)

Figure 2: Plots for solutions $x(t)$ (a) and $y(t)$ (b) of the original system (9) (solid) and the reduced system (10) (dashed).

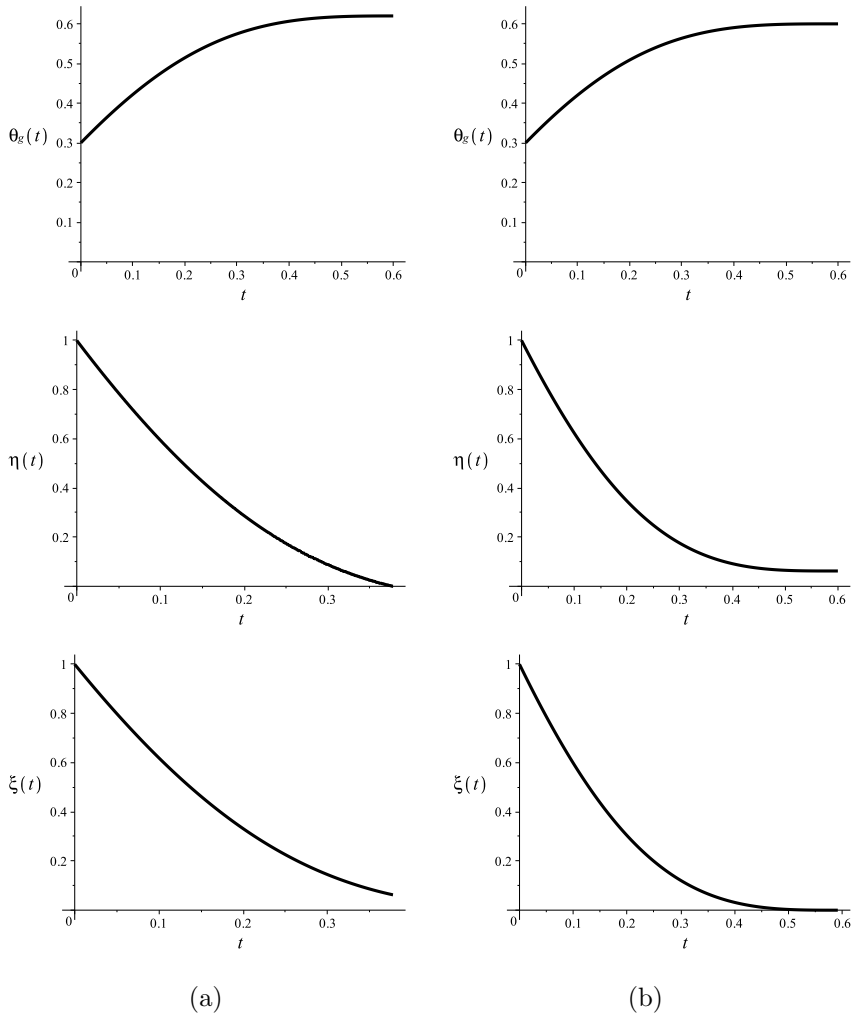


Figure 3: Plots of dimensionless gas temperature θ_g and the dimensionless concentrations η and ξ versus time for lean (Condition (35)) and rich (Condition (36)) fuel mixtures.