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Order reduction in models of spray ignition and combustion

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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 non-linearities 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 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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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 allow 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 [6–9]. In the case of autonomous systems this theory is known as the theory of invariant manifolds and is focused on the following equations:

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

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

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Nomenclature

a	coefficient introduced in Eq. (16) (m^{-b})
a_i	(i = 0, 1, 2) coefficients introduced in Eq. (16) (m^{-b} K^{-i})
af, bx	powers used in the definition of $\dot{\omega}$
A	pre-exponential factor ($\mathrm{kmol}^{1-(af+bx)}$ $\mathrm{m}^{3-3(af+bx)}$ s^{-1})
$\mathcal{A}, \mathcal{B}$	parameters introduced in Eq. (5)
b	coefficient introduced in Eq. (17)
b_i	(i = 0, 1, 2) coefficients introduced in Eq. (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 Eq. (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 Condition (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 Eqs. (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 Eqs. (18)–(22)
ε_i	($i = 1$, 2, 3, 4) dimensionless parameters introduced in Eqs. (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 Eq. (8)
$\wp$	parameter introduced in Eq. (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

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

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

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