Mathematical Modelling of Spray Combustion-Numerical and Analytical Analysis with application to Engineering Science

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Abstract

In the present paper we applied two well- known analytical method to the problem of thermal explosion of monodisperse and polydisperse fuel spray. The methods are the method of integral manifold (MIM) and the homotopy analysis method (HAM). The MIM method used as a basic tools for the analysis of SPS system of ordinary differential equations which means that the physical/ mathematical model should contain a small parameter in the governing equations. The HAM is always valid no matter whether there exist small physical parameters or not in contrast to the classical perturbation methods which requires the existence of a small parameter in the system (in general this is not the case). According to the theory of HAM, the convergence and the rate of solution series are dependent on the convergent control parameter $\hbar$. This means that this parameter gives one a convenient way to adjust and to control the convergent region of the solutions.

Keywords: Polydisperse and monodisperse spray, Homotopy analysis method, Method of invariant manifold, Asymptotic analysis, Partial differential equations

Nomenclature

A constant pre-exponential rate factor

C reactant concentration

c specific heat capacity

E activation energy

h heat transfer coefficient

h_m mass transfer coefficient

Q combustion energy

V total volume

T temperature

t time

r dimensionless radius

R universal gas constant

R droplet radii

L liquid evaporation energy (i.e., latent heat of evaporation, Enthalpy of evaporation)

n number of drops per unit volume

m mass

Greek symbols:

ρ reactant density

θ dimensionless temperature

β (conventional parameter of Semenov's theory of thermal explosion), reduced ambient temperature. This parameter is small compared with unity for most gaseous mixture due to the high exothermicity and activation energy of the chemical reaction

η dimensionless concentration

τ dimensionless time

α volumetric phase content

λ thermal conductivity

ψ represents the internal characteristics of the fuel (the ratio of the specific combustion energy and the latent heat of evaporation)

μ molar mass

σ Stefan-Boltzmann constant

$\chi(\cdot)$ Heaviside function

γ (conventional parameter of Semenov's theory of thermal explosion), the final dimensionless adiabatic temperature of the thermally insulated system after explosion. This parameter is small compared with unity for most gaseous mixture due to the high exothermicity and activation energy of the chemical reaction

κ = $2\epsilon_d/(2 - \epsilon_d)$ where ϵ_d is the emissivity of the droplet surface

$\epsilon_{1,2}$ dimensionless parameters, introduced for the first time (Gol'dshtein, Goldfarb, Shreiber, & Zinoviev, 1996) and describe the relations between the thermo physical properties of the gas and liquid phases

Subscript notations:

a ambient

b boiling point

ext external

0 initial state

ad adiabatic

re relaxation

g gas mixture

ox oxygen

L liquid phase

f combustible gas component of the mixture

d liquid fuel droplets

p under constant pressure

r reaction

s saturation line (surface of droplets)

1. Introduction

The present paper is concerned with theoretical and numerical investigation of combustion processes in multiphase media. The main topic under consideration is auto-ignition of polydisperse fuel spray. The research is motivated by a large number of industrial applications. For example, internal combustion and diesel engines, homogeneous chemical reactors, spontaneous insulation fires occurrence etc.

Thermo-chemical processes demonstrate a rich variety of complicated dynamical phenomena, which are not completely understood despite the relatively long history of combustion theory. Even in a relatively simple practical situation a large number of different chemical and thermo-physical processes are involved simultaneously. Therefore, attempts to give a detailed description of this processes lead to extremely complicated system of partial differential equations. Such models are almost useless for analytical extraction of main conceptual information about the dynamics of the processes, but the history of the thermal explosion theory shows that the main peculiarities of self-ignition in homogeneous case may be roughly described by simple Semenov's type model (Semenov, 1928). Semenov was the first who suggested a mathematical description of the thermal explosion phenomenon for highly exothermic chemical reaction. In his model the reactant consumption was neglected, which lead to the absence of energy conservation law, and the critical condition (i.e., thermal explosion limit) was described analytically as the loss of stability for the unique singular point of the single ODE. Stability means that the temperature is bounded at any time. The thermal explosion is an infinite increase of the temperature. In the Semenov's model, there are only two possible type of dynamical behavior : explosive and slow non-explosive regimes. Semenov's model become physically more realistic if the reactant concentration is taken into account. In this case the system is closed, which means that the mass and the energy conservation laws are valid.

The models that we present in this paper are includes an equations that described the combustion processes between a monodisperse/polydisperse fuel spray of droplets and oxidizer in the gas phase. In many practical combustion processes the fuel starts as a liquid that injected through an orifice into a gas-phase combustion environment. For example, Diesel engines, jet aircraft engines and so on. Once the droplets injected to a hot environment (hot gas) begins the process of heat transfer from the hot gas to the droplets which cause the droplets to evaporate until subsequent gas-phase start. What finally burn is the mixture of fuel vapor with oxygen and not the fuel liquid, this called spray combustion. When investigating the model of spray combustion one should take into account the following areas: single droplet combustion, combustion of monodisperse spray (all droplets have the same diameter), combustion of polydisperse spray (different size of radius's). The meaning in the first case is that the combustion of a dense cloud of many droplets can be viewed as an ensemble of single droplet combustion. In this case, one can take into account in details the description of the chemical reaction, evaporation, heat and mass transfer and many other chemical and physical processes which can be complicated from the other areas (spray combustion). This ensemble assumption enable one to understand the combustion process in more details than the spray combustion. In some special cases one can achieve an analytical expression to the dynamic variables of the model (Warnatz, Maas, & Robert, 2006). The monodisperse and polydisperse sprays combustion has been extensively studied both practically and theoretically. Various methods have been applied to these models as of numerical methods, asymptotic and analytical methods. Polydisperse fuel spray reflect reality better than the monodisperse one. On the other hand it is more complicated for research because of the large number of non-linear partial differential equations that take into account the velocity of the droplets, the collision between the droplets, the break-up of droplets, droplets distribution, droplets dispersion, droplets evaporation, gas-phase chemical kinetics, the change of the gas temperature, heat and mass transfer between the droplets and the gas and so on, i.e., all of the physical and chemical properties that should be include in order to describe the combustion of the spray that injected into a hot environment (Lefebvre, 1989; William, 1995). In some cases, the polydisperse spray can be described by a simpler model, often called a global or reduced model. Some knowledge of droplets size distribution is helpful in evaluating process application is sprays, especially in calculations of heat or mass transfer between the dispersed liquid and the surrounding gas. For predicting the mean drop size and drop size distribution only empirical correlations are available. When describing the droplets radii by distribution one should compare between the different distribution

parameters. All of them have deficiencies of one kind or another. In one distribution the maximum droplet diameter is unlimited, in another distribution the minimum possible diameter is zero or even negative. Hence, there is no single parameter emerged that has clear advantages over the other. For any given application the best distribution is one that is easy to manipulate and provides the best fit to the experimental date. The difficulties in specifying drop size distribution in sprays led the researches in the field to widespread use of various types of a mean or median diameter. For applications, it is very important therefore to decide which droplet size measure is the most suitable for the specific application. In many calculations of mass transfer and flow processes it is convenient to work with mean or average diameter instead of the complete drop size distribution. For example, in many engineering applications it is common practice to relate to the actual polydisperse spray as being equivalent to a monodisperse spray with all droplets therein having some average diameter. In combustion systems, the Sauter Mean Diameter (SMD) is frequently used for this purpose. The SMD based on the ratio between the total droplet volume and the total droplet surface area of all the droplets in the polydisperse spray. In general, for the discrete case the mean diameter given by Mugele and Evans (1951)

$$D_{pq} = \left[\frac{\sum_i N_i D_i^p}{\sum_i N_i D_i^q} \right]^{\frac{1}{(p-q)}}, \tag{1}$$

where N is the number of droplets and D is the diameter. For different values of D_{pq} see Table 1. For the continuous case the SMD is defined by the ratio of the third to the second moment of the probability density function.

Table 1. Mean diameter. The applications are: D_{10} for comparisons, D_{20} for surface area controlling, D_{30} for volume controlling, D_{21} for absorption, D_{31} for evaporation, molecular diffusion, D_{32} for mass transfer, reaction and D_{43} for combustion equilibrium

p	q	a+b (order)	Symbol	Name of mean diameter	Expression
1	0	1	D_{10}	Length	$\frac{\sum N_i D_i}{\sum N_i}$
2	0	2	D_{20}	Surface area	$\left(\frac{\sum N_i D_i^2}{\sum N_i} \right)^{1/2}$
3	0	3	D_{30}	Volume	$\left(\frac{\sum N_i D_i^3}{\sum N_i} \right)^{1/3}$
2	1	3	D_{21}	Surface area-length	$\frac{\sum N_i D_i^2}{\sum N_i D_i}$
3	1	4	D_{31}	Volume-length	$\left(\frac{\sum N_i D_i^3}{\sum N_i D_i} \right)^{1/2}$
3	2	5	D_{32}	Sauter (SMD)	$\frac{\sum N_i D_i^3}{\sum N_i D_i^2}$
4	3	7	D_{43}	De Brouckere	$\frac{\sum N_i D_i^4}{\sum N_i^3}$

$$D_32 = \frac{\int_{Dmin}^{Dmax} D^3 p(D)dD}{\int_{Dmin}^{Dmax} D^2 p(D)dD}. \tag{2}$$

The SMD is extensively used in the characterization of liquid/liquid or gas/liquid dispersions. This usage arises because the SMD, according to its definition, link the area of the dispersed phase to its volume and hence to mass transfer and chemical reactions rates. The SMD depends directly on d_{min} and d_{max} and the shape of the droplets size distribution (Pacek, Man, & Nienow, 1998).

Models that we investigated in this paper are including significantly different time scales, for example, the temperature change more rapidly then the concentration changes. Therefore, the natural way of modeling these processes is considered these models as Singular Perturbed Systems (SPS) of ordinary or partial differential equations. In order to investigate such system it is usual to apply different asymptotic methods. In this paper we use, in addition to different numerical methods, the geometric asymptotic method (Method of Integral Manifolds, MIM) which suggested by Bogolubov, and Mitropolsky (1974), Zadiraka, (1957), as a basic tools for the analysis of SPS system of ordinary differential equations. The MIM method has been successfully applied to the problem of combustion (for example, Babushok, Gol'dshtein, & Sobolev, 1990; Babushok, Gol'dshtein, Romanov, & Babkin, 1992; McIntosh, Gol'dshtein, Goldfarb, & Zinoviev, 1998; Goldfarb, Gol'dshtein, Kuzmenko, & Sazhin, 1999). The main idea

of this method is to reduce the dimension of the considered system by separate the system into fast and slow subsystems and studies these subsystems on the and slow integral manifolds.

Another analytical method that can be applied in general to nonlinear ordinary differential equations (ODEs) and partial differential equations and hence to combustion processes is the Homotopy Analysis Methods (HAM) (Liao, 2012). In general, perturbation method and asymptotic techniques are widely applied to obtain analytic approximations of nonlinear problems in science, and engineering problems. The biggest drawback of the traditional perturbation and asymptotic method is the dependence on the existence of a small parameter in the model, i.e., an explicit appearance of a small parameter in the governing equations. At this point the homotopy analysis method comes into play. In 1992, Liao (1992) employed the basic ideas of the homotopy in topology to propose a general analytic method for nonlinear problems. This method has been successfully applied to many types of nonlinear problems (see for example, Jafari & Seifi, 2008; Jafari, Seifi, & Saeidy, 2009; Mastroberardini, 2011). This analytical method is independent of any small/large physical parameters of the model.

2. The Method of Invariant Manifold (MIM)

In this section we review the general theory of the method of integral/invariant manifolds (Strygin & Sobolev, 1988) and its applications to problems of thermal explosion.

2.1 Mathematical background of the Method of Invariant Manifolds

Consider an ordinary differential equations which given in the form of SPS (singular perturbed system):

$$\frac{dy}{dt} = f(y, z, \epsilon), \ y(t_0) = y_0 \tag{3}$$

$$\epsilon \frac{dz}{dt} = g(y, z, \epsilon), \ z(t_0) = z_0, \tag{4}$$

where $y \in R^m$ (called *slow* variable), $z \in R^n$ (called *fast* variable) are vectors in Euclidean space, $t \in (t_0, \infty)$, $0 < \epsilon < \epsilon_0 << 1$, ϵ is a small parameter of the system, $f, (g) : R^m \times R^n \longrightarrow R^{m,(n)}$ are smooth functions for all y, z and ϵ.

The rate of change of the vector z tends to infinity when $\epsilon \longrightarrow 0$ if $g(y, z, \epsilon) \neq 0$. Hence, equation 4 describes the so-called fast sub-system, while equation 3 describes the so-called slow sub-system.

The MIM theory state that the above system has a unique integral (invariant) manifold that can be represented as a power series with respect to the small parameter ϵ. The advantage of the manifold's existence is the fact that in $O(\epsilon)$ approximation of the slow invariant manifold the analysis of the original system behavior can be considerably simplified by reducing the dimension of the system to the dimension of the slow variables. The determination of the exact and the location of the slow manifold is a rather complex problem, which can be eliminate the advantage of the dimension reduction. The zeroth approximation of the exact slow manifold can be found relatively simply just by equating the RHS of the fast equation to zero (i.e., $g(y, z, \epsilon) = 0$). This equation determines the so-called slow surface (in 2D its called curve) and the analysis of the original system can be reduced to the analysis on the slow surface. On the slow surface, the changes of the slow and fast variables are comparable (i.e., the fast and the slow processes are balanced). Beyond the slow surface, the slow variables are asymptotically constant (quasi-stationary - in an $O(\epsilon)$). Therefore, a trajectory of the system in the phase space (phase plane in 2D case) can be naturally decompose into fast parts (which are off the slow manifold) and slow parts (which are on the slow manifold). The fast and the slow parts of a trajectory can follow each other. The main types of system trajectories can be predicted by the slow surface.

Definition 1. *A smooth surface in the phase space $M \in R^m \times R^n \times R$ is called an invariant manifold of the system (2.1) and (2.2), if any phase trajectory $(y(t, \epsilon), z(t, \epsilon))$ such that $(y(t_1, \epsilon), z(t_1, \epsilon)) \in M$ belong to M for any $t > t_1$. If this condition holds only for $t \in [t_1, T]$, then M is called a local invariant manifold.*

If such manifolds are exist then the analysis of the system behavior can be considerably simplified by reducing the dimension of the system. The aim is to found an invariant manifolds of the dimension m (the dimension of the slow variable y) which can be represented as a graph:

$$z = h(y, \epsilon). \tag{5}$$

Such manifolds called *manifolds of slow motion*. The system dynamics of this manifold is given by the differential equations:

$$\frac{dy}{dt} = f(y, h(y, \epsilon), \epsilon). \tag{6}$$

The solution of the system 3-4 is given by $z = h(y(t, \epsilon), \epsilon)$ where the pair $(y(t, \epsilon), z(t, \epsilon))$ is the solution of 6.

In general, it is impossible to found the exact form and the location of the slow invariant manifolds. Hence, it is necessary to use an approximation methods. For example, the famous one is to represent the slow invariant manifold as a power series with respect to the small parameter of the considered system, i.e.,

$$z = h(y, \epsilon) = \sum_{i=0}^{\infty} \epsilon^i h_i(y), \tag{7}$$

which called *Asymptotic representation* of invariant manifolds. The slow surface $z = h_0(y)$ is $O(\epsilon)$ approximation of the slow invariant manifold. In order to get the zeroth approximation, $h_0(y)$, one should substituting the expansion of z as in eq. 7 into the SPS system and equating coefficient of the same powers of ϵ, or in another way, if we substitute $\epsilon = 0$ in the equations 3 and 4 we get the so-called the *degenerate system*:

$$\frac{dy}{dt} = f(y, z, 0) \tag{8}$$

$$0 = g(y, z, 0). \tag{9}$$

Equation 9 determines the slow surface (quasi steady state), which define the zeroth approximation to the slow invariant manifold. It is assumed the this equation has isolated smooth solution: $z = h_0(y)$, and fulfill the equation: $lim_{\epsilon \to 0} h(y, \epsilon) = h_0(y)$.

According to Tikhonov's theorem, the equation of stability of the invariant manifold can be reduced to the study of its zeroth approximation stability. Invariant manifold of the system 3 and 4 is stable (attractive), if the real parts of all eigenvalues of the matrix: $D_z g(y, h_0(y), 0)$ are negative. It means that if a solution $(y(t, \epsilon), z(t, \epsilon))$ of the system 3-4 which satisfies the initial conditions:

$$y(t_0) = y_0, \quad z(t_0) = z_0, \tag{10}$$

such that:

$$\|z_0 - h(t_0, x_0)\| < \delta, \tag{11}$$

for some positive number δ, can be represent as:

$$y(t, \epsilon) = u(t, \epsilon) + \psi_1(t, \epsilon) \tag{12}$$

and

$$z(t, \epsilon) = h(t, u(t, \epsilon), \epsilon) + \psi_2(t, \epsilon), \tag{13}$$

with the function $\psi_1(t, \epsilon)$ and $\psi_2(t, \epsilon)$ satisfy the condition:

$$lim_{t \to \infty} \psi_1(t, \epsilon) = lim_{t \to \infty} \psi_2(t, \epsilon) = 0. \tag{14}$$

Points of the surface which determined by equation 9 are subdivided into two types: *standard points* and *turning points* (or *stationary points*). A point (y, z) is a standard point of the slow surface if in some neighborhood of this point, the surface can be represented as a graph of the function $z = h_0(y)$ such that $g(y, h_0(y), 0) = 0$. It means that

the condition of the *Implicit Function Theorem* holds and the slow surface has the dimension of the slow variable. Turning point are defined as the solutions of the system:

$$g(y, z, 0) = \frac{\partial g(y, z, 0)}{\partial z} = 0. \tag{15}$$

The problems of existence, uniqueness and stability of integral manifold have been studied by many authors (for example, Zadiraka, 1957; Bogolubov, & Mitropolsky, 1974). The main results of these investigation are briefly summarized in the following theorems.

theorem 1. *(Mitropolsky and Lykova 1973) Let the system of 3 and 4 satisfy the following conditions:*

1: The equation $g(y, z, 0) = 0$ has an isolated solution $z = h_0(y)$ in some domain:

$$G = \{(y, z, \epsilon) : y \in R^m, 0 < \epsilon < \epsilon_0, \|z - h_0(y)\| \leq \mu\} \tag{16}$$

2: The functions f, g, h_0 and their first and second partial derivatives are uniformly continues and bounded in the domain G.

3: The eigenvalues $\lambda_1(y), \lambda_2(y), ..., \lambda_n(y)$ of the matrix $D_z g(y, h_0, 0)$ satisfy the condition that:

$$Re[\lambda_i(y)] \leq -\beta \, i = 1, 2, ..., n, y \in R^m \, for \, some \, \beta > 0. \tag{17}$$

Then there exists ϵ_1: $0 < \epsilon_1 < \epsilon_0$ such that for every ϵ: $0 < \epsilon < \epsilon_1$ the system 3 and 4 has a unique invariant manifold $z = h(y, h(y, \epsilon), \epsilon)$, where the function h satisfies the equation $h(y, 0) = h_0(y)$.

theorem 2. *(Strygin and Sobolev 1988) Let the assumptions of the above theorem holds. Then there exist an ϵ_1: $0 < \epsilon_1 < \epsilon_0$ such that for every ϵ: $0 < \epsilon < \epsilon_1$ the invariant manifold $z = h(y, \epsilon)$ is stable. Furthermore, for every $t > t_0$ the functions $\psi_1(t, \epsilon)$ and $\psi_2(t, \epsilon)$ which presented before in Equations 12 and 13, satisfy the conditions:*

$$\|\psi_1(t, \epsilon)\| \leq \epsilon C \|z_0 - h(t_0, y_0, \epsilon)\| \, exp\left(-\frac{\beta(t - t_0)}{\epsilon}\right) \tag{18}$$

$$\|\psi_2(t, \epsilon)\| \leq C \|z_0 - h(t_0, y_0, \epsilon)\| \, exp\left(-\frac{\beta(t - t_0)}{\epsilon}\right), \tag{19}$$

for some constant C, which is independent of t_0, y_0, z_0 and ϵ.

theorem 3. *(Strygin and Sobolev 1988) Let the assumptions of the above theorem holds. Then the invariant manifold $z = h(y, \epsilon)$ can be represented as:*

$$z = h(y, \epsilon) = h_0 + \sum_{i=1}^{k} \epsilon^i h_i(y) + h^*(y, \epsilon), \tag{20}$$

for some k, where $h^*(y, \epsilon)$ is a smooth function with a bounded norm, such that $\|h^*(y, \epsilon)\| = O(\epsilon^{k+1})$ for all R^m.

The last theorem is a methods of approximation in order to find the slow invariant manifold as a power series with the small parameter ϵ because in general situation, the determination of the exact form and the location of the slow invariant manifold is impossible.

In the zeroth approximation, the equation $z = h_0(y)$ is $O(\epsilon^k)$ approximation of the slow invariant manifold, except the turning points. Thus, the general case of the above technique for the SPS systems can be subdivided into two directions of analysis: the first is the analysis of the slow motion and second is the analysis of the fast motions. The analysis can be considerably simplified by this decomposition and by reducing the dimension of the system to the dimension of the slow variable y and the dimension of the fast variable z. It means that the zeroth approximation of the slow invariant manifold, the analysis of the original system can be reduced to the analysis of the system dynamics on the slow surface. As mention before, on the slow surface the change of the slow and the fast variables

are comparable. Beyond the slow surface, the slow variables are fixed (Quasi-stationary). Hence, each system's trajectory can be approximated by fast motions that are described by the fast sub-system:

$$\epsilon \frac{dz}{dt} = g(y_0, z, \epsilon); \ \ y = y_0 = constant, \tag{21}$$

and the slow motions (which are on the slow manifolds) that are given by the slow sub-system 6 with $z = h_0(y)$. In the next subsection we discuss in details with the asymptotic representation of the invariant manifold.

2.2 Asymptotic representation of the invariant manifold

In order to find the invariant manifold we should write the function $z = h(y, \epsilon)$ as an asymptotic expansion in power of the small parameter ϵ, i.e.,

$$z = h(y, \epsilon) = \epsilon^0 h_0(y) + \epsilon^1 h_1(y) + ... + \epsilon^n h_n(y) + ... \ . \tag{22}$$

Let $f(y, h(y, \epsilon, \epsilon))$ and $g(y, h(y, \epsilon, \epsilon))$ be a formal asymptotic representation which given as:

$$f(y, \sum_{k \geq 1} \epsilon^k h_k, \epsilon) = \sum_{k \geq 0} \epsilon^k f^{(k)}(y, h_0, h_1, ..., h_{k-1}), \tag{23}$$

and

$$g(y, \sum_{k \geq 0} \epsilon^k h_k, \epsilon) = \frac{\partial g}{\partial z}(y, h_0(y), 0) \sum_{k \geq 1} \epsilon^k h_k + \sum_{k \geq 1} \epsilon^k g^{(k)}(y, h_0, h_1, ..., h_{k-1}). \tag{24}$$

Let rewrite the fast equation in the form of

$$\epsilon \frac{dh}{dy} f(y, h(y, \epsilon, \epsilon)) = g(y, h(y, \epsilon, \epsilon)) \tag{25}$$

Which in an explicit terms has the form of:

$$\epsilon \sum_{k \geq 0} \epsilon^k \frac{dh_k}{dy} f(y, \sum_{k \geq 0} \epsilon^k h_k, \epsilon) = g(y, \sum_{k \geq 0} \epsilon^k h_k, \epsilon). \tag{26}$$

Now by substituting Equations 23 and 24 in 26 and equating the coefficient power of the small parameter ϵ, then one can get the equation:

$$h_k = (\frac{\partial g}{\partial z}(y, h_0(y)^{-1})(g^{(k)} - \sum_{0 \geq p \geq (k-1)} \frac{dh_p}{dy} f^{(k-1-p)}) \tag{27}$$

In particular:

$$h_0 : g(y, h_0(y), \epsilon) = 0, \tag{28}$$

which accordance to the equation 9 the zeroth approximation, $h_0(y)$, is applicable and has a sense.

In general, the coefficient $h_k(y)$ are found according to the next theorem:

theorem 4. *(Fenichel 1989, asymptotically stable slow manifolds). For any sufficiently small ϵ, there is a function h_k that is define on compact domain $K = [0, Y]^m$ in R^m such that the graph*

$$M_\epsilon = \{(y, z) : z = h_k, y \in K\} \tag{29}$$

is locally invariant under the dynamics of equations 3 and 4. The function h_k admits an asymptotic expansion,

$$h_k = h_0 + h_1 + h_2 + ... \; as \; \epsilon \to 0, \tag{30}$$

where the coefficient $h_k : K \to R^n$ are found successively from the equation:

$$
\begin{aligned}
(D_z g) h_l \;=\; & \sum_{i=0}^{l-1} D h_l f^{(l-1-i)} - \sum_{j=2}^{l} \frac{1}{j!} (D_z^j g) \sum_{|i|=l} (h_{i_1}, ..., h_{i_1}) \\
& - \sum_{k=1}^{l-1} \frac{1}{j!} \sum_{j=1}^{l-k} \frac{1}{j!} (D_z^j (\partial_\epsilon^k g)) \sum_{|i|=l-k} (h_{i_1}, ..., h_{i_1}) - \frac{1}{j!} (\partial_\epsilon^l g),
\end{aligned}
\tag{31}
$$

for $l = 1, 2, ...$ Here the functions f and g and their derivatives are evaluated at $(y, z = h_0, 0)$, and it is understood that a sum is empty when the lower bound exceeds the upper bound. In particular, h_1 and h_2 are given by:

$$(D_z g) h_1 = (D h_0) f - g_\epsilon \tag{32}$$

and

$$
\begin{aligned}
(D_z g) h_2 \;=\; & (D_z g) h_1 f + (D h_0)((D_z f) h_1 + f_\epsilon) \\
& - \frac{1}{2} (D_z^2)(h_1, h_1) - (D_z g_\epsilon) h_1 - \frac{1}{2} g_{\epsilon\epsilon},
\end{aligned}
\tag{33}
$$

Furthermore, $h \in C^r$ for any finite r, and the dynamics of the system of equations 3 and 4 on M_ϵ are given by the reduced equation

$$\frac{dy}{dt} = f(y, h_k(y), \epsilon). \tag{34}$$

In many instances - for example, in the Michaelis - Menten - Henri reaction mechanism, in combustion problems the reduced slow system, $\frac{dy}{dt} = f(y, h_0(y), 0)$, has an asymptotically stable fixed point at $(y_0, h_0(y_0))$. In such cases, the reaction schema has a global attracting equilibrium. Hence the system of Equations 3 and 4 has a fixed point at $(y_{0,\epsilon}, h_\epsilon(y_{0,\epsilon}))$, and the slow manifold, M_ϵ is its weak stable manifold.

2.3 Application of MIM to Thermal Explosion, fast and slow invariant manifold, Semenov's Model, Thermal Explosion Limit

Thermal explosion occurs when chemical reactions produce heat too rapidly for a stable balance between heat release and heat loss. Usually, chemical reaction modeled as a single step exothermic oxidation reaction obeying the Arrhenius temperature dependence. This approach enables one to extract the main features of the process under consideration and to explain the thermo physical phenomena of the model.

The first model for the self-ignition (i.e., a jump from slow to fast reaction) was constructed by Semenov (1928). The basic idea of the model was a competition between a heat production due to the exothermic reaction and heat losses (Newtonian cooling). The main physical assumptions of Semenov model was as follows: there is no reactant conversion during the fast highly exothermic chemical reaction, spatial uniformity of the temperature was also assumed. The governing equation of the temperature was a first-order ordinary differential equation in the form of:

$$\underbrace{\frac{dT}{dt}}_{\substack{Temperature \\ change}} = \underbrace{\frac{QC_0 A}{c_p \rho} exp\left(-\frac{E}{RT}\right)}_{\substack{Heat \\ release}} - \underbrace{\frac{h(T - T_a)}{V c_p \rho}}_{\substack{Heat \\ losses}}, \quad \underbrace{T(t = 0) = T_0}_{Initial \; condition}. \tag{35}$$

If one define the dimensionless temperature θ as:

$$\theta = \frac{T - T_a}{T_a} \beta, \tag{36}$$

where β is the reduced ambient temperature given by

$$\beta = \frac{RT_a}{E}. \tag{37}$$

This parameter is small for typical gas systems with high activation energy. Hence, $\beta\theta << 1$ which enable one to apply the Frank-Kamenetskii approximation given by

$$exp\left(-\frac{E}{RT}\right) = exp\left(-\frac{1}{\beta}\right) exp\left(\frac{\theta}{1+\beta\theta}\right) \approx exp\left(-\frac{1}{\beta}\right) exp\left(\theta\right). \tag{38}$$

Thus equation 35 becomes

$$\frac{d\theta}{dt} = \frac{QC_0 A}{c_p T_a \rho e^{\frac{1}{\beta}}} - \frac{h}{Vc_p\rho}. \tag{39}$$

The classical Semenov's theory of thermal explosion identifies the critical condition for thermal explosion as a loss of stability of an exothermic homogeneous reaction. Physical stability means that the temperature is bounded in time. According to Semenov's theory, the thermal explosion defined as an infinite growth of the temperature. The stability a steady state of a system can describe the reaction system behavior (explosive or non-explosive). The critical condition for self-ignition is the most important critical parameter in Semenov's model. Thermal explosion occurs if the curve of heat release lies above the line of heat losses. On the opposite case the explosion will not occurs. The criticality is defined by the condition of contact of these curves. The Semenov's explosion limit, the critical parameter for self-ignition defined by

$$\alpha_{cr} \equiv \frac{hRT_a^2}{VQC_0 AE} exp\left(\frac{E}{RT_a}\right) = e, \tag{40}$$

For $\alpha > e$ ($\alpha < e$) the solution of the temperature equation is bounded (unbounded). The maximum value of dimensionless temperature calculated under the critical parameter value $\alpha = \alpha_{cr}$ called a maximum sub critical temperature θ^* (see Figure) and equals to unity. If one take into account the reactant concentration in Semenov's model, then the physical model become more realistic. In this case the system of the governing equations is closed in the sense of the mass and energy conservation law. The first attempt to build such model belong to Todes (1936). His model was a system of two ordinary differential equations, the energy conservation equation and the concentration equation in the form of:

$$\frac{dT}{dt} = \frac{QA}{c_p\rho} C exp\left(-\frac{E}{RT}\right) - \frac{h\left(T - T_a\right)}{Vc_p\rho}, \tag{41}$$

$$\frac{dC}{dt} = -AC exp\left(-\frac{E}{RT}\right), \tag{42}$$

with the initial conditions:

$$T = T_0, \ C = C_0. \tag{43}$$

let us introduced some characteristics times: The first one is the reaction time t_r as a time required for the concentration to fall e times from its initial value under the isothermic condition $T = T_a$ given by the following formula:

$$t_r = \frac{1}{A} exp\left(-\frac{E}{RT_a}\right). \tag{44}$$

The second characteristic time is called the adiabatic time given by

$$t_{ad} = \frac{c_p\rho RT_a^2}{QC_0 AE} exp\left(-\frac{E}{RT_a}\right) \int_0^\infty exp\left(-\theta\right) d\theta. \tag{45}$$

The third characteristic time is the thermal relaxation time which in the absence of heat release, is the time that take the dimensionless temperature to decrease by the factor e from its initial value and given by

$$t_{re} = \frac{Vc_p\rho}{h}. \tag{46}$$

Applying 36, 37, 44, 45, 46 to the system 41-42 yields the following physical model

$$\frac{d\theta}{dt} = \frac{1}{t_{ad}}\eta exp\left(\frac{\theta}{1+\beta\theta}\right) - \frac{\theta}{t_{re}},$$ (47)

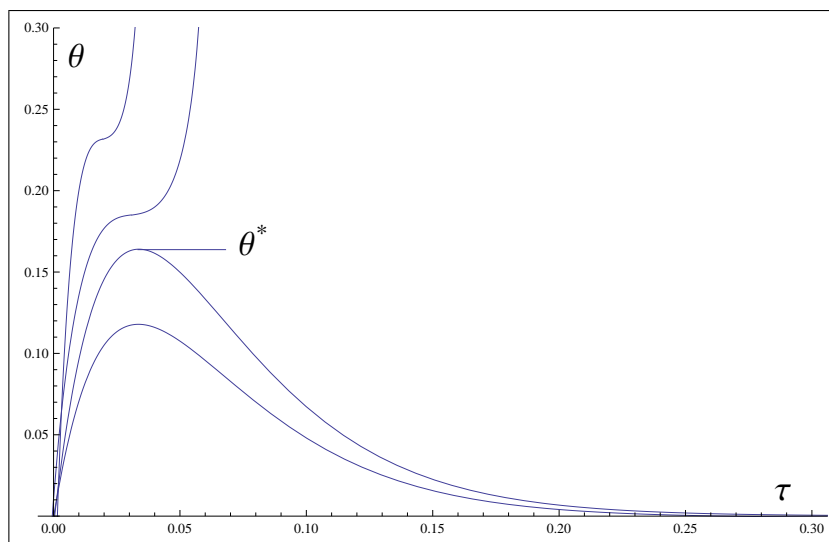$$\frac{d\eta}{dt} = -\frac{1}{t_r}\eta exp\left(\frac{\theta}{1+\beta\theta}\right).$$ (48)
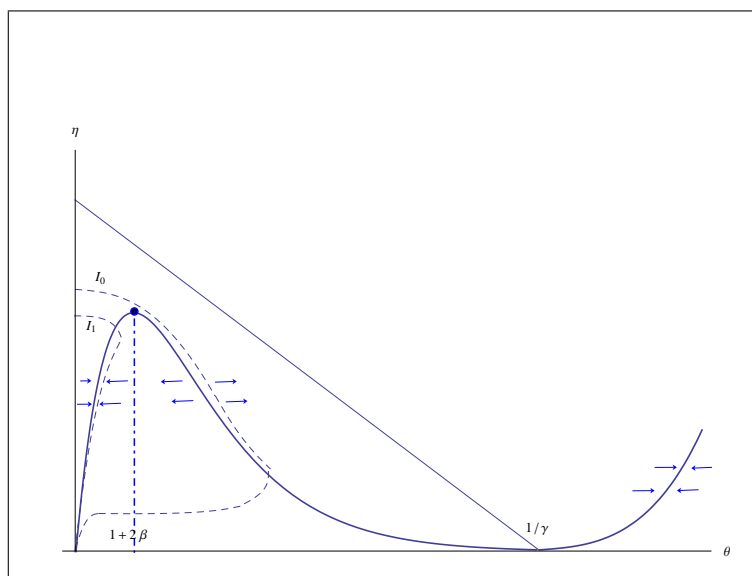

Figure 1. Semenov's temperature profile

Figure 2. Phase plane of the system 50-51, F_0, F_1 and F_2 are the slow curve branches

2.3.1 The motivation to applying the MIM

The analysis of the system 47-48 yield that the system has a unique steady state. This unique steady state is the final state with all the reactant converted i.e., $C = 0$ and the temperature equal to the ambient i.e.,m $T = T_a$. The final state bear no information about the dynamics of the system. Therefore, the classical Semenov's approach to criticality, which is based on the steady state analysis is no longer relevant. It is well known fact that significantly different time scales characterize a wide spectrum of thermo physical and chemical processes. Hence, a natural

way of the modeling of thermal explosion processes is to present the model in singularly perturbed system (SPS) of differential equations. The most common and successful way to study such systems is to apply a different asymptotic methods (for example, Kassoy & Liñan, 1978; Kotovich & Nesenenko, 2000).

In this paper we applied the method of invariant manifold that proposed by (Babushok & Goldshtein, 1988; Gol'dshtein & Sobolev, 1992) as a basic analytical tool. The main and basic idea of this method is to reduced the dimension of the governing equations and separate the system into fast and slow subsystems. According to this method the thermal explosion limit is a unique trajectory that contain an unstable invariant manifold. The critical Semenov's value is only the zero-order term corresponding asymptotic expansion in the sense of the small parameter. In order to apply this method to the system 47-48 let us introduce the following dimensionless parameters:

$$\tau = \frac{t}{t_r}, \ \gamma = \frac{t_{ad}}{t_r}. \tag{49}$$

Rewrite the system 47-48 using the above dimensionless parameters

$$\gamma \frac{d\theta}{d\tau} = \eta exp\left(\frac{\theta}{1 + \beta\theta}\right) - \alpha\theta, \ \theta = 0 \tag{50}$$

$$\frac{d\eta}{d\tau} = -\eta exp\left(\frac{\theta}{1 + \beta\theta}\right), \ \eta = 1. \tag{51}$$

For highly exothermic chemical system the parameters β and γ are rather small. For realistic combustible gas mixture the relation is satisfied: $\beta^2 < \gamma < \beta$. Therefore, the system 50 and 51 may be considered as a SPS of ordinary differential equations with the small parameter γ. The temperature is fast variable and the concentration is the slow one. The application to the division of the system into rapid and slow motion on the phase plane (η, θ) is applicable, see for example (Mischenko & Rozov, 1980).

For the above typical values of the parameters β and γ, there are two branches of the slow curve in a triangle on the phase plane bounded by coordinate axes and adiabatic line $\eta = 1 - \gamma\theta$ (see Figure). In order to apply the asymptotic method MIM let us define the slow curve of the system 50-51. According to MIM method the slow surface (curve in two dimensional case) is given by the equation:

$$F(\theta, \eta) \equiv \eta exp\left(\frac{\theta}{1 + \beta\theta}\right) - \alpha\theta = 0, \tag{52}$$

then there exist explicit function $\eta = \eta(\theta)$ which describing the slow curve in the phase plane $\eta - \theta$ and has the form of:

$$\eta = \alpha\theta exp\left(-\frac{\theta}{1 + \beta\theta}\right). \tag{53}$$

Remark: Applying the QSS approximation to equation 50 implies that:

$$\eta exp\left(\frac{\theta}{1 + \beta\theta}\right) - \alpha\theta = 0 \Rightarrow \eta = \alpha\theta exp\left(-\frac{\theta}{1 + \beta\theta}\right), \tag{54}$$

which means that the slow curve is the 0-isocline for the temperature. In other words, it is a curve of quasi steady state for the fast temperature process i.e., steady state for equation 50 with η considered as a parameter (i.e., constant when calculating the term $\frac{\partial F(\theta,\eta)}{\partial \theta}$). In this case the shape of slow curve is given by Figure .

The turning (jump) points A in Figure (at which $F(\theta, \eta) = 0, \frac{\partial F(\theta,\eta)}{\partial \theta} = 0$) of the slow curve dividends the slow curve into stable part (at which $\frac{\partial F(\theta,\eta)}{\partial \theta} < 0$) (the branch F_1) and unstable part (at which $\frac{\partial F(\theta,\eta)}{\partial \theta} > 0$) (the branch F_0. The third branch F_2 of the slow curve is stable. The branch of the slow curve is considered stable if in its neighborhood the vector motion field is directed to the branch and unstable if its direction is opposite. The stable part of the slow curve attract trajectories in the phase plane $\eta - \theta$ and the unstable part repel them. The trajectories in the $\gamma-$neighborhood of the stable integral manifold I_1 correspond to the slow reaction behavior. For some value of the parameter α the unstable integral manifold will be a part of phase trajectory of the system 50-51. Owing to the continuous dependence of system solutions on the initial conditions, there is a critical trajectory containing the unstable integral manifold I_0 as its own portion (Babushok & Goldshtein, 1988). According to MIM method the critical trajectory divides the phase plane into the non-explosive and the explosive region. The initial conditions that corresponding to I_0 can be considered as the explosion limit. The paths along and below I_0 describe the slow

transient behavior. They are characterized by a comparatively slow reaction with a considerable degree of reaction conservation followed by a sharp slowing down with the transition to a slow reaction proceeding-motion along I_1. The path along and above I_1 are typical for the explosive transient behavior. They are characterized by a rather slow reaction running up to substantial degrees of reactant consumption with subsequent transition to explosion-the motion parallel to the adiabatic line. What cause the ignition is the fact that the temperature is increase. The maximum temperature rise of the slow reaction is $1 + 2\beta + O(\gamma)$ taking the I_1 trajectory as critical one (Babushok, Goldshtein, & Sobolev, 1990). The critical trajectory determines the critical value of the parameter $\alpha = \alpha_{cr}$, i.e., the thermal explosion limit. The critical parameter value $\alpha = e$ that appear in Semenov and Todes is only the first term of the corresponding asymptotic expansion for α_{cr} in the sense of the small parameter γ. Using the asymptotic expansions for the invariant manifold yields (Gol'dshtein & Sobolev, 1992):

$$\alpha_{cr} = e(1 - \beta)\left(1 - 2.946(1 + 2\beta)\gamma^{2/3} - \left(\frac{4}{9}(1 + 6\beta)\gamma \cdot ln\left(\frac{1}{\gamma}\right)\right)\right). \tag{55}$$

This value is in a good agreement with the asymptotic results derived by others authors. In particular, Kassoy and Linan's formula (Kassoy & Liňan, 1978) for $\beta = 0$ reads as:

$$\alpha_{cr} = e(1 - 2.946\gamma^{\frac{2}{3}}). \tag{56}$$

Thomas (1961) and Frank-kamenetskii (1969) have obtained similar formula.

The mathematical interpretation of the thermal explosion phenomenon based on the integral manifold method enables to classify different types of behavior of the solution of the system, to calculate the maximum sub-critical temperature and to obtain an analytical estimation for the main quantitative characteristics of the system.

3. Homotopy Analysis Method (HAM)

Perturbations, approximations and other asymptotic techniques such as the method of multiple scale, the renormalization method, the method of matched asymptotic expansion, Pade approximation, variational iterations, Lyapunov's artificial small parameter, the δ-expansion, Adomian decomposition method, Lindstedt-Poincare method are widely in science and engineering, see for examples (Burke, 1971; Abbasbandy, 2003;). All these methods are based on small/large parameters of the systems of the governing equation. Applications of these methods is based on representations of solutions as series. Then nonlinear differential equation are replaced by an finite infinite number of linear sub-problems, which are completely determined by the original governing equation and especially by appearance small parameter. In general, and especially in combustion processes which are highly nonlinear an explicit small parameter does not appear in the governing equations. Besides that, even in presence of an explicit small parameter, the sub-problems might have no solutions, or might be so complicated that only a few sub-problems can be solved. Therefore, given a nonlinear problem with a multiple scale such that the small parameter is hidden in the governing equations, it is not guaranteed that one can always gain perturbation approximations. In addition, it is not guaranteed that a perturbation result is valid in the whole region of all physical parameters. In order to overcome the restrictions of perturbation techniques, some non perturbation methods are developed, such as Lyapunov's artificial small parameter method (Liao, 2003; Abbasbandy, 2006) the Adomian decomposition method (Wazwaz, 2005 Bildik & Konuralp, 2006) and so on. In general, all these methods are based on a so-called artificial parameter, and the approximation of solutions are due to series with the artificial small parameter. Given a physical model, one can put the artificial small parameter into the governing equations in many different ways, but there are no theories to guide how to put it in a better place so as to gain a better approximation. Generally speaking, all traditional non-perturbation methods as we mentions above, can not guarantee the convergence of approximation series. In this section we introduce the basic idea of the HAM as presented in the book of Shijun Liao (Liao, 2003, 2009, 2012).

3.1 Basic concepts of Homotopy Analysis Method (HAM)

To the best of our knowledge, the HAM is the only known analytical method that yields convergent solution for all the relevant parameters. Generally, combustion processes contain different scales in the mathematical/ physical model. Sometimes it is very difficult to identify the smallest parameter in the system. The most prominent advantage of this method is that it does not depend upon any small physical parameters at all and thus is more general than the traditional multiple-scale perturbation techniques. The HAM is a very effective analytical method for solving highly nonlinear problems in science and engineering, see for example in Mastroberardini (2011).

Consider the following differential equation:

$$N[\phi(\tau)] = 0, \tag{57}$$

where N is a nonlinear operator, τ is an independent variable and ϕ is an unknown function. For simplicity, we ignore all boundary or initial conditions, which can be treated similarly. By means of the homotopy method, Liao (1999) constructs the so-called zero-order deformation equation as follows:

$$(1 - \delta)\ell[\psi(\tau; \delta) - \phi_0(\tau)] = \delta\tilde{h}H(\tau)N[\psi(\tau; \delta)], \tag{58}$$

where $\delta \in [0, 1]$ is the embedding parameter, $\tilde{h}$ is a non-zero auxiliary parameter, which can choose freely in HAM, $H(\tau) \neq 0$ is an auxiliary function, ℓ is an auxiliary linear operator, ϕ_0 is an initial guess of $\phi(\tau)$, and $\psi(\tau, \delta)$ is an unknown function. When $\delta = 0$ and $\delta = 1$ we obtain the values $\psi(\tau; 0) = \phi_0(\tau)$ and $\psi(\tau; 1) = \phi(\tau)$ respectively. Thus, as δ increases from 0 to 1, the solution $\psi(\tau; \delta)$ varies from the initial guess to the solution. According to the HAM, we can first use the embedding parameter δ as a small parameter, and assume that the solutions of Equation 58 can be written as a power series in δ:

$$\psi = \phi_0(\tau) + \sum_{m=1}^{\infty} \phi_m(\tau)\delta^m. \tag{59}$$

If the auxiliary linear operator, the initial guess, the auxiliary parameter $\tilde{h}$, and the auxiliary function are properly chosen, the series in Equation 59 converges at $\delta = 1$, one has:

$$\phi(\tau) = \phi_0(\tau) + \sum_{m=1}^{\infty} \phi_m(\tau), \tag{60}$$

which must be one solution of the original nonlinear equation, as proved by Liao (1999).

3.1.1 The m-order deformation of HAM

Define the vector:

$$\vec{\phi}_n = \{\phi_0(\tau), \phi_1(\tau), ..., \phi_n(\tau)\}. \tag{61}$$

Differentiating Equation 58 m-times with respect to the embedding parameter δ, setting $\delta = 0$ and finally dividing the terms by $m!$, we obtain the mth-order deformation equation in the form of:

$$\ell[\phi_m(\tau) - \chi_m\phi_{m-1}(\tau)] = \tilde{h}H(\tau)R_m(\vec{\phi}_{m-1}(\tau)), \tag{62}$$

where,

$$R_m(\vec{\phi}_{m-1}(\tau)) = \frac{1}{(m-1)!}\frac{\partial^{m-1}N[\psi(\tau; \delta)]}{\partial\delta^{m-1}}|_{\delta=0}, \tag{63}$$

and χ_m is the unit step function.
Applying the inverse operator $\ell^{-1}(\cdot)$ on both sides of Equation 62, we obtain

$$\phi_m(\tau) = \chi_m\phi_{m-1}(\tau) + \tilde{h}\ell^{-1}[H(\tau)R_m(\vec{\phi}_{m-1}(\tau))]. \tag{64}$$

3.1.2 The convergence control parameter $\tilde{h}$ (the $\tilde{h}$-curve)

The homotopy perturbation method is based on the homotopy, a basic concept of topology. The role of the auxiliary parameter $\tilde{h} \neq 0$ is to construct the so-called zero-order deformation, which gives a more general homotopy than the traditional one. Thus, unlike all previous analytic methods, the convergence and the rate of solution series are dependent upon this parameter. This means that this technique gives one a convenient way to adjust and to control the convergent region of the solutions Liao (1999).

The solution of the mth-order deformation can be expressed according to Equation 64 which can be solved by symbolic software such as Mathematica 8.0, Maple, Matlab and so on. We obtain a family of solutions that depends on the auxiliary parameter $\tilde{h}$. So, regarding $\tilde{h}$ as an independent variable, it is easy to plot the $\tilde{h}$-curves. For example, we can plot the following curves:

$$\Gamma_1 = u(\vec{r}, t)_{|\vec{r}=0, t=0}, \, or \, \Gamma_2 = u'(\vec{r}, t)_{|\vec{r}=0, t=0}, \, or \, \Gamma_3 = u''(\vec{r}, t)_{|\vec{r}=0, t=0}.$$

The curves Γ_i ($i = 1, 2, 3$) are a function of $\tilde{h}$ and thus can be plotted by a curve $\Gamma \approx \tilde{h}$. According to Liao (1999) there exists a horizontal line segment (flat portion of the $\tilde{h}$-curve) in the figure of $\Gamma \approx \tilde{h}$ and called *the valid region*

of $\tilde{h}$ which corresponds to a region of convergence of the solutions. Thus, if we choose any value in the valid region of $\tilde{h}$ we are sure that the corresponding solutions series are convergent. For given initial approximation $u_0(\vec{r}, t)$, the auxiliary linear operator ℓ, and the auxiliary function $H(\vec{r}, t)$, the valid region of $\tilde{h}$ for different special quantities are often nearly the same for a given problem. Hence, the so-called $\tilde{h}$-curve provides us a convenient way to show the influence of $\tilde{h}$ on the convergence region of the solutions series.

3.2 Application the homotopy analysis method to thermal explosion model

In this section we applied the HAM to the model 50-51 with the application of Frank-kamenetskii (1969) approximation.

In order to apply the HAM let us define the following serieses:

$$\Phi_1 = \theta_0(\tau) + \sum_{m=1}^{\infty} \theta_m(\tau)\delta^m,$$

$$\Phi_2 = \eta_0(\tau) + \sum_{m=1}^{\infty} \eta_m(\tau)\delta^m.$$

The next step is to define the nonlinear operator $N[\cdot]$ for each function Φ_i $i = 1, 2$ which refer to the Equations 50-51 as follows:

$$N_\theta[\Phi_1] = \gamma \frac{d\Phi_1}{d\tau} - \Phi_2 exp\,(\Phi_1) + \alpha\Phi_1, \tag{65}$$

$$N_\eta[\Phi_2] = \frac{d\Phi_2}{d\tau} + \Phi_2 exp\,(\Phi_1). \tag{66}$$

Differentiating equations 66-66 m-times with respect to the small parameter δ, then setting $\delta = 0$, and finally dividing these equations by $(m - 1)!$, we obtained the so-called $m-$th order equation for θ and η:

$$\ell\left[\theta_m - \chi_m\theta_{m-1}\right] = \tilde{h}R_{m_\theta},$$
$$\ell\left[\eta_m - \chi_m\eta_{m-1}\right] = \tilde{h}R_{m_\eta}. \tag{67}$$
$$\tag{68}$$

According to Liao (2009) let:

$$D_m(\cdot) = \frac{1}{m!}\frac{\partial^m(\cdot)}{\partial\delta^m}|_{\delta=0}, \tag{69}$$

then the expressions for $R_{m_{(\cdot)}}$ are as follows:

$$R_{m_\theta}(\theta_{m-1}) = \frac{d\theta_{m-1}}{d\tau} - \eta_m \sum_{k=0}^{m-1}\left(1 - \frac{k}{m}\right)D_k(e^{\theta_m})\theta_{m-k} + \alpha\theta_m, \tag{70}$$

$$R_{m_\eta}(\eta_{m-1}) = \frac{d\eta_{m-1}}{d\tau} + \eta_m \sum_{k=0}^{m-1}\left(1 - \frac{k}{m}\right)D_k(e^{\theta_m})\theta_{m-k} \tag{71}$$

To solve the model 50-51 by means of HAM, we choose the initial guess to be $\theta_0 = 0$ and $\eta_0 = 1$ which satisfies the initial conditions in 50 and 51. In addition we choose the linear operator

$$\ell_{\theta,\eta}[\cdot] = \frac{d}{d\tau} \tag{72}$$

with the property $\ell[C] = 0$ where C is the integral constant. The inverse operator ℓ^{-1} is given by

$$\ell_\theta^{-1}[\cdot] = \int_0^\tau (\cdot)d\tau, \;\; \ell_\eta^{-1}[\cdot] = \int_1^\tau (\cdot)d\tau. \tag{73}$$

Now, the solutions of the mth-order deformation equations of θ_m and η_m given by

$$\theta_m = \chi_m\theta_{m-1} + \ell_\theta^{-1}\left[\tilde{h}R_{m_\theta}\right],$$
$$\eta_m = \chi_m\eta_{m-1} + \ell_\eta^{-1}\left[\tilde{h}R_{m_\eta}\right]. \tag{74}$$

The solutions profiles of the temperature and concentration given by the application of the HAM are presented in Figure -Figure correspondingly.
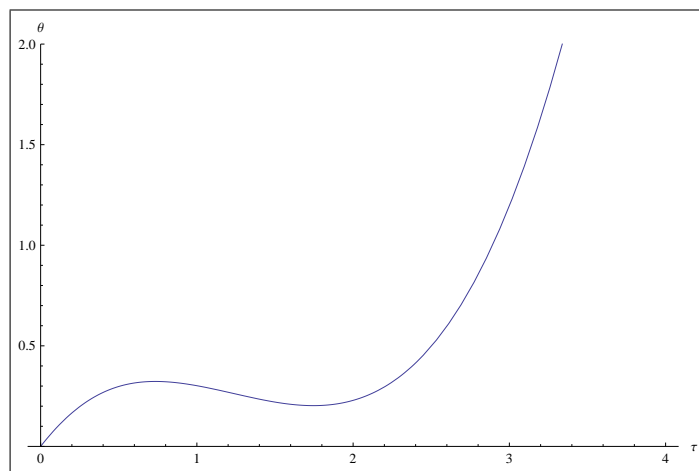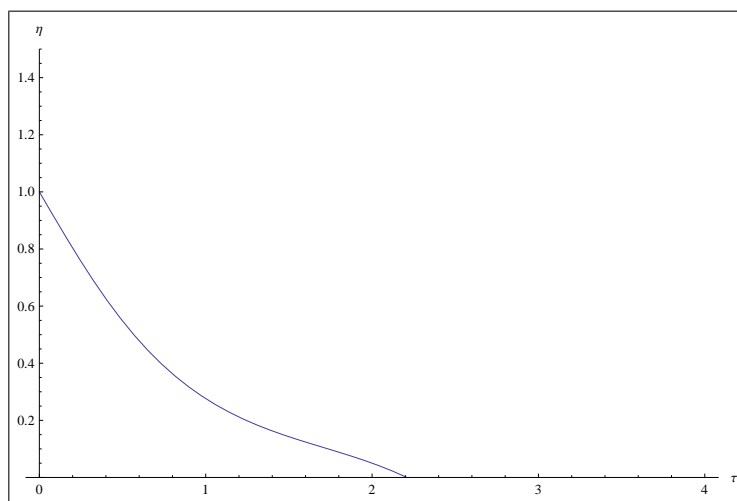

Figure 3. HAM's temperature profile

Figure 4. HAM's concentration profile

4. Thermal explosion of monodisperse spray combustion

Spray ignition represents phenomenon of great fundamental and practical engineering interest and have been widely discussed in the literature (Clift, Grace, & Weber, 1978Faeth, 1983 William, 1995; Kuo, 1996; Aggarwal, 1998; Lefebvre, 1989; Abramzon & Sirignano, 1989Abramzon & Sirignano, 1989; Sirignano, 1999; Dombrovsky et al., 2001), . Spray combustion is employed in numerous practical systems including industrial furnaces, boilers, gas turbines, diesels, spark ignition engines, and rocket engines. Ignition is a crucial event in the operation of these systems. The ignition of fuel sprays injected in jet engine combustors is an important phenomenon due to the desirability of fast ignition and its relation to the issue of flame stabilization. Similar considerations apply to spark ignition engines, where fast, well-controlled ignition is important to engine efficiency and emissions. In diesel engines, the ignition of fuel sprays injected into a high temperature and pressure environment reached by establishing a high compression ratio, considerably exceeding the compression ratio in gaseous fuel and carburetor engines, represents a critical event in their operation. Another issue, more specific to spray ignition, deals with the occurrence of ignition in the vicinity of an individual droplet, cluster of droplets, or globally in a spray, and which one is likely to occur depends upon the flow conditions, spray properties, liquid fuel loading, and wall temperature etc.

Let us explain every mode: (1) The state of ignition for an individual droplet represents the appearance of a flame surrounding the droplet or in the wake region, with a dimension on the order of the droplet diameter. An ignition event for a droplet distinguishes the state of pure vaporization from that of a diffusion flame around the droplet. This has significant implications for spray flames with regard to flame stability and the amount of pollutants formed. In spray combustion modeling, the identification of this event is important since it determines the amount of heterogeneous burning involved, and the rates of mass and heat transport are significantly altered following its occurrence. (2) For a liquid fuel spray, on the other hand, ignition represents the appearance of a global sheath flame that is associated with the entire spray and not with any individual droplet, and has a dimension few orders of magnitude larger than the droplet diameter. (3) The ignition of a droplet cloud or cluster represents an intermediate situation, and can be utilized to bridge the results of studies dealing with modes (1) and (2).

Our models that we investigated in this paper are analyzed the effects of the thermal radiation on thermal explosion in combustible gas containing fuel droplets. An adequate treatment of thermal radiation is essential to develop a mathematical model of the combustion system. The level of detail required for radiative transfer depends on whether one is interested in determining the instantaneous spectral local radiative flux, flame structure, scalar properties of the flame, formation of flame-generated particles (largely soot), local radiative flux and its divergence or the temperature distribution. For example, when the model is used to predict pollutant concentrations, accurate temperatures are especially important since the chemical kinetics involved are extremely temperature dependent. The fraction of the total heat transfer due to radiation grows with combustor size, attaining prominence for gaseous firing at characteristic combustion lengths of about 1(m). Radiation heat transfer then, plays a dominant role in most industrial furnaces. Unfortunately, it is governed by a complex integro-differential equation which is time consuming to solve. In a combustion chamber, radiation heat transfer from the flame and combustion products to the surroundings walls can be predicted if the radiative properties and temperature distributions in the medium and on the walls are available. Usually, however, temperature itself is an unknown parameter, and as a result of this, the total energy and radiant energy conservation equations are coupled, as in many heat transfer applications. Solution of the thermal energy equation can be obtained if several other physical and chemical processes can be modeled. The major processes which need to be considered in a combustion system in addition to radiation include: chemical kinetics, thermal chemistry, molecular diffusion, laminar and turbulent fluid dynamics, phase transitions, such as evaporation and condensation, surface effects. Since the physical and chemical processes occurring in combustion chambers are very complicated and cannot be modeled on the micro scale, there is a need for physical models to simulate these processes. And the main thermo-physical assumptions are as follows: (1) the spray ignition is considered as an explosion problem, where droplets are regarded as the source of endothermicity. (2) the system is adiabatic; the medium is modeled as a spatially homogeneous mixture of an optically thin, combustible gas with a mono-dispersed spray of evaporating fuel droplets. (3) the medium is modeled as a spatially homogeneous mixture of an optically thin, combustible gas with a mono-dispersed spray of evaporating fuel droplets; (4) with a view to the application of the results to diesel engines the variations of the pressure in the enclosure are ignored as well as their influence on the combustion process; (5) the heat flux from the burning gas to droplets is assumed to consist of the convection and radiation fluxes; (6) the thermal conductivity of the liquid phase is much greater than that of the gas phase; (7) the volume fraction of the gas is much greater than that of the liquid phase. Thus, the heat transfer coefficient of the mixture is controlled by the thermal properties of the gaseous component; (8) the fuel droplets are assumed to be semitransparent and the radiation flux at their surface is described by the Stephan-Boltzman law; (9) the burning gas is optically thick; the walls of enclosure are perfect reflectors or circular; (10) the burning process takes place in the gaseous phase only, and it is described as a first order exothermic reaction; (11) the droplets surfaces are assumed to be on the saturation line Katz (2005).

The problem of a thermal explosion in a mixture containing fuel droplets and gas, in most cases, has been studied based on the application of Computational Fluid Dynamics (CFD packages) (see for example, Aggarwal, 1998; Chiu & Hu, 1998; Stapf, Dwyer, & Maly, 1998; Bykov et al., 2007). This is a numerical method and has a number of attractive feature since it potentially allows us to take into account various heat and mass transfer and combustion processes in the mixture of gas and fuel droplets in a self-consistent way. The benefit of this approach is that it could take into account the complicated geometry of the enclosure and chemistry of the processes involved. This is very attractive for engineering applications including the modeling of combustion precesses in diesel engine (Sazhin et al., 2000). The downside of this approach is that it does not allow us to separate the contribution of different processes and as a result it is not particularly helpful in understanding the relative contribution of these processes.

An alternative approach to this problem is based on an analytical study of the underlying equations in different

limiting cases (i.e., asymptotic analysis). This approach cannot replace the CFD code but can complement it. One of the methods is based on the applications of the zero-order approximation of the geometric version of the asymptotic method of integral manifold as mention before. This method is a convenient tool for the investigation of singular perturbed system of differential equations. Its allows to investigate the dynamics of the system on a subsystem with reduced dimensional. The definition of the integral manifold of the system in the standard form and the theorems of the conditions of existence have been introduced in Bogolubov (1945). Significant influence on the development of the method has been made by Bogolubov and Mitropolsky (1963). Another results of the theory of integral manifolds are presented by Mitropolsky (1973), and in Sazhin et al. (2001) the MIM was applied to a specific problem of modeling of the ignition process in diesel engine.

4.1 The thermal explosion of a gas mixture in monodisperse fuel spray

The first model that we investigate in this paper is presented by Goldshtein, Goldfarb, and Zinoviev (1996) and described the thermal explosion in a two-phase medium. When authors applied the method of the invariant manifold to the model they found three options of physical dynamics behavior: slow regimes, fast explosion regimes, and explosion with freeze delay, i.e., decrease of the temperature before the explosion. The main physical assumptions of the are as following: the process of the thermal explosion is considered in a combustible gas mixture containing evaporating liquid drops, the system is adiabatic, the pressure changes are negligible in the reaction volume and its influence on the combustion process, the quantity of vapor generated during the process is sufficiently small and does not change the essential combustible gas concentration, the thermal conductivity of the liquid phase is much greater than that of the gas phase, quasi-stationary approximation is valid for the combustion process, the drop boundary is assumed to be on a saturation line, i.e., the liquid temperature is constant and is equal to a liquid saturation temperature, the drop size distribution is supposed to be monodisperse spray, the combustion reaction is modeled as a first-order, highly exothermic chemical reaction. Under the above assumptions the system of the governing equations are presented as:

$$c_{pg}\rho_g\alpha_g\frac{dT_g}{dt} = C_f\rho_g Q_f\alpha_g A exp\left(-\frac{E}{RT_g}\right) - 4\pi R_d\lambda_g n_d\left(T_g - T_d\right), \tag{75}$$

$$\frac{dR_d^3}{dt} = -\frac{3\lambda_g}{\rho_L L}\left(T_g - T_d\right), \tag{76}$$

$$\frac{dC_f}{dt} = -C_f A exp\left(-\frac{E}{RT_g}\right). \tag{77}$$

The initial conditions are:

$$at T = 0 : T_g = T_{go}, \ C_f = C_{f0}, \ R_d = R_{d0}, \ T_d = T_{g0}. \tag{78}$$

The system of Equation 75-77 includes the energy equation, the mass equation for the liquid drop, and the concentration equation for the reacting gas respectively. This model has been investigated qualitatively. Using the assumption that the system is adiabatic, dynamical variable C_f can be extracted in explicit form using the energy integral procedure. This procedure reduce the system from three ordinary differential equation into two ordinary differential equation only. The small parameter of the system is:

$$\gamma = (c_{pg}T_{g0}^2 R)/(C_{f0}Q_f E). \tag{79}$$

According to the MIM method, the reduce system includes two equations: fast heat emitting process i.e., the temperature is the fast variable (because of the small parameter that conjugate to the change of the temperature $\gamma \cdot d\theta/d\tau$), and slow process of combustible gas concentration change, i.e., the concentration is the slow variable of the system. By applying the MIM method and the Frank-Kamenetskii approximation to the reduce model and restrict the analysis to a zero approximation for the small parameter $\gamma = 0$ of the system, the authors of Goldshtein, Goldfarb, and Zinoviev (1996) obtained the slow curve of the system in non dimensional form as:

$$F(\theta, \eta)|_{\gamma=0} = \eta e^\theta - \epsilon_1\theta\sqrt[3]{1 + \epsilon_2(\eta - 1)} = 0, \tag{80}$$

where:

$$\eta = \frac{C_f}{C_{f0}}, \quad \theta = \frac{E(T_g - T_{g0})}{RT_{g0^2}}, \epsilon_1 = \frac{4\pi n_d R_{d0} \lambda_g \beta T_{g0}}{A C_{f0} Q_f \alpha_g} e^{\frac{1}{\beta}},$$

$$\beta = \frac{RT_{g0}}{E}, \quad \epsilon_2 = \frac{c_{pg} T_{g0} \beta}{C_{fo} Q_f}.$$

The shape and the position of the allow curve on the phase plane $\theta - \eta$ depend on the combination of the parameters ϵ_1 and ϵ_2. A maximum point, which obtain from the solution of the system $F(\theta, \eta) = dF(\theta, \eta)/d\theta = 0$, divides the slow curve into stable and unstable parts. The maximum temperature is $\theta^*_{max} = 1$, and the thermal explosion criterion (limit) is $\epsilon_1 = e$ which obtained earlier by Semenov's theory. The unexpected fact of the existence of an explosion limit in the adiabatic system is caused by the presence of additional liquid phase that plays the role of energy sink. The trajectories lying above the critical trajectory (for $\epsilon_1 < e$) describe conventional explosion regimes with fast increase in the temperature. The trajectories that lying below the critical trajectory (for $\epsilon_1 > e$) depict the so-called *delay time* (which discuss in details in the following section).

4.1.1 The delay time in the model of thermal explosion of a gas mixture

The delay time defined mathematically as the time period during which the trajectory moves along the slow curve until the fast thermal explosion is occurred, i.e., time period between the intersection point of the trajectory with the slow curve on the phase plane up to the so-called the turning point. The physical meaning of the delay time is as follows: the rate of change of the slow and fast variables become comparable in the phase plane, when the trajectory is attracted by the stable slow curve. Moving along the stable slow curve physically means delay effects before the final explosion (Goldfarb, Gol'dshtein, & Zinoviev, 2002). The system trajectory stays on the slow curve till it reach the turning point and then jump from the the slow curve. Jumping from the slow curve corresponds to transition to the fast explosive behavior. The time during which the trajectory stays on the slow curve represents a delay time before the final explosion, which is extremely important from the practical point of view (see Figure). In some cases it is possible to estimate the delay time analytically. In this model the delay time is computable analytically. For this purpose we rewrite the slow curve as a function of the dimensionless radius $r = R_d/R_{d0}$ and the dimensionless temperature θ in the form of:

$$\tilde{F}(\theta, r)|_{\gamma=0} = \frac{\epsilon_2 - (1 - r^3)}{\epsilon_2} e^\theta - \epsilon_1 r \theta = 0. \tag{81}$$

The solution of the system $\tilde{F}(\theta, \eta) = d\tilde{F}(\theta, \eta)/d\theta = 0$ is $\theta = 1$. The next step is to find the turning point i.e., r_T. The value of r_T is given by the (numerical) solution of the following equation:

$$\tilde{F}(\theta = 1, r_T)|_{\gamma=0} = \frac{\epsilon_2 - (1 - r_T^3)}{\epsilon_2} e^1 - \epsilon_1 r_T = 0. \tag{82}$$

Substituting the expression $\epsilon_1 r \theta$ from Equation 81 into the RHS of the radius equation i.e., Equation 76 in non dimensional form:

$$\frac{dr^3}{d\tau} = -\epsilon_1 \epsilon_2 r \theta, \tag{83}$$

where the dimensionless time τ define by:

$$\tau = \frac{t}{exp\,(1/\beta)\,/A}. \tag{84}$$

$$\frac{dr^3}{d\tau} = -\left[\epsilon_2 - (1 - r^3)\right] e^\theta. \tag{85}$$

Integrating Equation 85

$$\tau_{delay} = -\int_1^{r_T} \frac{3r^2 dr}{\left[\epsilon_2 - (1 - r^3)\right] e^{\theta(r)}}. \tag{86}$$

The integration with respect to r is carried out from its initial value to its value at the turning point, the latter being determined from Equation 82. In addition, this integration can only be performed analytically if an explicit

expression for $\theta(r)$ is known, which is generally not the case. However, the fact that during the delay period the inequality

$$1 = e^0 < e^\theta < e^1 = e, \tag{87}$$

is valid enable one to obtain the upper bound and the lower bound for the delay time in the form of

$$\frac{1}{e} ln\left(\frac{\epsilon_2}{\epsilon_2 - (1 - r_T^3)}\right) < \tau_{delay} < ln\left(\frac{\epsilon_2}{\epsilon_2 - (1 - r_T^3)}\right). \tag{88}$$

To summarize the results of the model that presented by (Goldfarb, Gol'dshtein, & Zinoviev, 2002) and describe the thermal explosion of monodisperse fuel spray in two-phase medium (combustible gas mixture/liquid drops) has been assumed adiabatic and hence the first energy integral process has been applied. This procedure enable to reduced the model from three ordinary differential equation into two ordinary differential equation. By algebraic manipulations the authors obtained the so-called the slow curve of the system. The dynamic of the system on the slow curve depend on two new dimensionless parameters ϵ_1 and ϵ_2. The combination between these two parameter determined the shape and the position of the slow curve. This qualitative analysis enable to classify main dynamic regimes of the system into a slow regime, a conventional thermal explosion with the criterion for explosion $\epsilon_1 = e$ which congruence with the Semenov's theory, and a new type of thermal explosion with delay before the ignition i.e., thermal explosion with freeze delay. Freeze means that the temperature has been significant decrease before explosion. The delay time was evaluated analytically.
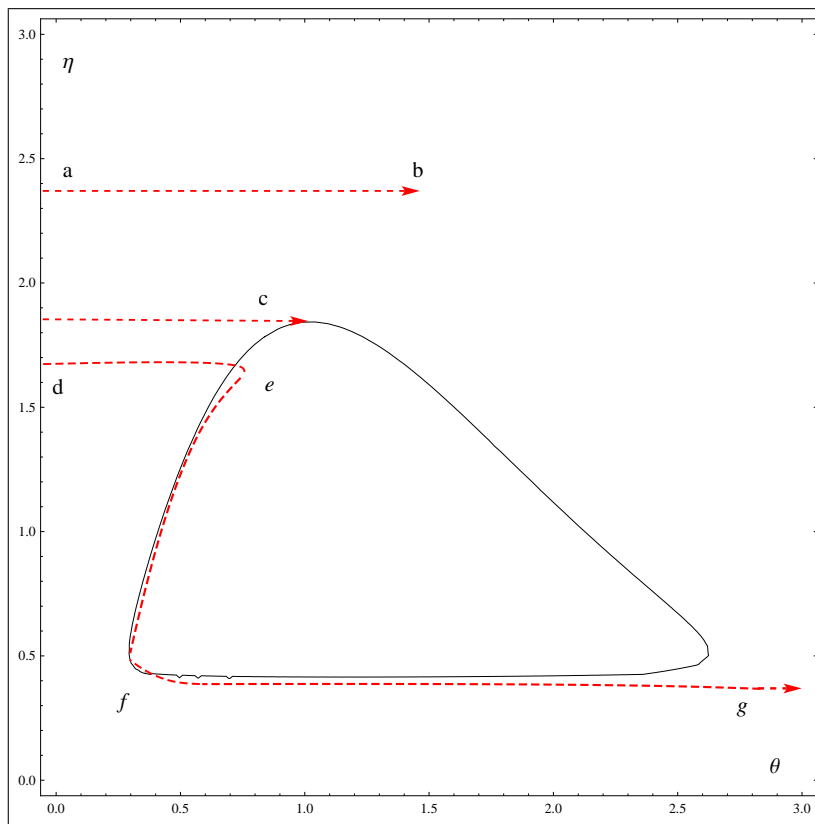

Figure 5. Slow curve. The typical phase trajectories describing different dynamic behavior. Trajectory $a - b$ is fast explosive; c is the critical trajectory (passing through jump (turning)point c), and $d - e - f - g$ describe the delay time

The model that presented by Goldshtein, Goldfarb, and Zinoviev (1996) has been extended (Goldfarb, Gol'dshtein, Kuzmenko, & Greenberg, 1998) in such way that the concentration equation for the reacting gas mixture include a term that describe the addition to the concentration C_f due to the evaporation process. The model that proposed

by the authors of (Goldfarb, Gol'dshtein, Kuzmenko, & Greenberg, 1998) differs from the model presented in Goldshtein, Goldfarb, and Zinoviev (1996) only in the following concentration equation 77:

$$\frac{dC_f}{dt} = -C_f A exp\left(-\frac{E}{RT_g}\right) + \frac{4\pi R_d \lambda_g n_d}{L \rho_g \alpha_g}\left(T_g - T_d\right).$$ (89)

The set of the governing Equations 75-76 with 89 and with the initial conditions 78 describe the effect of a flammable spray on thermal explosion in a preheated combustible gas mixture. The spray is a monodisperse one and the droplets are taken to be a source of endothermicity. An analytical formulas are developed for ignition delay times by exploiting the sensitivity of the process to the chemical activation energy. The qualitative analysis of the model has been done by applying the MIM method and the isocline method. The qualitative analysis of the model divided into two main regimes, upper limit activation energy and low limit activation energy. The first one leads to a relatively small heat release due to chemical reaction, i.e., for the fixed temperature, the Arrhenius term does not take into account in the model. This case characterized by the fact that at the initial stage of the ignition gas mixture cooling represents the dominant process in comparison with heat release. This allow one to apply the theory of the isocline method. This method enable one to compute the ignition time before the conventional thermal runaway in pure combustible gas mixture.

In order to compute the cooling dimensionless time, $\tau_{cooling}$, the energy and the radius equation in dimensionless form as presented in (Goldfarb, Gol'dshtein, Kuzmenko, & Greenberg, 1998) are:

$$\frac{d\theta}{d\tau} = \eta exp\left(\frac{\theta}{1 + \beta\theta}\right) - \epsilon_1 r\theta,$$ (90)

$$\frac{dr^3}{d\tau} = -\epsilon_1 \epsilon_2 r\theta.$$ (91)

Applying the assumption of the high activation energy the energy equation 90 become:

$$\frac{d\theta}{d\tau} = -\epsilon_1 r\theta.$$ (92)

From Equation 91 and 92 one obtained the relation:

$$\frac{d\theta}{dr} = \frac{3r^2}{\gamma\epsilon_2}.$$ (93)

Integrating this equation yield the expression for the temperature θ in the form of:

$$\theta = \theta_0 - \frac{1 - r^3}{\gamma\epsilon_2}.$$ (94)

Substituting the functional relation 94 into Equation 91 and integrate with respect to the variable θ and r yield the cooling time:

$$\tau_{cooling} = \frac{\gamma}{2\epsilon_1 r_c}\left[ln\left(\frac{1 - r_c + r_c^2}{(1 + r_c)^2}\right) + \frac{\pi}{\sqrt{3}} + 2\sqrt{3}arctan\left(\frac{2 - r_c}{\sqrt{3}r_c}\right)\right],$$ (95)

where

$$r_c = (\gamma\epsilon_2\theta_0 - 1)^{1/3}.$$ (96)

The second approximation, the low limit activation energy, assumed that the heat release term on the RHS of the energy equation 90 is dominant in comparison with the term that responsible for Newtonian cooling. In this case on can compute the total time of ignition, i.e., the time from the beginning of the process (from the initial conditions) up to the moment when the system almost reaches its final adiabatic temperature. For this purpose the authors of (Goldfarb, Gol'dshtein, Kuzmenko, & Greenberg, 1998) applied the MIM method since the model is in the form of a singular perturbed system.

In order to compute the total time of ignition, τ_{total}, the energy equation in dimensionless form as presented in (Goldfarb, Gol'dshtein, Kuzmenko, & Greenberg, 1998) is:

$$\gamma\frac{d\theta}{d\tau} = \left(\eta_0 + \frac{1}{\epsilon_2}(\psi-1)(1-r^3) - \gamma(\theta-\theta_0)\right)exp\left(\frac{\theta}{1+\beta\theta}\right) - \epsilon_1 r\theta, \tag{97}$$

where

$$\psi = \frac{Q_f}{L}. \tag{98}$$

When obtained Equation 97 one apply the energy integral procedure. The second term on the RHS of Equation 97 should be neglected according to the assumption of low activation energy. The slow curve of the model in this case (low activation energy) has the form of:

$$\eta_0 + \frac{1}{\epsilon_2}(\psi-1)(1-r^3) - \gamma(\theta-\theta_0) = 0. \tag{99}$$

Extracting θ from Equation 99 as a function of r, i.e., $(\theta(r))$ and substituting into Equation 91 and integrating with respect to r yield the total time of ignition as:

$$\tau_{total} = \frac{\gamma}{2(1-\psi)\epsilon_1 r_p}\left[ln\left(\frac{(1+r_p)^2}{1-r_p+r_p^2}\right) - \frac{\pi}{\sqrt{3}} + 2\sqrt{3}arctan\left(\frac{2-r_p}{\sqrt{3}r_p}\right)\right], \tag{100}$$

where

$$r_p = \left(\frac{\epsilon_2(\gamma\theta_0+\eta_0)}{\psi-1} + 1\right)^{1/3}. \tag{101}$$

The above theoretical results for the ignition time 95 and 100 were compared with experimental results presented in the paper (Miyasaka & Mizutani, 1975). The precision of Equation 95 is extremely high, i.e., the relative deviation of less than 0.1% was found, and less than 0.8% for the total of ignition.

The model will be more practical if one consider the effect of thermal radiation radiation on the thermal explosion of a flammable gas mixture with the addition of volatile fuel droplets (Goldfarb, Gol'dshtein, Kuzmenko, & Sazhin, 1999). The thermal radiation energy exchange between the evaporating surface of the fuel droplets and burning gas is describing using the $P-1$ model with the Marshak boundary conditions. The governing equations are a nonlinear ordinary differential equations in the form of singular perturbed system and describe the effects of heating, evaporation and the combustion of fuel of droplets. Due to the form of the governing equations (SPS form) one can apply the advanced geometric asymptotic technique the MIM method for the qualitative analysis of the behavior of the solution.

The physical assumptions for the thermal explosion in a two-phase medium (a combustible gas mixture containing evaporating fuel droplets) are as follows: The adiabatic approach is applied, the spray of the fuel droplets is a monodisperse spray and the medium is assumed to be spatially homogeneous, the variation in pressure is neglected (this assumption is justified in many industrial applications including diesel engines), the heat flux from the burning gas to the droplets is assumed to consist of two components: convection and radiation fluxes, the thermal conductivity of the liquid phase is much greater than that of the gas phase and the volume fraction of the liquid phase is much less than that of the gas phase, the droplets are not transparent, their surface are grey and that the radiation heat fluxes at these surfaces are described by Stefan-Boltzmann law (Siegel & Howell, 2002) with a given emissivity at the droplets' surfaces, the burning gas is optically thick and the walls of the enclosure are ideal reflectors, the droplets's boundaries are assumed to be on the saturation line (Incroperra & DeWitt, 2006), the Reynolds, Prandtl and Schmidt numbers are sufficiently small so that the Nusselt number and the Sherwood number can be taken to equal to 2, the changes in the droplets' temperature can be ignored, the combustion takes place in the gas phase only and the combustion is a first order exothermic reaction. Under the above assumptions the governing equations are:

$$c_{pg}\rho_g\alpha_g\frac{dT_g}{dt} = C_f\mu_f Q_f\alpha_g A exp\left(-\frac{E}{RT_g}\right) - 4\pi R_d n_d \lambda_{g0}\sqrt{\frac{T_g}{T_{g0}}}\left(T_g - T_d\right), \tag{102}$$

$$\frac{dR_d^3}{dt} = -\frac{3\lambda_{g0}}{\rho_L L} R_d \sqrt{\frac{T_g}{T_{g0}}} \left(T_g - T_d\right) - \frac{3R_d^2 \sigma \kappa}{\rho_L L} \left(T_g^4 - T_d^4\right), \tag{103}$$

$$\frac{dC_f}{dt} = -C_f A exp\left(-\frac{E}{RT_g}\right) \quad + \quad \frac{4\pi R_d \lambda_{g0} n_d}{L \mu_f \alpha_g} \sqrt{\frac{T_g}{T_{g0}}} \left(T_g - T_d\right)$$
$$+ \quad \frac{4\pi R_d^2 \sigma \kappa n_d}{\mu_f L \alpha_g} \left(T_g^4 - T_d^4\right). \tag{104}$$

where $\kappa = \frac{2\epsilon_d}{2-\epsilon_d}$ and ϵ_d is the emissivity of the droplet's surface. The initial conditions are:

$$at \ T = 0 : T_g = T_{go}, \ C_f = C_{f0}, \ R_d = R_{d0}, \ T_d = T_{g0}. \tag{105}$$

Appropriate combination of Equations 102-104 and integration with respect to time yields the energy integral. Addition simplification of this model can be done by applying the Frank-Kamenetskii approximation. The MIM method states that the zero-order approximation of the manifold lies within the γ-neighborhood of the exact manifold position. The dimensionless parameter γ which multiply the term $\frac{d\theta}{d\tau}$ defined as:

$$\gamma = \frac{c_{pg} T_{g0} \rho_{g0}}{C_{f0} Q_f \mu_f} \beta, \tag{106}$$

where β defined in 81. The slow curve of the model 102-104 in non dimensional form presented in (Goldfarb, Gol'dshtein, Kuzmenko, & Sazhin, 1999) is:

$$F(\theta, r) = \left(1 - \frac{(\psi - 1)(1 - r^3)}{\tilde{\epsilon}_2}\right) e^{\theta} - \tilde{\epsilon}_1 r\theta - \tilde{\epsilon}_1 \epsilon_3 r^2 \theta = 0, \tag{107}$$

where

$$
\begin{aligned}
r &= \frac{R_d}{R_{d0}}, \ \epsilon_3 = \frac{4T_{g0}^3 \sigma \kappa R_{d0}}{\lambda_{g0}}, \ \tilde{\epsilon}_1 = \frac{4\pi n_d R_{d0} \lambda_g \beta T_{g0}}{A C_{f0} Q_f \alpha_g} e^{\frac{1}{\beta}}, \\
\beta &= \frac{RT_{g0}}{E}, \ \tilde{\epsilon}_2 = \frac{c_{pg} T_{g0} \beta}{C_{fo} Q_f}.
\end{aligned}
\tag{108}
$$

and θ, ψ defined in 81 and 98 respectively. The shape and the position of the slow curve in the phase plane $\theta - r$ depends on the combination of the value of the dimensionless parameters $\tilde{\epsilon}_1$, $\tilde{\epsilon}_2$, ϵ_3 and ψ.

The turning points on the slow curve are defined as the points adhere the slow curve has the horizontal tangent i.e., the solution of the system

$$F(\theta, r) = 0 = \frac{\partial F(\theta, r)}{\partial \theta}. \tag{109}$$

The turning points divide the slow curve into stable and unstable parts. The stable parts attract trajectories and the unstable parts repel them. According to MIM method, when a trajectories approaches to the stable parts of the slow curve, the trajectories moves along the slow curve within γ-neighborhood. In other words, the trajectories adhere to the stable parts of the slow curve. The movement along the stable (attractive) parts of the slow curve continues until the trajectories reaches the unstable parts of the slow curve, i.e., until the turning points of the slow curve. The solution for the temperature of the system 109 is $\theta = 1$. The r-coordinate, r_T, of the turning point is found from the solution of:

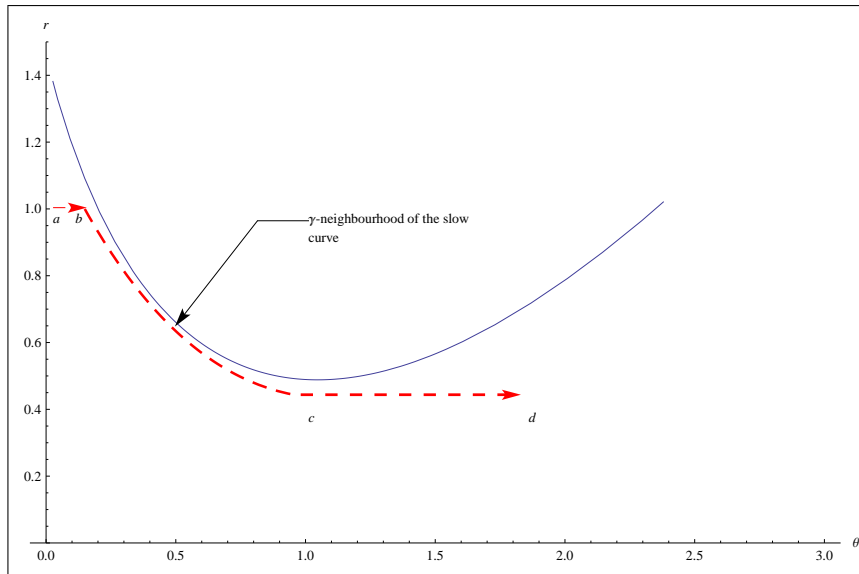$$F(1, r_T) = 0, \tag{110}$$

(f in Figure A).

Figure 6. Slow curve. The trajectory $a - b$ is a fast motion, the part $b - c$ of the trajectory adhere to the stable part of the slow curve (within its γ-neighbourhood) and describe the so-called the delay time, the point c is the turning point of the slow curve with the coordinate $(\theta = 1, r_T)$

A solution of the model begins with fast motion from the initial condition $(\theta = 0, r = 1)$ (dimensionless initial conditions of the model 102-104) parallel (in the zero-order approximation) to the θ-axis. One should distinguish between three cases: 1: If a trajectory passes below the slow curve (Figure B) then it describes the conventional fast explosive regime (chemical reaction overrides the evaporation process, the system explodes and the gas mixture temperature rises sharply), 2: Trajectories that starting at the initial point and reaching the slow curve. When these fast trajectories touches the turning point (point f in Figure A) then they called the critical trajectories, 3: A trajectories that start at the initial point with fast motion ($a - b$ in Figure) reach the stable branch of the slow curve ($b - c$ in Figure) adhere to the slow curve (because $b - c$ is the stable part of the slow curve) and move along to the slow curve within the γ-neighborhood of the slow curve until the turning point c with the coordinates $(\theta = 1, r_T)$. This trajectories defined the so-called the delay time.

Let us detail cases 2 and 3. Case 2: the critical trajectory determines the critical combination of the values of parameters which can be found from the equation $F(1, 1) = 0$. Hence, the critical condition for thermal explosion is

$$\tilde{\epsilon}_1(1 + \epsilon_3) = e. \tag{111}$$

As in the classical Semenov's theory, this critical combination 111 of parameters allows one to conclude that in a system with $\tilde{\epsilon}_1(1 + \epsilon_3) < e$ only a conventional thermal explosion can be expected. In the opposite case where $\tilde{\epsilon}_1(1 + \epsilon_3) > e$ one can expect to the so-called the delay time i.e., case 3. Hence, a trajectories starting at the initial point (point a in Figure) reach the stable branch of the slow curve (branch $b - c$ in Figure) after the fast part of the trajectories i.e., the temperature is the fast variable of the system. The radius of the droplets, which is the slow variables of the system, cannot increase within the framework of the model. Therefore, the trajectory along the slow curve should describe the decreasing radius until it reaches the turning point (point c in Figure). In other words, after the initial period of rapid temperature increase the intensities of the two processes (heat release and heat loss) are balanced and the droplets' radius begins to decrease slowly. After the turning point c the system blows up and the gas phase temperature rises sharply (part $c - d$ in Figure). The turning point describing, from physical point of view, the intensity of the reaction which is so high that it cannot be controlled by the evaporation process.

Because the delay time is important for engineering applications we present here the results obtained by (Goldfarb, Gol'dshtein, Kuzmenko, & Sazhin, 1999). The delay phenomenon is the result of a competition between heat release process due to the exothermic chemical reaction and internal heat losses due to droplets evaporation process.

Equation 107 describes the slow curve with the effect of the thermal radiation. In order to analyzed the effect of
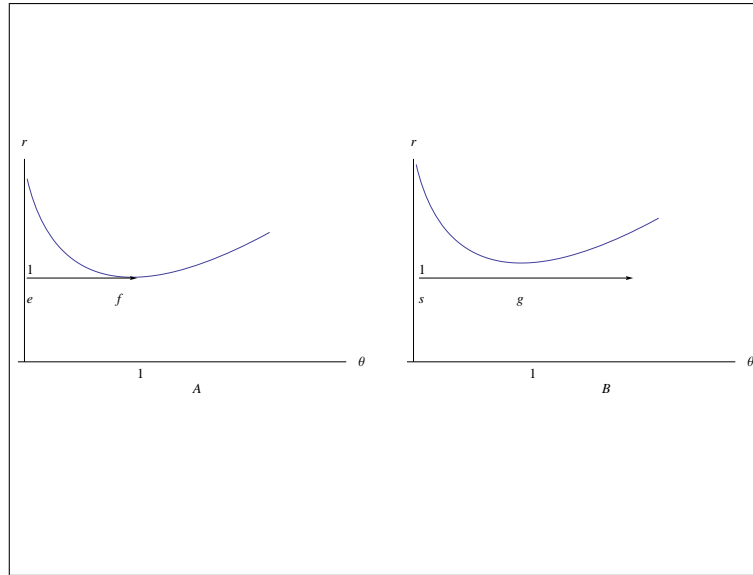
Figure 7. Two different types of the slow curve. If a trajectory pass below the slow curve ($s − g$ in figure B) then it describes the conventional fas explosive regime. If a trajectory reach the slow curve ($e − f$ in figure A) then it define the so-called the critical trajectory

the thermal radiation on the delay time one should rewrite the slow curve without the expression that responsible to the thermal radiation i.e., the slow curve in the form of:

$$f(\theta, r) = \left(1 - \frac{(\psi - 1)(1 - r^3)}{\tilde{\epsilon}_2}\right) e^{\theta} - \tilde{\epsilon}_1 r\theta = 0. \tag{112}$$

We first compute the delay time with the effect of the thermal radiation (τ_{delay}^{CR}) (*CR-Convection+Radiation*) using the slow curve 107. For this purpose we write the mass equation (Equation 103) in non-dimensional form as presented in (Goldfarb, Gol'dshtein, Kuzmenko, & Sazhin, 1999):

$$\frac{dr^3}{d\tau} = -\tilde{\epsilon}_2 \tilde{\epsilon}_1 r\theta(1 + \epsilon_3 r). \tag{113}$$

Rewrite Equation 107 to the following form:

$$\tilde{\epsilon}_2 \tilde{\epsilon}_1 r\theta(1 + \epsilon_3 r) = \left(1 - \frac{(\psi - 1)(1 - r^3)}{\tilde{\epsilon}_2}\right) e^{\theta}. \tag{114}$$

Substituting Equation 114 into Equation 113 integrating over r from its initial value ($r = 1$) up to the turning point r_{TF} (here the subscript relate the turning point that belongs to the slow curve $F(\theta, r)$ presented in Equation 107) and using the fact presented in Equation 87 yield the analytical bounded for the delay time with taking into account the effect of the thermal radiation in the form of:

$$\frac{1}{e(\psi - 1)} ln\left(1 + \frac{(\psi - 1)(1 - r_{TF}^3)}{\tilde{\epsilon}_2}\right) < \tau_{delay}^{CR} < \frac{1}{(\psi - 1)} ln\left(1 + \frac{(\psi - 1)(1 - r_{TF}^3)}{\tilde{\epsilon}_2}\right). \tag{115}$$

Repeating the above analysis for the case without the effect of the thermal radiation. In the mass equation (Equation 113) one should delete the term $\epsilon_3 r$. For this case the turning point defined by r_{Tf} (here the subscript relate the

turning point that belongs to the slow curve $f(\theta, r)$ presented in Equation 112) and the delay time defined by τ_{delay}^{C} (C for convection without radiation). The quantity that express the effect of the thermal radiation on the delay time is the difference between the upper limit of the delay time i.e., the following quantity:

$$\Delta\tau = \tau_{delay}^{CR} - \tau_{delay}^{C}, \tag{116}$$

which given analytically by:

$$\Delta\tau = ln\left(\frac{1 + [(\psi - 1)/\tilde{\epsilon}_2](1 - r_{TF}^3)}{1 + [(\psi - 1)/\tilde{\epsilon}_2](1 - r_{Tf}^3)}\right)^{1/(\psi-1)}. \tag{117}$$

The next step is to approximate asymptotically the value of Δ for the case when $\tilde{\epsilon}_2 >> 1$. The physical meaning of this parameter is the ratio of two energies ($\tilde{\epsilon}_2 \propto \frac{Q_f}{L}$): the chemical energy contained in the gaseous mixture at the beginning of the process and the energy required to evaporate the liquid phase of the fuel (Gol'dshtein, Goldfarb, Shreiber, & Zinoviev, 1996; Goldfarb et al., 1997; Goldfarb, Gol'dshtein, Kuzmenko, & Greenberg, 1998). This parameter is approximately unity when the chemical reaction is highly exothermic and the initial concentration of the gaseous fuel is not too small. Hence, all the fractions with this parameter in the following equations 107 and 112 can be ignored. This assumption enable one to obtain the following turning points:

$$r_{TF} \approx \frac{e}{\tilde{\epsilon}_1}, \;\; r_{Tf} \approx \frac{e}{\tilde{\epsilon}_1} - \frac{\epsilon_3 e^2}{\tilde{\epsilon}_1^2}. \tag{118}$$

This simplification allows the authors of (Goldfarb, Gol'dshtein, Kuzmenko, & Sazhin, 1999) to simplify the expression for $\Delta\tau$ to:

$$\Delta < \frac{1}{\tilde{\epsilon}_2}\left(r_{Tf}^3 - r_{TF}^3\right) \approx \frac{3e^4\epsilon_3}{\tilde{\epsilon}_2\tilde{\epsilon}_1^4}. \tag{119}$$

The theoretical and experimental results are summarized in Tables 2, 3 and 4 for the following $n - decane$ data:

$$\begin{aligned} E &= 1.26 \cdot 10^8 (J/kg), A = 1.91 \cdot 10^7 (s^{-1}), \; T_{g0} = 490(K), \\ Q &= 4.42 \cdot 10^7 (J/kg), \; L = 3.2 \cdot 10^5 (J/kg), \; c_p = 1050(J/(Kkg)), \\ \rho_L &= 730(kg/m^3), \; \mu_f = 142(kg/kmol), \; C_{f0} = 10^{-5}(kmol/m^3). \end{aligned}$$

According to Equation 119 one can see that the approximation for $\Delta\tau$ depends on the dimensionless parameter ϵ_3 which accounts for the thermal radiation effects. According to Tables 2, 3 and 4. One can see that the effects of the thermal radiation to the delay time for $Tetralin$ spray is negligibly and substantial for $n - decane$.

To summarizing the paper presented by (Goldfarb, Gol'dshtein, Kuzmenko, & Sazhin, 1999) the system of equations that described the effect of thermal radiation on the thermal explosion of a combustible gas mixture with evaporating fuel droplets has been transformed to the form of singularly perturbed system (SPS). The model takes into account the heat release due to exothermic oxidation of gaseous fuel, heat losses due to liquid fuel evaporation, gaseous fuel consumption as a result of a chemical reaction, gaseous fuel supply by evaporated liquid fuel, and two mechanisms of heat transfer from the burning gas to the evaporating fuel fuel droplets: convection and radiation.

The SPS form of the model enable the authors to applied the method of integral manifold (MIM) and hence to write the slow curve of the model. Two main types of dynamic behavior are found for the system: fast explosion regimes and explosion with delay. Using the slow cure of the governing equations of the model enable the authors to obtained an analytical expression for the lower and upper limits for the delay time with and without the impact of the thermal radiation. The experimental results takes into account two types of fuel: tetralin and n-decane. The final conclusion of the results was that the effects of the thermal radiation can be ignored in the case of tetralin fuel, while in the case of n-decane the effects of the thermal explosion can be dominant.

Table 2. Analytical lower limit for the delay time applied to the model 102-104

Fuel	R_{d0}	n_d	Lower τ_{delay}	
	(m)	(m^{-3})	Without radiation	With radiation
n-decane	10E-5	10E+4	No delay	No delay
n-decane	10E-5	5·10E+4	0.0272	0.0278
n-decane	10E-5	10E+5	0.07398	0.07405
n-decane	10E-5	10E+6	0.7676	0.7676
n-decane	10E-4	10E+3	No delay	No delay
n-decane	10E-4	5·10E+3	2.720	3.118
n-decane	10E-4	10E+4	7.389	7.449
n-decane	10E-4	10E+5	75.956	75.956
Tetralin	10E-5	10E+0	51.16	51.16
Tetralin	10E-5	10E+1	511.61	511.61
Tetralin	10E-5	10E+2	51161.4	51161.4

Table 3. Analytical upper limit for the delay time applied to the model 102-104

Fuel	R_{d0}	n_d	Lower τ_{delay}	
	(m)	(m^{-3})	Without radiation	With radiation
n-decane	10E-5	10E+4	No delay	No delay
n-decane	10E-5	5·10E+4	0.07404	0.07562
n-decane	10E-5	10E+5	0.201	0.201
n-decane	10E-5	10E+6	2.087	2.087
n-decane	10E-4	10E+3	No delay	No delay
n-decane	10E-4	5·10E+3	7.394	8.475
n-decane	10E-4	10E+4	20.085	20.249
n-decane	10E-4	10E+5	206.469	206.469
Tetralin	10E-5	10E+0	139.07	139.07
Tetralin	10E-5	10E+1	1390.71	1390.71
Tetralin	10E-5	10E+2	13907.1	13907.1

Table 4. The relative difference in (%) for the delay time refer to Tables 2 and 3 applied to the model 102-104

Fuel	$R_{d0}(m)$	$n_d(m^{-3})$	Relative difference
n-decane	10E-5	10E+4	No delay
n-decane	10E-5	5·10E+4	2.1
n-decane	10E-5	10E+5	0.1
n-decane	10E-5	10E+6	10E-5
n-decane	10E-4	10E+3	-
n-decane	10E-4	5·10E+3	12.8
n-decane	10E-4	10E+4	0.8
n-decane	10E-4	10E+5	10E-4
Tetralin	10E-5	10E+0	0
Tetralin	10E-5	10E+1	0
Tetralin	10E-5	10E+2	0

The physical model written by (Goldfarb, Gol'dshtein, Kuzmenko, & Sazhin, 1999) extended by (Goldfarb, Gol'dshtein, Greenberg, & Kuzmenko, 2000) in such way that the model takes into account the equations for the oxidizer molar concentration, and hence the equations for the fuel and oxidizer takes into account the contribution of the exothermic chemical reaction and fuel evaporation, and also a balance equation for a single droplet due to the using the infinite conductivity model for the droplet. The main physical of the model are as follows: An adiabatic approach is adopted for the analysis, Frank-Kamenetskii approximation for thermal explosion is applied, the pressure change in the reaction volume is negligible, the thermal conductivity of the liquid phase is much greater than the gas phase, the volumetric fraction of the liquid phase is supposed to be much less than that of the gas phase, the spray is in the form of monodisperse fuel spray, the combustion reaction is modeled as a first-order, highly exothermic chemical reaction, the effective Nusselt number Nu_{eff} which is corrected to account for that part of the total heat flux that is spent of droplet heating is of order 1 i.e., $Nu_{eff} \approx O(1)$. Under the above assumptions the governing equations of

the physical model are as follows:

$$c_{pg}\rho_g\alpha_g\frac{dT_g}{dt} = C_fC_{ox}\mu_fQ_f\alpha_gAexp\left(-\frac{E}{RT_g}\right)$$
$$- 4\pi R_dn_d\frac{\lambda_g\tilde{L}}{c_p}ln\left(1 + \frac{c_p}{\tilde{L}}\left(T_g - T_d\right)\right),$$

$$\frac{d}{dt}\left(\frac{4\pi}{3}R_d^3\right)\rho_d = -\dot{m} = -4\pi R_d\frac{\lambda_g}{c_p}ln\left(1 + \frac{c_p}{\tilde{L}}\left(T_g - T_d\right)\right), \tag{120}$$

$$\frac{dC_f}{dt} = -C_fC_{ox}Aexp\left(-\frac{E}{RT_g}\right) + \frac{\dot{m}n_d}{\mu_f\alpha_{g0}}, \tag{121}$$

$$\frac{dC_{ox}}{dt} = -C_fC_{ox}Aexp\left(-\frac{E}{RT_g}\right), \tag{122}$$

$$\rho_dc_d\frac{d}{dt}\left(\frac{4\pi}{3}R_d^3T_d\right) = 4\pi R_d\lambda_gNu_{eff}ln\left(1 + \frac{c_p}{\tilde{L}}\left(T_g - T_d\right)\right)\chi\left(T_s - T_d\right), \tag{123}$$

where:

$$\tilde{L} = L + \frac{\frac{4}{3}\pi R_d^3\rho_dc_{pd}\frac{dT_d}{dt}}{-\frac{d}{dt}\left(\frac{4}{3}\pi R_d^3\rho_d\right)}, \quad \tilde{L} \geq L. \tag{124}$$

The initial conditions are:

$$atT = 0 : T_g = T_{go}, \;\; C_f = C_{f0}, \;\; C_{ox} = C_{ox0} \;\; R_d = R_{d0}, \;\; T_d = T_{d0} = T_{g0}. \tag{125}$$

In this case it is necessary to rewrite the above physical model in non dimensional form because the model is in the form of multi-scale system which contained two small parameter. For this purpose let us introduce the following dimensionless parameters:

$$\zeta_1\frac{d}{d\tau}(r^3(1 + \beta\theta_d)) = rln\left(1 + \zeta_2(\theta_g - \theta_d)\right)\chi\left(T_s - T_d\right), \tag{126}$$

$$\gamma\frac{d\theta_g}{d\tau} = \eta exp\left(\frac{\theta_g}{1 + \beta\theta_g}\right) - \frac{\epsilon_1r}{\zeta_2}ln\left(1 + \zeta_2(\theta_g - \theta_d)\right)(1 + \beta\theta_g), \tag{127}$$

$$\frac{dr^3}{d\tau} = -\frac{\epsilon_1\epsilon_2r}{\zeta_2}ln\left(1 + \zeta_2(\theta_g - \theta_d)\right), \tag{128}$$

$$\frac{d\eta}{d\tau} = -\frac{1}{1 + \beta\theta_g}exp\left(\frac{\theta_g}{1 + \beta\theta_g}\right) + \frac{\epsilon_1\psi r}{\zeta_2}ln\left(1 + \zeta_2(\theta_g - \theta_d)\right), \tag{129}$$

where the dimensionless parameters are as follows:

$$r = \frac{R_d}{R_{d0}}, \; t_r = \frac{1}{A}exp\left(\frac{E}{RT_s}\right), \; \theta_g = \frac{E(T_g - T_s)}{RT_s^2}, \; \theta_d = \frac{E(T_d - T_s)}{RT_s^2},$$

$$\eta = \frac{C_f}{C_{f0}}, \; \hat{\epsilon}_2 = \frac{Q_fC_{f0}\alpha_g\mu_f}{\rho_dL\alpha_d}, \; \hat{\epsilon}_1 = \frac{4\pi n_dR_{d0}\lambda_g\beta T_s}{AC_{f0}Q_f\alpha_g\mu_f}e^{\frac{1}{\beta}}, \; \beta = \frac{RT_s}{E},$$

$$\gamma = \frac{c_{pg}T_s\rho_{g0}\beta}{C_{f0}Q_f\mu_f}, \psi = \frac{Q_f}{L}, \; \alpha_g = 1 - \alpha_d, \; \tau = \frac{t}{t_r},$$

$$\alpha_d = \frac{4\pi}{3}R_{d0}^3n_d, \; \zeta_1 = \frac{R_{d0}^2\rho_dc_d}{3Nu_{eff}t_r\lambda_g}, \; \zeta_2 = \frac{c_{dp}\beta T_s}{L},$$

and c_d is the thermal capacity of the liquid fuel droplet.

The initial condition of the non dimensional model are:

$$\theta_{g0} = \theta_{d0} = \frac{\frac{T_{g0}}{T_s} - 1}{\beta}, \quad \eta = 1 = r. \tag{130}$$

The dynamical of the system 126-129 depends on the dimensionless parameters: β, γ, $\hat{\epsilon}_1$, $\hat{\epsilon}_2$, π, ζ_1 and ζ_2. The parameters ζ_1 and ζ_2 relate to the heat transfer processes between the host gas phase and the droplets. As one can see from the system 126-129 there are two small parameters $\zeta_1 \ll 1$ and $\gamma \ll 1$ which appear on the LHS of Equation 126 and 126 respectively. They typically satisfy that $\zeta_1 \ll \gamma$. This means that the temperature variable of the droplet (θ), at the initial process, is change faster that the others variables i.e., r, θ_g and η are the slow variables of the system. In order to determined the internal hierarchy of the system one should assumed that $\gamma_{\text{ii}} 1/\hat{\epsilon}_2$. Hence, θ_d and θ_g, which are the faster variables of the system will reached the quasi stationary state and at the same time the slower variables r and η will be frozen. In general, The quasi stationary state can be temporary and in a finite period of time, the it can be fast again. This parametric analysis leads the authors to conclude that the system can be decomposed into two subproblems. The first one describe the process of droplet heating from the initial temperature up to the saturation line, and the second one relates to the process of thermal explosion that starting at the saturation line. The application of the MIM to the model 126-129 can be apply due to the decomposition of the model into slow and fast variable (due to the existence of a small parameters). Using the approximation of $ln(1 + c_{dp}(T_g - T_d)/\tilde{L})$, and substituting $\gamma \ll 1$, $\beta \ll 1$ the slow curve has the following form of:

$$\hat{F}(\theta, r) = \left(1 + \frac{(\psi - 1)(1 - r^3)}{\hat{\epsilon}_2}\right)e^\theta - \hat{\epsilon}_1 r\theta = 0. \tag{131}$$

The shape and the position of the slow curve depend on the parameters: ψ, $\hat{\epsilon}_2$, and $\hat{\epsilon}_1$. The analysis of the slow curve was divided into two different values of ψ, $\psi < 1$ and $\psi > 1$. The value $\psi = 1$ belong to bifurcation point in which the shape of slow curve change. Substituting $\theta = 0$ into Equation 131 one can obtain the r-coordinate of the intersection of the slow curve and the r-axis which satisfy the following inequalities:

$$r_0 = \left(1 + \frac{\hat{\epsilon}_2}{\psi - 1}\right) > 1, \quad \forall \psi > 1, \quad and \quad r_0 = \left(1 + \frac{\hat{\epsilon}_2}{\psi - 1}\right) < 1, \quad \forall \psi < 1. \tag{132}$$

The dynamical behavior of the system based on the following different regimes (Goldfarb, Gol'dshtein, Greenberg, & Kuzmenko, 2000):

$$\begin{aligned}
\hat{\epsilon}_1 &< e, \ conventional \ fast \ explosion, \\
\hat{\epsilon}_1 &> e, \ 0 < \psi < 1 - \hat{\epsilon}_2, \ non-explosive \ slow \ regime, \\
\hat{\epsilon}_1 &> e, \ 1 - \hat{\epsilon}_2 < \psi < 1 - \hat{\epsilon}_2/3, \ thermal \ explosion \ with \ freeze \ delay, \\
\hat{\epsilon}_1 &> e, \ 1 - \hat{\epsilon}_2/3 < \psi < 1, \ thermal \ explosion \ with \ delay, \ concentration \ decreases, \\
\hat{\epsilon}_1 &> e, \ \psi > 1 \ thermal \ explosion \ with \ delay, \ concentration \ increases.
\end{aligned} \tag{133}$$

The delay time, which is important from practical point of view, is computed for the relevant above regime. In order to compute the delay time one should first find the θ and r-coordinates of the turning point. The turning point can be found by the solution of the system: $\hat{F}(\theta, r) = 0 = \partial\hat{F}(\theta, r)/\hat{F}(\theta, r)\partial\theta$ which implies that $\theta = 1$. The r-coordinate can be fond numerically by the solution of the equation $\hat{F}(1, r_{T\hat{F}}) = 0$. The upper and the lower bounded approximation of the delay time can be found by the same algebraic manipulations as we have already done before. The analytical expression are as follows:

$$\frac{1}{e(\psi - 1)}ln\left(1 + \frac{(\psi - 1)(1 - r_{T\hat{F}}^3)}{\hat{\epsilon}_2}\right) < \tau_{delay} < \frac{1}{(\psi - 1)}ln\left(1 + \frac{(\psi - 1)(1 - r_{T\hat{F}}^3)}{\hat{\epsilon}_2}\right). \tag{134}$$

If the chemical energy release while burning the fuel vapor in the initial gas mixture (per unit volume) is much greater than the energy needed to evaporate all the droplets (in the same unit volume) than one implies that $\hat{e}_2 << \psi$ i.e.,

$$\frac{Q_f C_{f0} \alpha_g \mu_f}{\rho_L L \alpha_L} << 1. \tag{135}$$

Using Equation 135 implies the following approximation for the delay time:

$$\frac{1}{\hat{e}_2 e}\left(1 - r_{T\hat{F}}^3\right) < \tau_{delay} < \frac{1}{\hat{e}_2}\left(1 - r_{T\hat{F}}^3\right). \tag{136}$$

The experimental data for the analysis are summarized in Table 5.

To summarize the paper that presented by (Goldfarb, Gol'dshtein, Greenberg, & Kuzmenko, 2000) the model in the paper described the effects on the thermal explosion of monodisperse fuel spray in a gas-cloud. The model, in contrast to the conventional model that we review here in this paper, contain two different small parameters. The appearance of a small parameters in the model enable the authors of this paper to applied the MIM method. The original model decompose into two sub-models. The first one relates to the heat up period of the droplets, and the second one begins at the saturation point. Five main dynamical regimes were identifies: fast explosion regime, slow regime, thermal explosion with freeze delay, thermal explosion with delay where concentration increases, and thermal explosion with delay where concentration decreases. Upper and lower bounded approximation for the delay time are derived analytically and compared with numerical simulations. The relative error (%) in the delay time upper bound versus the initial radius of droplets and Relative error (%) in the delay time upper bound versus the number of dropelts per unit volume are presented in Figure .

Table 5. Thermophysical experimental data applied to the model 120-122

Property	n-decane	tetralin
c	1050	1256
L	3.21E+05	3.17E+05
ρ_g	0.712	0.727
T_0	450	480
ρ_d	730	971
μ_f	142	132
Q_f	4.42E+07	1.266E+07
E	1.257E+08	2E+08
λ	0.0193	0.084
A	1.9E+07	3.3E+08

The next model that have been presented by the authors of (Babushok & Goldshtein, 1988; Gol'dshtein & Sobolev, 1992; Goldfarb et al., 1997; Goldfarb, Gol'dshtein, Kuzmenko, & Greenberg, 1998; McIntosh, Gol'dshtein, Goldfarb, & Zinoviev, 1998; Goldfarb, Gol'dshtein, Greenberg, & Kuzmenko, 2000; Sazhin et al., 2001;) generalized the model of in such way that the model take into account the effect of thermal radiation of heat transfer between the droplet and gas in different way and more precisely. The main physical assumption of the model are: The contribution of the thermal radiation based on the $P - 1$ approximation for the thermal radiation transfer with Marshak boundary condition (Modest, 1993; Sazhin et al., 1996; Siegel & Howell, 2002;), the spray is monodisperse spray, the droplets are opaque, their surface are gray, and the radiative temperature T_r is equal to the gas temperature T_g, the Spalding number is small, the characteristic time of droplet t_d and gas t_g for typical diesel engine parameters satisfies the inequality $t_d << t_g$ and the droplet heating can be neglected. This approximation allow to assume that the temperature of droplet surface, T_s, is constant, The Nusselt number and Sherwood number are equal to 2 i.e., the droplet are suspended in stationary environment, The chemical term is presented in the Arrhenius form with the pre-exponential factor calculated from the enthalpy equation using the Shell autoignition model.

Under these assumptions the governing equations of the model that described the effects of heating, evaporation and combustion of fuel droplets has the form of 102-104. The difference between the model presented by (Goldfarb, Gol'dshtein, Kuzmenko, & Sazhin, 1999; Sazhin et al., 2001)is the qualitative analysis. The last one (Sazhin et
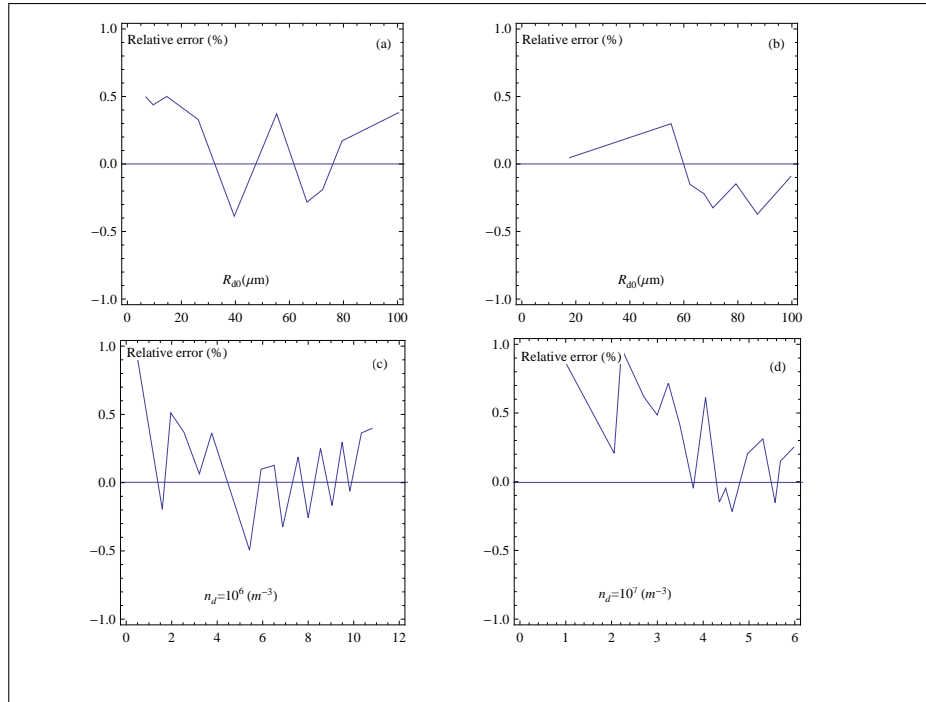
Figure 8. Relative error (%) in the delay time upper bound versus the initial radius of droplets: (a) *tetralin* fuel, $C_{f0} = 10^{-2}(kmolm^{-3})$, $R_{d0} = 10^{-6}(m^{-3})$, (b) $n - decane$ fuel, $C_{f0} = 10^{-4}(kmolm^{-3})$, $R_{d0} = 10^{-5}(m^{-3})$. Relative error (%) in the delay time upper bound versus the number of droplets per unit volume: (c) *tetralin* fuel, $C_{f0} = 10^{-4}(kmolm^{-3})$, $N_d = 10^4(m^{-3})$, (d) $n - decane$ fuel, $C_{f0} = 10^{-4}(kmolm^{-5})$, $N_d = 10^6(m^{-3})$

al., 2001) divided the ignition process into two stages: droplet evaporation and ignition of the gaseous mixture. Results predicted by the analytical solutions are compared with those predicted by the CFD package VECTIS code. Whereas the analysis of the first model (Goldfarb, Gol'dshtein, Kuzmenko, & Sazhin, 1999) concentrated on the effect of the thermal radiation on the delay time. Let us summarize the results of Sazhin et al. (2001): Let θ be the dimensionless gas temperature. The assumption that the gas temperature remains close to its initial condition T_{g0} during the heating, evaporation and initial combustion processes enable the authors to write θ as $\theta = \theta_0 + \theta_1$ where $|\theta_1| << \theta_0$. This case is important for diesel where the evaporation time of the droplets and the values of gas temperature, fuel concentration and droplet radii can be estimated before explosion. Analysis of critical conditions for thermal explosion process requires different approximations (Babushok, Gol'dshtein, & Sobolev, 1990). Using this approximation one can rewrite the energy equation and the mass equation in non-dimensional form as:

$$\frac{d\theta_1}{d\tau} = \quad a_{\theta 0} + a_{\theta 1}r + a_{\theta 2}r^2 + a_{\theta 3}r^3$$
$$+ \quad (b_{\theta 0} + b_{\theta 1}r + b_{\theta 2}r^2 + b_{\theta 3}r^3)\theta_1, \tag{137}$$

$$r\frac{dr}{d\tau} = a_{r0} + a_{r1}r + (b_{r0} + b_{r1}r)\theta_1, \tag{138}$$

The expressions $a_{\theta i}$ and $b_{\theta i}$ can be found in their explicit form in Sazhin et al. (2001). Appropriate algebraic manipulations one can obtain the solution for θ_1 as:

$$\theta_1 = exp\left(\int_0^1 \left(\frac{b_r a_\theta}{a_r^2} - \frac{b_\theta}{a_r}\right)rdr\right)\int_1^r \frac{ra_\theta}{a_r} \cdot exp\left(-\int_0^1 \left(\frac{b_r a_\theta}{a_r^2} - \frac{b_\theta}{a_r}\right)rdr\right)dr,$$
$$\tag{139}$$

where

$$
\begin{aligned}
a_\theta &= a_{\theta 0} + a_{\theta 1} r + a_{\theta 2} r^2 + a_{\theta 3} r^3 \\
b_\theta &= b_{\theta 0} + b_{\theta 1} r + b_{\theta 2} r^2 + b_{\theta 3} r^3 \\
a_r &= a_{r0} + a_{r1} r \\
b_r &= b_{r0} + b_{r1} r.
\end{aligned}
\tag{140}
$$

Substituting Equation 139 into Equation 138 and assuming that $r = 0$ yield the explicit form for the complete evaporation time of fuel droplet as:

$$
\tau_{evaporation} = - \int_0^1 \frac{r}{a_r + b_r \theta_1(r)} dr.
\tag{141}
$$

This evaporation time is accurate if the condition $|\theta_1| \ll \theta_0$. If it is not the case, then Equation 141 represents the upper limit of the physical ignition time delay (Sazhina, Sazhin, Heikal, & Marooney, 1999). If the temporal dependence of temperature and droplet radii are obtained, using the assumption that $|\theta_1| \ll \theta_0$, and the changes in T_g is ignored, and assumed that T_s=const, and finally using the assumption that the contribution of the thermal radiation is small i.e., $|a_0| \ll |a_1|$ then the total time can be simplified to

$$
\tau = \frac{L\rho_L R_{d0}^2}{2\lambda_{g0}(T_{g0} - T_s)} \left\{ (1 - r^2) - \frac{2\sigma\kappa(T_{g0}^4 - T_s^4)R_{d0}}{\lambda_{g0}(T_{g0} - T_s)}(1 - r^3) \right\}.
\tag{142}
$$

The first term is the d^2-law for droplets evaporation, and the second term describes the correction due to the contribution of the thermal radiation. When one substitute $r = 0$ which means that the droplets are evaporate, then the expression for droplet evaporation time can be obtained in the form of:

$$
\tau_{evaporation} = \tau_{evaporation(0)}(1 - \tilde{\kappa}).
\tag{143}
$$

where

$$
\tau_{evaporation(0)} = \frac{L\rho_L R_{d0}^2}{2\lambda_{g0}(T_{g0} - T_s)} \quad \tilde{\kappa} = \frac{2\sigma\kappa(T_{g0}^4 - T_s^4)R_{d0}}{\lambda_{g0}(T_{g0} - T_s)},
\tag{144}
$$

where $\tau_{evaporation(0)}$ is the evaporation time in the absence of the thermal radiation, and $\tilde{\kappa}$ accounts for the effect of the thermal radiation.

Experimental data for approximate diesel fuel by n-dodecane ($C_{12}H_{26}$) (Sazhin et al., 2000) and Sazhina, Sazhin, Heikal, & Marooney (1999) (the spray is a monodisperse fuel spray):

$$
\begin{aligned}
R_0 &= 6(\mu m), \ n_d = 3.02 \times 10^{12}(m^{-3}), \ \alpha_L = 2.73 \times 10^{-3} \ T_{d0} = 300(K), \\
\rho_d &= 744(kg/m^3), \ T_{g0} = 880(K), \ T_s = 600(K), \ C_l = 2.83(kJ/(kgK)), \\
\rho_L &= 600(kg/m^3), \ L = 250(kJ/kg), \ Q_f = 43(MJ/kg), \\
\mu_f &= 170(kg/kmol), \ \lambda_{g0} = 6.1 \times 10^{-2}(W/mK), \\
\kappa\sigma &= 11.3 \times 10^{-8}(W/m^2K^4), \ \alpha_g = 1, A = 10^7(1/s).
\end{aligned}
\tag{145}
$$

The results of the model are compared with those that predicted by the CFD code VECTIS of Ricardo Consulting Engineering. The governing equations for the gas phase are solved by using the Eulerian approach, and the governing equations for the droplets are solved using the Lagrangian approach. The model solved for three dimensional space. The VECTIS turbulence modeling is based on the conventional and RNG version of the $k - \epsilon$ model. The Magnussen-Hjertager model is valid for high-temperature combustion. The physical model take into account the thermal radiation effect based on the version conventional $P - 1$ model, i.e., the radiative energy exchange between the fuel droplets surface and gas is described using the well known $P - 1$ model with Marshak boundary conditions. Convective and a radiative heat exchange of the monodisperse spray with the surrounding gas have taken into account. The results are compared for three different values of the pre-exponential factor 3×10^6, 6×10^6 and 3×10^7. Due to the presence of a small parameter in the model, the MIM method have been applied, and the ignition process is subdivided into two stages: droplet evaporation and ignition of gaseous mixture. When the gas

temperature has been assumed to be equal local temperature in the vicinity of droplet, then the evaporation time (that the authors of Sazhin et al. (2001) obtained analytically from the model), agree with the evaporation time that predicted by CFD. The thermal radiation, for high temperature and large droplets cannot be ignored.

Another important paper that investigated the effect of radiative heat loss (rather than convective) of gas on thermal explosion have been presented by (Goldfarb, Gol'dshtein, Greenberg, & Kuzmenko, 2002). The mathematical model includes two highly nonlinear ordinary differential equations: an energy equation and a concentration equation. In general , a physical model that describe a thermal explosion of a gas should take into account two basic and important mechanisms of heat and mas transfer between the gas phase and the liquid phase: heat loss due to thermal radiation of the burned gas and heat release associated with the exothermic oxidation reaction. The competition between these two processes determines the behavior of the exploding system. Thermal explosion means that at the initial stages of the temperature begins to rise and the aforementioned competing mechanisms are called into play. Because the gas-phase temperature changes very quickly due to the highly exothermic reaction and the concentration of the combustible mixture change relatively slowly (i.e., the system is considered as a multiple-scale), one can apply a geometric asymptotic method such as the MIM method.

The main physical assumptions of the model presented by these authors, which is a modification of Semenove's classical model of thermal explosion in a combustible gas mixture, are as follows: the changes in the pressure in the reacting mixture and its influence on the combustion process are neglected, the heat transfer to the ambient is due to the thermal radiation only (there are no heat losses of any other kind), the combustible component of the mixture is supposed to be deficient, and is mainly dictated by flammable mixture and by its temperature. The expression for the thermal radiation suggested by (Sohrab, Linan, & Williams, 1982) is

$$q_{radiation} = \approx B_r exp\left(-\frac{E_r}{RT_g}\right)\chi(T - T_\infty),$$ (146)

and is rather than the well-known Stefan-Boltzman law. Here B_r ($J/m^3 s$) is plays the role of a constant preexponential factor and E_r ($J/kmol$) is a parameter similar to the conventional activation energy. These coefficients are chosen in such a way as to minimize the difference between Equation 146 and the Stefan-Boltzman law within a given limited temperature interval.

Comment : 1:This form for $q_{radiation}$ was based on nothing the high sensitivity of the T^4-law to temperature variations and expanding the radiation heat loss in an appropriate power series about a reference temperature. More generally, the expression for $q_{radiation}$ can be derived directly from the standard expression for black-body radiation by taking some average value for the wave number of the gaseous species involved. 2: The appearance of the Heaviside function $\chi(\cdot)$ in Equation 146 ensures that the radiation is cut off when the temperature of the emitting medium reaches the ambient temperature ($T_g = T_\infty$).

The concentration of the oxidizer is taken to be approximately constant, the combustion reaction is modeled as a first order, one step highly exothermic chemical reaction, the gas is taken to be optically thin. Under these assumptions the model include two governing equations: an energy equation for the reacting gas and a concentration equation for the reacting fuel in the form of

$$c_{pg}\rho_g \frac{dT_g}{dt} = C_f \mu_f Q_f \frac{T_{g0}}{T_g} A exp\left(-\frac{E}{RT_g}\right) - q_{radiation},$$ (147)

$$\frac{dC_f}{dt} = -C_f \frac{T_{g0}}{T_g} A exp\left(-\frac{E}{RT_g}\right),$$ (148)

with the initial conditions:

$$T = T_{g0}, \;\; C = C_{f0}.$$ (149)

In order to apply the MIM method one should rewrite Equations 147-148 in non-dimensional form. The slow cure of the model 147-148, in non-dimensional form, have the form

$$\check{F}(\theta_g, \eta) = \eta exp\left(\frac{\theta_g}{1 + \beta\theta_g}\right) - \kappa_1(1 + \beta\theta_g)exp\left(\frac{\kappa_2}{1 + \beta\theta_g}\right)\chi(\theta_g - \theta_{g\infty})$$ (150)

where:

$$\kappa_2 = \frac{E - E_r}{RT_{g0}}, \;\; \kappa_1 = \frac{B_r}{C_{f0}\mu_f AQ_f}, \;\; \beta = \frac{RT_{g0}}{E}, \;\; \theta_g = \frac{1}{\beta}\frac{T_g - T_{g0}}{T_{g0}}, \;\; \eta = \frac{C_f}{C_{f0}}.$$ (151)

The small dimensionless parameter of the system is

$$\gamma = \frac{c_{pg} T_g \rho_{g0} \beta}{C_{f0} Q_f \mu_f}.$$ (152)

When $E < E_r$ i.e., the activation energy is less than the radiation energy, than $\kappa_2 < 0$, and in the opposite case (when $E > E_r$) than $\kappa_2 > 0$. This separation into two cases of κ_2 affects the qualitative analysis of the curve curve $\check{F}(\theta_g, \eta)$. The shape and the position of the slow curve in the $\theta_g - \eta$ phase plane depend on the combination of the values of the dimensionless parameters κ_1, κ_2 and β. The slow curve is an explicit, analytical single-valued function $\eta(\theta_g)$ in the $\theta_g - \eta$ phase plane, and any combination of the parameters dictates its location relative to the initial conditions $\theta_{g0} = 0$ and $\eta_0 = 1$. When $\kappa_2 = 0$ than it represent a bifurcation point for the slow curve 150 and it is a straight line $\eta = \kappa_1(1 + \beta)$. When $\kappa_2 > 0$ than the slow curve 150 has two branches with vertical asymptote, and when $\kappa_2 < 0$ that the slow curve 150 is monotonic.

In order to find the criterion condition for thermal explosion one should solve the system $\check{F}(\theta_g, \eta) = 0 = \frac{\partial}{\partial \theta} \check{F}(\theta_g, \eta)$. Let us follow the qualitative analysis of the slow curve as presented in (Goldfarb, Gol'dshtein, Greenberg, & Kuzmenko, 2002) and separate the qualitative analysis into two cases: $\kappa_2 > 0$ and $\kappa_2 < 0$.

1: The first case when $\kappa_2 > 0$ than the slow curve 150 has a single turning point θ_{gT} with the coordinate

$$\theta_{gT} = \frac{1}{\beta}(\kappa_2 - 1),$$ (153)

if $\theta_{gT} > \theta_{g\infty}$, or has no turning point at all if $\theta_{gT} \leq \theta_{g\infty}$. In addition the slow curve 150 has a vertical asymptote at the point $\theta_g = -1/\beta$.

2: The second case when $\kappa_2 < 0$ than the slow curve 150 has no turning point at all and intersects the θ_g-axis at the single point $\theta_g = -1/\beta$.

The next step in the qualitative analysis is to find the criterion for thermal explosion. The above analysis enable one to distinguish between the conventional explosive regimes and the slow regimes. Explosive behavior of the mixture temperature occurs when $\kappa_1 exp(\kappa_2) < 1$. This means that $kappa_1$ and κ_2 are connected parameters i.e., the pre-exponential factor B_r and the radiative activation energy E_r are connected. These two parameters dictate the intensity of the radiative heat flux from the burned gas to the ambient (see Figure).
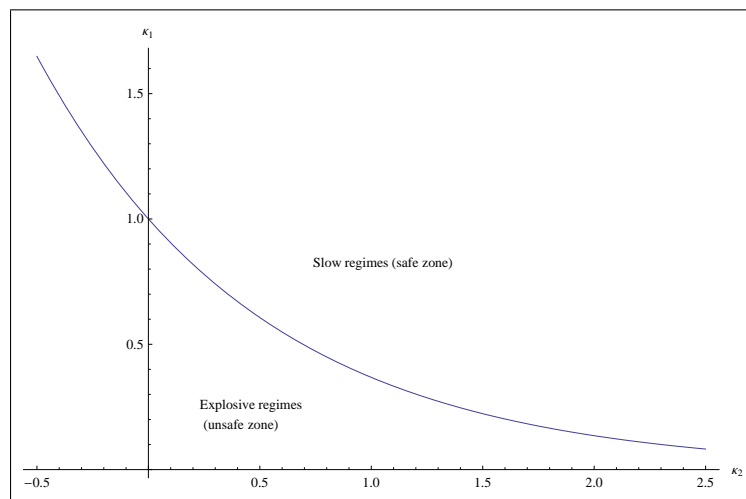

Figure 9. Regime graph (safe-unsafe zones) in the $\kappa_1 - \kappa_2$ parameter plane

For practical applications, the approximate of the expression for the maximum temperature of the burning system can be obtained in the process of thermal explosion. In order to get this approximation one should explore the quasi-stationary approximation for the slow variable η. Substituting $\eta_0 = 1$ in the slow curve (Equation 150) the authors of (Goldfarb, Gol'dshtein, Greenberg, & Kuzmenko, 2002) obtained the maximum temperature with the approximation of Frank-Kamenetskii has the form of

$$\theta_g^{max} \approx \frac{1 - \kappa_1 exp(\kappa_2)}{\beta \kappa_1 (1 - \kappa_2) exp(\kappa_2)}.$$ (154)

The theoretical results compared to three kinds of fuel: $n-$decane, $n-$heptane and tetralin presented in Table 6.

Table 6. Thermophysical experimental data applied to the model 147-148

Property	n-decane	n-heptane	tetralin
c	1050	1256	1256
L	3.21E+05	3.2E+05	3.17E+05
T_{g0}	1100	1100	1100
μ_f	142	100	132
Q_f	4.42E+07	4.54E+07	1.266E+07
E	1.257E+08	1.257+08	2.8E+08
λ	0.0193	0.0193	0.084
A	0.95E+07	0.95E+07	1.15E+08

Applied the experimental data for these three kinds of fuels implies that the influence of the thermal radiation changes strongly with the physic-chemical properties of the fuel and depends on the radiative properties of the original gaseous mixture. Numerical simulations confirmed that radiative losses cannot be ignored for tetralin from the beginning of the combustion process, whereas for normal hydrocarbon the effects of the thermal radiation can be ignored at the fast explosive stages of the thermal explosion. In addition, the qualitative analysis and the numerical simulations indicates the critical role of the fuel type and the ambient conditions in determining the influence of thermal radiation on the maximum explosive temperature.

In order to extend analysis of the model of thermal explosion in a hot gas-droplets mixture one should permit a more complete description of the chemistry via a single-step two reactant model of general order, rather than the prior deficient reactant model. This expansion was made by authors of the paper (Bykov, Goldfarb, Gol'dshtein, & Greenberg, 2002). The physical model encompasses oxidizer effects on the thermal explosion of a hot combustible mixture of gases and cool evaporating fuel droplets, i.e., the physical model take into account the effects of oxidizer and fuel concentrations on the thermal explosion of a flammable spray in a pre-heated gas mixture. The main physical assumptions are as follows: The medium is infinite and filled with a combustible gas mixture (oxidant and gaseous fuel) and liquid fuel droplets, the spray are monodisperse fuel spray (i.e., the droplets are distributed uniformly), the system is adiabatic, the pressure change in the reaction is negligible, all the droplets are at the same constant temperature (on the saturation line) which differs from that of the hot gas, heat flux from the burning gas to the droplets is supposed to be proportional to the temperature difference between the liquid and the gas phases, the chemistry is modeled as a one-step highly exothermic chemical reaction, the reaction rate contains the multiple of non-integer powers of the fuel and oxidizer concentration in addition to the usual Arrhenius exponential term. Under these assumptions the model consists of four highly non-linear ordinary differential equations: an energy equation, a mass equation for a single droplet, concentration equations for the fuel and oxidizer and have the form

$$
c_{pg}\rho_g\alpha_g\frac{dT_g}{dt} = C_f^a C_{ox}^b \mu_f Q_f \alpha_g A exp\left(-\frac{E}{RT_g}\right)
$$
$$
- 4\pi R_d n_d \lambda_g \left(T_g - T_d\right), \tag{155}
$$

$$
\frac{dR_d^3}{dt} = -\frac{3R_d n_d \lambda_g}{\rho_L L}\left(T_g - T_d\right), \tag{156}
$$

$$
\frac{dC_f}{dt} = -\nu_f C_f^a C_{ox}^b A exp\left(-\frac{E}{RT_g}\right) + \frac{4\pi\lambda_g R_d n_d}{\mu_f L\alpha_g}\left(T_g - T_d\right), \tag{157}
$$

$$
\frac{dC_{ox}}{dt} = -\nu_{ox} C_f^a C_{ox}^b A exp\left(-\frac{E}{RT_g}\right), \tag{158}
$$

with the initial conditions

$$
at\ t = 0:\ T_g = T_{g0},\ R_d = R_{d0},\ C_f = C_{f0},\ C_{ox} = C_{ox0}. \tag{159}
$$

When one rewrite the model in non-dimensional form the system consists two small parameters which enable one to investigate the model as multi-scale system and hence to apply an asymptotic methods such as the MIM methods. The non-dimensional model has the form (Bykov, Goldfarb, Gol'dshtein, & Greenberg, 2002)

$$\gamma \frac{du}{d\tau} = \eta^a \zeta^b exp\left(\frac{u}{1+\beta u}\right) - \epsilon_1 r(u + \theta_0), \tag{160}$$

$$\frac{1}{\epsilon_2} \frac{dr^3}{dt} = -\epsilon_1 r(u + \theta_0), \tag{161}$$

$$\tilde{v}_f \frac{d\eta}{d\tau} = -\eta^a \zeta^b exp\left(\frac{u}{1+\beta u}\right) + \tilde{v}_f \psi \epsilon_1 r(u + \theta_0), \tag{162}$$

$$\tilde{v}_{ox} \frac{d\zeta}{d\tau} = -\eta^a \zeta^b exp\left(\frac{u}{1+\beta u}\right), \tag{163}$$

with the initial conditions

$$at \ \tau = 0: \ u = u_0 = 0, \ r = r_0 = 1, \ \eta = \frac{C_{f0}}{C_{ff}}, \ \zeta = \zeta_0 = 1, \tag{164}$$

where C_{ff} is the overall fuel concentration. The following dimensionless parameters have been introduced:

$$\beta = \frac{RT_{g0}}{E}, \ \tau = \frac{t}{t_{react}}, \ t_{react} = \frac{e^{1/\beta}}{AC_{ff}^{a-\frac{1}{2}}C_{ox}^{b-\frac{1}{2}}}, r = \frac{R_d}{R_{d0}},$$

$$\psi = \sqrt{\frac{C_{ff}}{C_{ox0}}} \frac{Q_f}{L}, \ \zeta = \frac{C_{ox}}{C_{ox0}}, \ \theta_g = \frac{1}{\beta} \frac{T_g - T_d}{T_{g0}}, \ \theta_0 = \frac{1}{\beta} \frac{T_{g0} - T_d}{T_{g0}},$$

$$\tilde{v}_{ox} = \frac{1}{v_{ox}} \sqrt{\frac{C_{ox0}}{C_{ff}}}, \ \tilde{v}_f = \frac{1}{v_f} \sqrt{\frac{C_{ff}}{C_{ox0}}}, \ \eta = \frac{C_f}{C_{ff}}, \ \epsilon_1 = \frac{4\pi\lambda_g R_{d0}\beta T_{g0} n_{d0}}{C_{ff}^a C_{ox0}^b A Q_f \alpha_g \mu_f} e^{\left(\frac{1}{\beta}\right)},$$

$$\epsilon_2 = \frac{\sqrt{C_{ff}C_{ox0}}Q_f\mu_f\alpha_g}{\rho_L L \alpha_L}, \ \gamma = \frac{\beta c_{pg}T_{g0}\rho_g}{\sqrt{C_{ff}C_{ox}}Q_f\mu_f}, \ u = \theta_g - \theta_0. \tag{165}$$

The dynamical behavior of the system depends on the dimensionless parameters: $\beta, \gamma, \epsilon_1, \epsilon_2, \psi, \tilde{v}_f, \tilde{v}_{ox}, a, b$ and on the initial condition: η_0, θ_0.

Appropriate combinations of Equations 160-163 and integration with respect to the initial conditions 164 one can obtained an explicit expressions for η and ζ as a functions of the temperature u and the radius r.

$$\eta(u, r) = \eta_0 - \frac{\gamma u \epsilon_2 - (\tilde{v}_f \psi - 1)(1 - r^3)}{\tilde{v}_f \epsilon_2}, \tag{166}$$

$$\zeta(u, r) = 1 - \frac{\gamma u \epsilon_2 + (1 - r^3)}{\tilde{v}_o \epsilon_2}. \tag{167}$$

Because the analysis focused on the initial stages of the behavior of the combustible medium as its temperature begins to rise, then it is reasonable to apply the Frank-Kamenetskii approximation $\beta\theta << 1, \gamma\theta << 1$. Hence, the model 160-163 reduce to the pair of ordinary differential equations

$$\gamma \frac{du}{d\tau} = \eta(u, r)^a \zeta(u, r)^b exp\left(\frac{u}{1+\beta u}\right) - \epsilon_1 r(u + \theta_0), \tag{168}$$

$$\frac{1}{\epsilon_2} \frac{dr^3}{dt} = -\epsilon_1 r(u + \theta_0). \tag{169}$$

The parameters γ and $1/\epsilon_2$ are small. $\gamma << 1$ due to the exothermicity of the chemical reaction, and $1/\epsilon_2 << 1$ as a result of the appropriate combination of physical properties of the system. Hence, at the initial stage the system 168-169 represents a singular perturbed system of ordinary differential equations with appreciably different rates of change of the dependent variables. Three different scenarios are possible 1: $\gamma << 1$ and $\gamma << 1/\epsilon_2$ which means that the temperature changes much faster the the droplet radius, i.e., Equation 168 describes a fast heat release process, whereas Equation 169 describes the slow process of the reduction in the droplets' radius, 2: $1/\epsilon_2 << \gamma << 1$ which means that the radius of the droplets changes much faster than the gas temperature, i.e., Equation 168 describes a slow heat release process, whereas Equation 169 describes the fast process of the reduction in the droplets' radius due to intensive evaporation, 3: $1/\epsilon_2 \approx \gamma << 1$ which means that the rates of changes of the droplets radius and the gas temperature are approximately the same. In this intermediate case, the equations cannot be separated according to their rates of change.

Due to the appearance of the small parameters in the system 168-169 one can apply an asymptotic methods such as the MIM method. Hence, the system 168-169 have two slow curves

$$\breve{F}_u(u,r) = \eta(u,r)^a \zeta(u,r)^b exp(u) - \epsilon_1 r(u + \theta_0) = 0, \tag{170}$$

$$\breve{F}_r(u,r) = -\epsilon_1 r(u + \theta_0)) = 0. \tag{171}$$

Let us details the different scenarios mentioned above. 1: The temperature is the fast variable and the radius is the slow one, $\gamma << 1$ and $\gamma << 1/\epsilon_2$, in this case we substitute $\gamma = 0$ in Equation 170 and obtain the slow curve in the form

$$\breve{F}_u(u,r) = \left(\eta_0 + \frac{(\tilde{v}_f \psi - 1)(1 - r^3)}{\tilde{v}_f \epsilon_2}\right)^a \left(1 - \frac{(1 - r^3)}{\tilde{v}_o \epsilon_2}\right)^b exp(u)$$
$$- \epsilon_1 r(u + \theta_0) = 0. \tag{172}$$

The turning point of the slow curve 172 can be obtain from the solution of the system $\breve{F}_u(u,r) = 0 = \frac{\partial \breve{F}_u(u,r)}{\partial u}$. The $u-$coordinate of the turning point, i.e., the solution of this system for the variable u is $u_T = 1 - \theta_0$, and the $r-$coordinate of the turning point can be calculate from the equation $\breve{F}_u(u_T, r) = 0$.

In order find the inclusion of thermal explosion theory of Semenov one should find the critical trajectory which describes the critical dynamical regime. Substituting $r = 1$ and $u = 1 - \theta_0$ into Equation 172 for the slow curve yield the critical condition for thermal explosion limit in the form

$$\epsilon_1 = \eta_0^a \cdot exp(1 - \theta_0). \tag{173}$$

When $\theta_0 = 0$ and $\eta_0 = 1$ then ϵ_1 is the condition for thermal explosion limit of Semenov.

The next step in this case (when the temperature is the fast variable and the radius is the slow one) is to find the delay time. For this purpose one should substitute the expression $\epsilon_1 r(u + \theta_0)$ form Equation 172 and integrate Equation 171 with respect to the initial conditions 164 (i.e., $r_0 = 1$) until the turning point r_T. This procedure yields

$$\tau_{delay} = -\frac{3}{\epsilon_2} \int_0^{r_T} \frac{exp(u(r)) r^2 dr}{\left(\eta_0 + \frac{(\tilde{v}_f \psi - 1)(1 - r^3)}{\tilde{v}_f \epsilon_2}\right)^a \left(1 - \frac{(1 - r^3)}{\tilde{v}_o \epsilon_2}\right)^b}. \tag{174}$$

During the delay time one can approximate the integral in Equation 174 using the inequality

$$e^{(-\theta_0)} < e^{(u)} < e^{(1-\theta_0)}. \tag{175}$$

This inequality is valid due to the u coordinate of the turning point T that was found earlier $u_T = 1 - \theta$. Hence, using Equation 175 when the temperature is the fast variable and the radius is the slow one the approximation of the delay time is

$$\Gamma e^{(\theta_0 - 1)} < \tau_{delay} < \Gamma e^{(\theta_0)} \tag{176}$$

where

$$\Gamma = \frac{3}{\epsilon_2} \int_1^{r_T} \left(\eta_0 + \frac{(\tilde{v}_f \psi - 1)(1 - r^3)}{\tilde{v}_f \epsilon_2}\right)^{-a} \left(1 - \frac{(1 - r^3)}{\tilde{v}_o \epsilon_2}\right)^{-b} r^2 dr. \tag{177}$$

This integral can be calculated analytically (Bykov, Goldfarb, Gol'dshtein, & Greenberg, 2002).

2: The radius is the fast variable and the temperature is the slow one, $1/\epsilon_2 << \gamma << 1$. Then the equation of the slow curve is $r = 0$. This means that the axis of the temperature u is the slow curve and it consists a single attractive branch and all possible trajectories are similar to each other, i.e., there is no dependence on the location of the initial conditions. The next step in this case (when the radius is the fast variable and the temperature is the slow one) is to find the delay time. In this case, when the trajectory reaches the slow curve and there is no motion along the slow curve because that the conventional explosion begins, the system describes the extinction of droplet. The time before the final thermal explosion is therefore the time during the process of evaporation occurs fast and the temperature vary slowly. Hence, taking the temperature u as constant and equal to its initial value $u_0 = 0$ and integrating Equation 171 the delay time before the thermal explosion can be calculated analytically as

$$\tau_{delay} = -\int_1^0 \frac{3r^2}{\epsilon_1 \epsilon_2 r(\theta_0)} dr = \frac{3}{2\epsilon_1 \epsilon_2 \theta_0}. \tag{178}$$

3: The radius and the temperature are fast and of the same order $1/\epsilon_2 \approx \gamma << 1$. Then the original system contains two fast variables of the same order and the situation is much more complex and its beyond in the scope of this paper (for more details please see Bykov, Goldfarb, Gol'dshtein, & Greenberg, 2002). The delay time can be calculated analytically as

$$\tau_{delay} = \frac{\gamma}{2\epsilon_1 p}\left(\frac{\pi}{\sqrt{3}} + 2\sqrt{3}\arctan\left(\frac{2-p}{\sqrt{3}p}\right) + \ln\left(\frac{1-p+p^2}{(1+p)^2}\right)\right), \tag{179}$$

where $\sqrt[3]{\gamma\theta_0\epsilon_2 - 1}$.

Let us summarize the results of the model that presented by (Bykov, Goldfarb, Gol'dshtein, & Greenberg, 2002) and permit a more complete description of the chemistry via single-step-reactant model of general order, rather than the prior deficient reactant model. The governing equations of the physical model involves a singular perturbed system (SPS system) of four highly non-linear ordinary differential equations. The SPS form enable the authors to applied the MIM method due to the appearances of a small parameters. The system contains two small parameters γ and $1/\epsilon_2$. This multi-scale system requires separation of the dynamical behavior of the model into the following cases, 1: the temperature is vast variable and the radius is the slow one, 2: the radius is the fast variable and the temperature is the slow one, 3: the radius and the temperature are of the same order. At each case the delay time have been approximated analytically which is very practical important. When the authors investigated each case they found a new physical phenomenon which called freeze delay time. This freeze delay cause by the fact that the model take into account two-reactant single-step reaction, with the reaction rate depending much more strongly on the oxidizer concentration than the fuel concentration ($a = 0.25$ and $b = 1.5$). The model have been investigated using the thermo physical properties of $n-$ decane given in Tables 7-8.

Table 7. Thermophysical experimental data applied to the model 155-158

Property	n-decane
c_{pg}	1050
L	3.21E+05
ρ_f	730
T_{g0}	550
ρ_d	730
μ_f	142
Q_f	4.42E+07
E	1.257E+08
λ_g	0.0193
n_{d0}	10^7
A	1.9E+07

The natural generalization of the model presented by (Bykov, Goldfarb, Gol'dshtein, & Greenberg, 2002) is to take into account the effect of the thermal radiation on thermal explosion. This generalization have been done by the authors of (Goldfarb, Sazhin, & Zinoviev, 2004; Goldfarb, Gol'dshtein, Katz, & Sazhin, 2007). The model described

Table 8. Dimensionless parameters applied to the dimensionless model 160-163

Dimensionless parameter	Conventional explosion	Explosion with delay	Explosion with freeze delay
γ	0.01	0.001	0.001
ϵ_1	0.1	1	1.5
ϵ_2	0.001	0.1	0.333
θ_0	1.5	1.5	3
$\tilde{v}_f$	0.1	0.127	0.4
$\tilde{v}_o$	0.9	0.327	0.5
η_0	0.15	0.25	0.1
ψ	15	15	3

the radiation effect on thermal explosion in a gas containing evaporating fuel monodisperse spray. The physical assumptions of the model are as follows: the difference between gas temperature (responsible for convective heating of droplets) and external temperature (responsible for radiative heating of droplets) is taken into account, the droplets are regarded as the source of endothermicity, the medium is modeled as a spatially homogeneous mixture of an optically thin, combustible gas with monodisperse spray of evaporating fuel droplets, the distortion of the incident radiation by surrounding droplets is ignored, the effects of droplet movement and the effect of temperature gradient inside the droplets are ignored, the incident radiation has a black-body spectrum, the system is adiabatic, the gas pressure is constant, convective and radiative heating of droplets are taken into account, the thermal conductivity of the liquid phase is assumed to be infinity large, the volume fraction of the liquid phase is assumed to be much less than that of the gaseous phase (hence, the heat transfer coefficient of the mixture is controlled by the thermal properties of the gaseous component), the burning process described by a first order exothermic reaction and takes place in the gaseous phase only, the velocity of the droplets and the effects of natural convection are neglected (hence, the effects of the Stefan flow are neglected), Nusselt and Sherwood numbers are taken equal to 2, Reynolds number is less than 1 ($Re \ll 1$). Under these assumptions the physical model that describe the thermal explosion in a fuel droplets/ hot air mixture contains highly nonlinear ordinary differential equations: an energy balance equation for the gas phase, a equation of the droplet average temperature, an equation for the rate of fuel evaporation, an equation for the combustible gas and oxygen concentration and have the form

$$\alpha_g \rho_g c_{pg} \frac{dT_g}{dt} = C_f^a C_{ox}^b \alpha_g \mu_f Q_f A exp\left(-\frac{E}{RT_g}\right) - 4\pi R_d^2 n_d (q_c + q_r), \tag{180}$$

$$C_f m_d \frac{dT_d}{dt} = 4\pi R_d^2 (q_c + q_r)\left(\frac{T_d - T_{d0}}{T_b - T_{d0}}\right). \tag{181}$$

$$\frac{d}{dt}\left(\frac{4\pi}{3} R_d^3 \rho_L\right) = \frac{dm_d}{dt} = -4\pi R_d^2 \frac{(q_c + q_r)}{L}\left(\frac{T_d - T_{d0}}{T_b - T_{d0}}\right), \tag{182}$$

$$\frac{dC_f}{dt} = -v_f C_f^a C_{ox}^b A exp\left(-\frac{E}{RT_g}\right) + 4\pi R_d^2 n_d \frac{(q_c + q_r)}{\mu_f L \alpha_g}\left(\frac{T_d - T_{d0}}{T_b - T_{d0}}\right), \tag{183}$$

$$\frac{dC_{ox}}{dt} = -v_0 C_f^a C_{ox}^b A exp\left(-\frac{E}{RT_g}\right), \tag{184}$$

Where,

$$q_c = \frac{\lambda_g}{R_d}(T_g - T_d), \quad q_r = a\sigma R_d^b T_{ext}^4, \quad a = a_0 + a_1 10^{-3} T_{ext} + a_2 10^{-6} T_{ext}^2,$$
$$b = b_0 + a_1 10^{-3} T_{ext} + b_2 10^{-6} T_{ext}^2. \tag{185}$$

Here, q heat flux (c for convective and r for radiative), a, a_0, a_1, a_2, b, b_0, b_1 and b_2 are coefficients introduced in Goldfarb, Gol'dshtein, Katz, and Sazhin (2007).

The initial conditions are:

$$t = 0 : \quad T_g(t = 0) = T_{g0}, \quad R_d = R_{d_0}, \quad T_d = T_{d0}, \quad C_f = C_{f0}, \quad C_{ox} = C_{ox0}. \tag{186}$$

The analysis of the model 180-184 is based on the geometrical version of the method of integral manifold (MIM). In order to apply the MIM method the authors of (Goldfarb, Gol'dshtein, Katz, & Sazhin, 2007) transform the Equations 180-184 to the SPS form (singular perturbed system). The non-dimensional model is

$$\gamma \frac{d\theta_g}{d\tau} = \eta^a \zeta^b exp\left(\frac{\theta_g}{1+\beta\theta_g}\right) - \epsilon_1 r \sqrt{\frac{T_{d0}(1+\beta\theta_g)}{T_{go}}}(\theta_g - \theta_d), \tag{187}$$

$$\frac{d\theta_d}{d\tau} = \frac{\epsilon_2}{\epsilon_4 r^3}\left\{\epsilon_1 r \sqrt{\frac{T_{d0}(1+\beta\theta_g)}{T_{go}}}(\theta_g - \theta_d) + \frac{\epsilon_1\epsilon_3}{4\beta}r^{2+b}(1+\beta\theta_g^{ext})^4\right\}\xi(\theta_d), \tag{188}$$

$$\begin{aligned} \frac{1}{\epsilon_2}\frac{dr^3}{dt} = & - \epsilon_1 r \sqrt{\frac{T_{d0}(1+\beta\theta_g)}{T_{go}}}(\theta_g - \theta_d)(1 - \xi(\theta_d)) \\ & - \frac{\epsilon_1\epsilon_3}{4\beta}r^{2+b}(1+\beta\theta_g^{ext})^4(1 - \xi(\theta_d)), \end{aligned} \tag{189}$$

$$\begin{aligned} \tilde{v}_f\frac{d\eta}{d\tau} = & - \eta^a\zeta^b exp\left(\frac{\theta_g}{1+\beta\theta_g}\right) \\ & + \frac{\psi}{\tilde{v}_f}\epsilon_1 r \sqrt{\frac{T_{d0}(1+\beta\theta_g)}{T_{go}}}(\theta_g - \theta_d)(1 - \xi(\theta_d)) \\ & + \frac{\psi}{\tilde{v}_f}\frac{\epsilon_1\epsilon_3}{4\beta}r^{2+b}(1+\beta\theta_g^{ext})^4(1 - \xi(\theta_d)), \end{aligned} \tag{190}$$

$$\tilde{v}_{ox}\frac{d\zeta}{d\tau} = -\eta^a\zeta^b exp\left(\frac{\theta_g}{1+\beta\theta_g}\right), \tag{191}$$

with the initial conditions

$$at \ \tau = 0 : \ \theta_g = \theta_{g0}, \ \theta_d = \theta_{d0} \ r = r_0, \ \eta = \frac{C_{f0}}{C_{ff}}, \ \zeta = \zeta_0 = 1. \tag{192}$$

The following dimensionless variables are used

$$\begin{aligned} \beta &= \frac{RT_{g0}}{E}, \ \tau = \frac{t}{t_{react}}, \ t_{react} = \frac{e^{1/\beta}}{AC_{ff}^{a-\frac{1}{2}}C_{ox}^{b-\frac{1}{2}}}, r = \frac{R_d}{R_{d0}}, \ \theta_g = \frac{1}{\beta}\frac{T_g - T_{d0}}{T_{d0}} \\ \psi &= \sqrt{\frac{C_{ff}}{C_{ox0}}}\frac{Q_f}{L}, \ \zeta = \frac{C_{ox}}{C_{ox0}}, \ , \ \theta_d = \frac{1}{\beta}\frac{T_d - T_{d0}}{T_{d0}}, \ \theta_g^{ext} = \frac{1}{\beta}\frac{T_{ext} - T_{d0}}{T_{d0}}, \\ \tilde{v}_{ox} &= \frac{1}{v_{ox}}\sqrt{\frac{C_{ox0}}{C_{ff}}}, \ \tilde{v}_f = \frac{1}{v_f}\sqrt{\frac{C_{ff}}{C_{ox0}}}, \ \eta = \frac{C_f}{C_{ff}}, \ \epsilon_1 = \frac{4\pi\lambda_g R_{d0}\beta T_{d0}n_d}{C_{ff}^a C_{ox0}^b AQ_f\alpha_g\mu_f}e^{\left(\frac{1}{\beta}\right)}, \\ \epsilon_2 &= \frac{\sqrt{C_{ff}C_{ox0}}Q_f\mu_f\alpha_g}{\rho_L L\alpha_L}, \ C_{ff} = \frac{4\pi}{3\mu_f}R_{d0}^3\rho_f n_d(1 + w_f), \ w_f << 1 \\ \gamma &= \frac{\beta c_{pg}T_{d0}\rho_g}{\sqrt{C_{ff}C_{ox}}Q_f\mu_f}, \ \epsilon_3 = \frac{4T_{d0}^3\sigma R_{d0}\kappa_{10}}{\lambda_{g0}}, \ \epsilon_4 = \frac{c_f T_{d0}\beta}{L}, \\ \xi(\theta_d) &= \left(\frac{T_b - T_{d0}(1 + \beta\theta_d)}{T_b - T_{d0}}\right). \end{aligned} \tag{193}$$

where κ_{10} is the efficiency factor of absorption at the initial stage.

The following term clarify the impact of the thermal radiation, which is measured in percent, on the delay time before the final explosion

$$\delta(\%) = \frac{\tau_{delay}^{CR} - \tau_{delay}^{C}}{\tau_{delay}^{CR}} \cdot 100\%, \tag{194}$$

where τ_{delay}^{CR} and τ_{delay}^{C} are the dimensionless delay time with and without taking into account the effect of the thermal radiation respectively, $\epsilon_3 \neq 0$ and $\epsilon_3 = 0$ respectively.

The authors of (Goldfarb, Gol'dshtein, Katz, & Sazhin, 2007) investigated the parameters given in tables 9 for the model 180-184 and found that the only possible dynamical scenarios, when the MIM can be applied, are those when the fast dimensionless variables are gas temperature θ_g and droplet temperature θ_d.

Scenario 1: The gas temperature is the fas variable. In this, according to MIM method the slow curve of the system 187-191 is

$$\hat{F}(\theta_g, r) = \eta^a \zeta^b exp\left(\frac{\theta_g}{1+\beta\theta_g}\right) - \epsilon_1 r \sqrt{\frac{T_{d0}(1+\beta\theta_g)}{T_{go}}}(\theta_g - \theta_d) = 0. \tag{195}$$

The delay time can be formally obtained by integration Equation 187 from the initial condition of the dimensionless gas temperature θ_{g0} until the final value of the dimensionless gas temperature θ_{gf}

$$\tau_{delay} = \gamma \int_{\theta_{g0}}^{\theta_{gf}} \frac{d\theta_g}{\left((1+\beta\theta_g)\left(\eta_0^a \zeta_0^b exp\left(\frac{\theta_g}{1+\beta\theta_g}\right) - \epsilon_1 r_0 \sqrt{\frac{T_{d0}(1+\beta\theta_g)}{T_{go}}}(\theta_g - \theta_{d0})\right)\right)}. \tag{196}$$

From practical applications, Equation 196 is limited due to the fact that θ_{gf} is unknown value. In order to compute this integral one should solve numerically the system 187-191 and receive an approximate solution to the final dimensionless gas temperature. In addition delay time predicted by Equation 196 in not the total ignition delay which defined as the time span between droplet injection and the time when the fuel vapor/air mixture reaches an a priori chosen temperature (typically $1100(K)$) (Sazhina, Sazhin, Heikal, & Marooney (1999); Sazhin et al., 1999). From physical point of view the delay time the delay times increase with increasing droplet number density n_d and droplet initial radii r_{d0}. If the volume fraction of the liquid fuel is too high then the drop of gas temperature due to droplet evaporation would lead to the additional delay in the setup of the ignition. When the initial gas temperature is increased then the ignition delay time is decreased. In this scenario, the thermal radiation leads to decrease of the ignition delay. These results is expected from the point of view of the underlying physics of the process. The more heat is absorbed by the droplet via thermal radiation-the quicker it is evaporated. The energy for this evaporation is taken mainly from the external source of thermal radiation and not from the surrounding gas. When the number density of droplet present in the system and their radii increase, then the amount of the thermal radiation absorbed by the liquid fuel is expected to increase as well. This result consistent with the increase of the thermal radiation impact with increased droplet number density and droplet radii.

Scenario 2: The droplet temperature is the fast variable. In this scenario, the thermal explosion process should be divided into two separate consecutive sub-processes: A-The heat-up and evaporation (time) process and, B-the induction (time) process. Let us review these two processes as presented in (Goldfarb, Gol'dshtein, Katz, & Sazhin, 2007). Case A: Heat-up and evaporation time: during the heat-up and evaporation time the dimensionless droplet temperature rises from its initial value θ_{d0} to its boiling point θ_b and the droplets evaporate (during this time the fuel droplets evaporate completely). During the heat-up and evaporation time the droplet dimensionless temperature θ_d is the fast variable whereas the others variables are constants. The slow curve in this case has the form

$$\check{\check{F}}(\theta_g, \theta_d) = \quad \frac{\epsilon_2}{\epsilon_4 r(\theta_d)^3} \epsilon_1 r(\theta_d) \sqrt{\frac{T_{d0}(1+\beta\theta_g)}{T_{go}}}(\theta_g - \theta_d)$$

$$+ \quad \frac{\epsilon_2}{\epsilon_4 r(\theta_d)^3} \frac{\epsilon_1 \epsilon_3}{4\beta} r(\theta_d)^{2+b}(1+\beta\theta_g^{ext})^4 \xi(\theta_d) = 0, \tag{197}$$

where $r(\theta_d)^3 = \left(exp(\theta_d)\,\xi(\theta_d)^{\theta_{db}}\right)^{\epsilon_4}$ obtained by appropriate combination of Equations 188 and 189 (this is a partial integral of this system).

According to MIM method a trajectory of the system starts with the fast motion from the initial condition $(\theta_{g0}, \theta_{d0})$ toward the attractive branch of the slow curve (Equation 197). After a short period of time, it intersects with the slow curve at the point which coordinates $(\theta_{g0}, \theta_d^*)$ and satisfy the equation $\check{F}(\theta_{g0}, \theta_d^*) = 0$ (See Figure). Thereafter, it start a relatively slow movement along the attractive branch of the slow curve until the trajectory reaches the point $(\theta_{gd}, \theta_{db})$, where, θ_{gb} is the dimensionless gas temperature corresponding to the dimensionless fuel boiling temperature θ_b. This point $(\theta_{gd}, \theta_{db})$ is the so-called the turning point of the slow curve 197 (See Figure) and satisfies the equations: $\check{F}(\theta_{gb}, \theta_{db}) = 0 = \partial\check{F}(\theta_{gb}, \theta_{db})/\partial\theta_d$. If one ignoring the contribution of the initial fast part of the system trajectory i.e., the part of the trajectory from the point $(\theta_{go}, \theta_{d0})$ until the point $(\theta_{go}, \theta_d^*)$, then the heat-up and evaporation period, taking into account the convective and radiative heating (labeled CR), can be approximate as

$$\tau_{delay,hp}^{CR} = \int_{\theta_{g0}}^{\theta_{gb}} \frac{\gamma d\theta_g}{(1+\beta\theta_g)\left(\eta_0^a\zeta_0^b exp\left(\frac{\theta_g}{1+\beta\theta_g}\right) + \frac{\epsilon_1\epsilon_3}{4\beta}r(\theta_g)^{2+b}(1+\beta\theta_g^{ext})^4\right)},$$

(198)

where the subscript hp indicate the heat-up time. The heat-up and evaporation period, without taking into account the thermal radiation i.e., $\epsilon_3 = 0$ and labeled as C, Equation 198 simplified to

$$\tau_{delay,hp}^{C} = \int_{\theta_{g0}}^{\theta_{gb}^*} \frac{\gamma d\theta_g}{(1+\beta\theta_g)\eta_0^a\zeta_0^b exp\left(\frac{\theta_g}{1+\beta\theta_g}\right)}$$

(199)

where the point θ_{gb}^* is the turning point of the slow curve given in Equation 197 when $\epsilon_3 = 0$ i.e., $\check{F}(\theta_g, \theta_d)_{|\epsilon_3=0}$.

Case B: Induction time process: During the heat-up time the droplet temperature reach its boiling point and the droplets evaporate. Hence, the one can excluded Equation 188 and 189 from the system of equations. In addition, when the droplets have evaporated the heat exchange between the gaseous and liquid phases are disappears. Thus, all the relevant terms that responsible for these processes (heat exchange) should be remove from the system of equations under consideration. The new model contains the following dynamical variables: θ_g, η and ζ. The fast variable of the system is the dimensionless gas temperature. In this case the induction time can be calculated as (Goldfarb, Sazhin, & Zinoviev, 2004)

$$\tau_{induction} = \frac{\gamma}{\eta_b^a\zeta_b^b},$$

(200)

where $\eta_b = \eta_{|\theta_d=\theta_{db}}$ and $\zeta_b = \zeta_{|\theta_d=\theta_{db}} = 1$.
The total ignition of the delay time is

$$\tau_{delay,total} = \tau_{hp} + \tau_{induction}.$$

(201)

The set of equations 180-184 has been analyzed for the set of parameters typical for diesel engines and presented in Table 9 (Sazhin et al., 2001). By applying different numerical simulations, the authors of (Goldfarb, Goldshtein, Katz, & Sazhin, 2007) observed that the delay time increases with increasing droplet number density and radius, and decreases with increasing the initial gas temperature (these results are for the case when the gas temperature is the fast variable). The impact of the thermal radiation increases with increasing the droplet number density and droplet radii, and decreasing with increasing the initial gas temperature.

Let us summarize the results of the model that presented by (Goldfarb, Gol'dshtein, Katz, & Sazhin, 2007). The physical model which includes a non-linear ordinary differential equations take into account the oxidizer and thermal radiation effects on the thermal explosion of a hot combustible mixture of air and evaporating fuel of monodisperse spray. The physical model take into account the heat release due to the exothermic oxidation of fuel vapor, heat losses due to the liquid fuel evaporation, fuel vapor consumption as a result of a chemical reaction, fuel vapor supply by the evaporated liquid fuel and two mechanisms of heating of evaporating fuel droplets: convection and radiation. The physical properties of the set of parameters are taken those for n-dodecane, except for the spectrum of the thermal radiation absorption which was based on the direct measurements for low sulphur ESSO AF1313 diesel fuel as reported (Sazhin et al., 2004). By rewrite the model in dimensionless form the model

transform to a SPS form. This SPS form enables the authors of (Goldfarb, Gol'dshtein, Katz, & Sazhin, 2007) to apply the MIM method. By applying the MIM method the model contains two fast variables (and hence the model investigated as a multi-scale system): the gas temperature θ_g and the droplet temperature θ_d. When θ_d identified as the fast variable the ignition time presented as a sum of heat-up and evaporation time (physical delay time) and induction time (chemical delay time) i.e., ($\tau_{totalignition} = \tau_{heat-up+evaporation} + \tau_{induction}$) (Induction time is the time of gas heating from the initial point to the slow curve, At this time evaporation almost does not exists, because it is comparatively fast process. The heat-up time is the time when the process is in the slow curve. It is heat-up time due to the fuel evaporation and grows of concentration). In this case the authors in (Goldfarb, Gol'dshtein, Katz, & Sazhin, 2007) obtained an analytical expression for the heat-up and evaporation delay time and an analytical expression for the induction delay time. The total ignition delay time and the effects of the thermal radiation increase with increase of the droplet number density and radius. On the other hand, the total ignition delay time and the effects of the thermal radiation decrease when the initial gas temperature increase. The results of the total ignition delay time predicted by (Goldfarb, Gol'dshtein, Katz, & Sazhin, 2007) and Goldfarb, Gol'dshtein, and Zinoviev, (2002) agree with the experimental data and the predictions from CFD simulations predicted (Flynn et al., 1999; Sazhin et al., 2000).

Table 9. Thermophysical experimental data applied to the model 180-184 and to the parameters in Equation 185 except for the spectral properties. This physical parameters are taken for *n*-dedecane fuel. The spectral properties are based on direct measurements for low sulphur ESSO AF1313 diesel fuel as reported (Sazhin et al., 2004). The values of the initial gas temperature, droplets radii and droplet concentrations are taken in the range $\left(T_{g0}, R_{d0}, n_{d0}\right) = [600, 1100] \times \left[5 \cdot 10^{-6}, 5 \cdot 10^{-5}\right] \times \left[10^6, 10^{12}\right]$.

Property	n-dodecane
c_{pg}	1120
L	3.6×10^5
ρ_{g0}	23.8
ρ_f	600
μ_f	170
Q_f	4.32×10^7
E	7.6×10^7
λ_{g0}	0.061
σ	5.67×10^{-8}
T_b	600
T_{d0}	300
T_{ext}	2500
a_0	$0.104(m^{-b})$
a_1	$-0.05432(m^{-b}K^{-1})$
a_2	$0.008(m^{-b}K^{-1})$
b_0	0.49162
b_1	$0.098369(K^{-1})$
b_2	$-0.007857(K^{-2})$

5. Polydisperse fuel spray combustion

In many practical engineering combustion processes fuel start as a liquid spray, for example diesel engines, jet aircraft engines and so on. The combustion of liquid is atomized into a gas-phase combustion environment. The liquid in then break-up into large number of small droplets which increase the overall surface area exposed to the oxidizer and enhance the rates of heat and mass transfer (the atomization of a 1cm diameter droplet of liquid into droplets of 100 μm diameter, for example, produces a million droplets and increases the overall surface area by a factor of 10^4). The droplets distribution range from few microns to around 500 μm, primarily because practical nozzles cannot produce sprays of uniform drop size at typical operating conditions. Furthermore, many of the larger droplets produced in the initial liquid disintegration undergo further breakup into smaller droplets. When the droplets injected into a hot gas environment (combustion zone) then the mechanism of heat transfer to the droplets come into play. This mechanism increases the vapor pressure, and thus fuel evaporation into the gas phase, until subsequent gas-phase ignition come into play (Warnatz, Maas, & Robert, 2006). When researchers modeled a spray combustion they should take into account all physical processes of droplets spray combustion such as jet
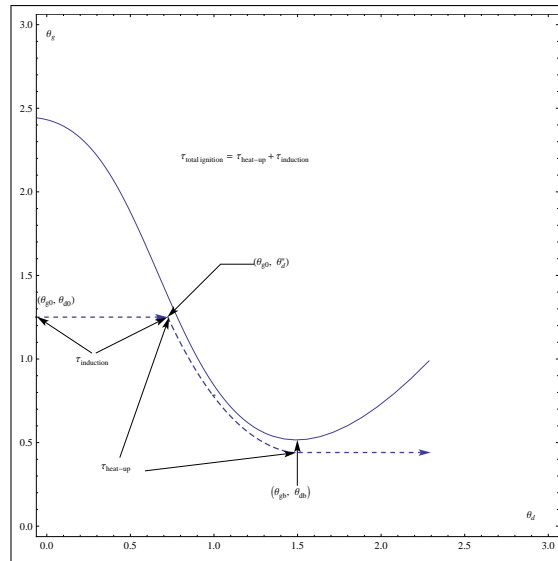
Figure 10. The slow curve obtained from Equation 197 when the droplet temperature θ_d is the fast variable

break-up, droplet dispersion, droplet evaporation, turbulent mixing, gas phase chemical kinetics, droplet velocity, collision between the droplets, coalescence between droplets, heat and mass transfer, ignition and so on. From practical point of view it is useful to split these into simply sub-models called reduced model.

Evaporation of the droplets and diffusion of the fuel into the gas phase leads to the formation of a combustible mixture, which sufficiently high temperature. If the spray is dilute, i.e., the distance between the droplets is large in comparison to the droplet diameter, then the processes during ignition and combustion can be considered as as isolated examination of the droplets. If the spray is dense, i.e., the droplets are too close for their interaction to be neglected, then in order to modeled the spray combustion one should take into account the spray as an ensemble of single non-interacting burning droplets, i.e., group/cloud of droplets.

5.1 Statistical description of fuel spray

One successful method to model a spray combustion is to characterize the the distribution of the droplets diameters by using various distribution function with associated moments that evolve in time. For simplicity, the distribution function will only depends on the radius, location and velocity of the droplets i.e., the distribution function have the form William (1995).

$$P_i(R, x, y, z, v_x, v_y, v_z, t)dRdxdydzdv_xdv_ydv_z. \tag{202}$$

which is the probable number of particle of chemical composition i in the radius range dR about R located in the spatial range $dxdydz$ about (x, y, z) with velocities in the range $dv_xdv_ydv_z$ about (v_x, v_y, v_z) at time t. In general the distribution function is largely determined by the nature of the injection and flow in the combustor. An equation governing the evolution of P_i reads as

$$\frac{\partial P_i}{\partial t} = -\frac{\partial(\dot{R}P_i)}{\partial R} - \sum_{j=1}^{3} v_j \frac{\partial P_i}{\partial x_j} - \sum_{j=1}^{3} v_j \frac{\partial P_i}{\partial v_j} \left(\vec{F}P_i\right) + S_D + S_C, \tag{203}$$

where $\dot{R}$ is the rate of change of the radius R of the droplet, $\vec{F}_j = dv_j/dt, (j = x, y, z)$ ($\vec{F}$ is the change of droplet velocity according to the friction), S_D is the change of P_i due to a source term, and S_C is the change of P_i do to the droplet collisions (S_D and S_C are a function of the droplet radii, the spatial location of the droplet and on the velocities of the droplets).

If the spray distribution is known, then one can obtain an average values of the spray properties. From practical point of view the magnitudes that are interested in among engineers are the droplet diameter distribution at the certain location in the flow which can be obtained as a marginal probability density functions (PDF) by integrating

the spray density function over velocity space and conditioning on the spatial location. This results in a probability density function $P_R(R, x, y, z, t)dr$ for the droplet radius at a given location at a given time. The average droplet radius is

$$\langle R \rangle = \int_0^\infty R P_R(R, x, y, z, t)dR. \tag{204}$$

The overall mass of droplet is proportional to the volume of the droplet $4\pi R^3/3$ and the rate of evaporation is proportional to the surface area of the droplet $4\pi R^2$. According to the above introduction the natural way to generalize the SMD given in Equation 2 to its continuous form is as follow

$$\langle R \rangle_{32} = \frac{\int_0^\infty R^3 P_R(R, x, y, z, t)dR}{\int_0^\infty R^2 P_R(R, x, y, z, t)dR}. \tag{205}$$

The advantages of the spray density function is that it reduces the governing equation of the discrete model and it reduced the computer time which is very expensive for researchers in this area of combustion.

Our aim in this section is to review the papers that presents a models that transform the models that reviewed above in a discrete form to continuous form. The first stage is transform the model that describe the thermal explosion of monodisperse fuel spray to polydisperse spray.

5.2 Polydisperse fuel spray droplet combustion: the discrete model

In this section we will investigate the model presented by (Bykov et al., 2007) and describes the effects of fuel polydisperse fuel spray on the auto-ignition process in fuel cloud. In more details, the model that describes the problem of thermal explosion in a combustible gaseous mixture that contains vaporizing fuel droplets of different radii (polydisperse spray). The physical assumptions of the model are as follows: The combustible liquid droplets are considered to comprise a polydisperse spray. The adiabatic approach is applied due to an extremely short period of ignition relative to the heat diffusion time of the system (during this period there is almost no heat transfer out of the system). Changes in the pressure relative to the mean pressure are negligible during the ignition process Semenov (1928) and Frank-Kamenetskii (1969). The thermal diffusivity of the liquid phase is greater than that of the gas phase (Sazhin et al., 2007). Thus, the heat transfer coefficient in the liquid gas mixture is supposed to be defined by the thermal properties of the gas phase. The quasi-steady state approximation is valid for the vaporizing droplets William, 1995. The droplet boundaries are assumed to be on the saturation line (i.e., the liquid temperature is constant and is equal to the liquid saturation temperature). The combustion reaction is modeled as a first order, highly exothermic chemical reaction. The governing equations are a system of non-linear ordinary differential equations. Under these assumptions, the system of the governing equations as given in (Bykov et al., 2007) is:

$$\alpha_g \rho_g c_{pg} \frac{dT_g dt}{=} \alpha_g \mu_f Q_f A C_f e^{(-\frac{E}{RT_g})} - 4\pi\lambda_g (T_g - T_d) \times \sum_{i=1}^m R_{d_i} n_{d_i}, \tag{206}$$

$$\frac{d(R_{di}^2)}{dt} = -\frac{2\lambda_g}{\rho_L L}(T_g - T_d), \ i = 1, ..., m, \ (m \ equations) \tag{207}$$

$$\frac{dC_f}{dt} = -A C_f e^{(-\frac{E}{RT_g})} + \frac{4\pi\lambda_g}{L\alpha_g \mu_f}(T_g - T_d) \times \sum_{i=1}^m R_{d_i} n_{d_i}. \tag{208}$$

The initial conditions are:

$$at \ t = 0: \ T_g(t = 0) = T_{g0}, \ R_{d_i} = R_{d_{i0}}, \ C_f = C_{f0}. \tag{209}$$

Equations 206-208 include an energy equation for the reacting gas, a mass equation for liquid droplets, and a concentration equation for the reacting gas mixture, respectively.

The behavior of the system is driven by two main processes: heat transfer from the gas phase to the liquid phase due to the evaporation process, and heat release, which is associated with an exothermic reaction in the gas phase and is described by the Arrhenius equation. Competition between these two processes determines the main dynamic peculiarities of the system.

Using the approximation of Frank-Kamenetskii i.e., $\beta << 1$ the dimensionless form of the model 206-208 is

$$\gamma \frac{d\theta_g d\tau}{=} \eta exp\left(\frac{\theta_g}{1 + \beta\theta_g}\right) - \theta_g \sum_{i=1}^{m} \epsilon_i r_i, \tag{210}$$

$$\frac{d(r_i^2)}{d\tau} = -\frac{2}{3}\epsilon_i k_i \theta_g, \ \ i = 1, ..., m, \ \ (m \ equations), \tag{211}$$

$$\frac{d\eta}{d\tau} = -\eta exp\left(\frac{\theta_g}{1 + \beta\theta_g}\right) + \psi\theta_g \sum_{i=1}^{m} \epsilon_i r_i, \tag{212}$$

where the following dimensionless variables are used

$$\tau = \frac{t}{t_{react}}, \ \ t_{react} = A^{-1}exp\left(\frac{E}{RT_{g0}}\right), \ \ \beta = \frac{RT_{g0}}{E}, \ \ \gamma = \frac{c_{pg}T_{g0}\rho_g}{C_{f0}Q_f\mu_f}\beta,$$

$$\theta_g = \frac{E}{RT_{g0}}\frac{T_g - T_{g0}}{T_{g0}}, \ \ \eta = \frac{C_f}{C_{ff}}, \ \ r_i = \frac{R_{d_i}}{R_{d_{i0}}}, \ \ \psi = \frac{Q_f}{L}, \tag{213}$$

$$\epsilon_i = \frac{4\pi R_{d_{i0}}\lambda_g T_{g0} n_{d_i} A C_{f0} Q_f \mu_f \alpha_g^{(1/\beta)}}{e}, \ \ C_{ff} = \frac{4\pi\rho_L}{3\mu_f}\sum_{i=1}^{m} R_{d_{i0}}^3 n_{d_i} + C_{f0},$$

$$\alpha_{L_i} = \frac{4\pi}{3}R_{d_i}^3 n_{d_i}, \ \ k_i = \frac{\alpha_g \mu_g C_{ff}\psi}{\alpha_{L_i}\rho_L}.$$

where C_{ff} is the total fuel concentration in both liquid and gas phases.
The initial dimensionless conditions are

$$at \ \tau = 0 : \ \theta_g = \theta_{g0} = 0, \ R_{d_i} = R_{d_{i0}} = 1, \ (i = 1, ..., m) \ C_f = C_{ff}. \tag{214}$$

Appropriate combination of Equations 210-212 and integration with respect to the initial condition 214 yields the energy integral

$$\eta = \eta_0 - \gamma\theta_g + (1 - \psi)\sum_{i=1}^{m} \frac{r_i^3 - 1}{k_i}. \tag{215}$$

From Equation 215 one can derive the final adiabatic temperature of the system after the combustion and evaporation processes are completed. Hence, substituting the final values of the dimensionless concentration and radius, i.e., $\eta_{final} = 0 = r_{i,final}$ we obtain the adiabatic temperature of the system

$$\theta_g^{(adiabatic)} = \frac{1}{\gamma}\left(1 + (\psi - 1)\sum_{i=1}^{m} \frac{1}{k_i}\right). \tag{216}$$

The following algorithm is used in order to reduce the system 210-212 from three non-linear ordinary differential equation into two non-linear ordinary differential
1: Use Equation 215 to express η explicitly as a function of $(\theta_g, r_1, ..., r_m)$,
2: Substitute η in Equations 210 and exclude η form the system,
3: Divide the equation of the i radius by the equation of the j radius, i.e, dr_i^2/dr_j^2, and substitute the dimensionless parameters ϵ_i and k_i from Equation 213 to receive the following relations,

$$\frac{dr_i^2}{dr_j^2} = \frac{R_{d_{j0}}^2}{R_{d_{i0}}^2}. \tag{217}$$

4: Substitute the expression form step 3 into the m differential equations 211,
5: Integrate the resulting equations from step 4 and order the droplet t radii such that $r_1 <, ..., r_m$ and receive the following relations

$$r_i = \left(1 + \frac{R_{d_{j0}}^2}{R_{d_{i0}}^2}(r_j^2 - 1)\right)^{1/2} \cdot \chi\left(1 + \frac{R_{d_{j0}}^2}{R_{d_{i0}}^2}(r_j^2 - 1)\right). \tag{218}$$

6: Using step 5 to exclude (in addition to η) $m - 1$ variables $(r_1, ..., r_m, \eta)$ from the system of Equations 210-212.

Applying the above steps $(1) - (6)$, the model 210-212 finally reduce the original system of $(m + 2)$ nonlinear ordinary differential equations to a system containing only two variables and has the form

$$\gamma \frac{d\theta}{d\tau} = \left(\eta_0 - \gamma \theta_g + (1 - \psi) \sum_{i=1}^{m} \frac{r_i^3(r_m) - 1}{k_i} \right) exp \left(\frac{\theta_g}{1 + \beta \theta_g} \right) - \theta_g \sum_{i=1}^{m} \epsilon_i r_i(r_m), \tag{219}$$

$$\frac{d(r_m^2)}{d\tau} = -\frac{2}{3} \epsilon_m k_m \theta_g. \tag{220}$$

The dynamical behavior of the system 219-220 depends on the following $(2m + 4)$ dimensionless parameters $\beta, \gamma, \psi, \eta_0, k_i, \epsilon_i$.

Due to the small parameter in Equation 219 the system 219-220 has the SPS form and hence one can apply the MIM method. The fast variable of the system is the gas temperature θ_g, heat emitting process (Equation 219), and the slow variable of the system is the maximum radius r_m (Equation 220 describes the slow process of the reduction of the radius of the largest droplets). By applying the MIM method and the Frank-Kamenetskii approximation $\beta \theta_g << 1$ the slow curve of the considered system in the $\theta_g - r_m$ phase plane has the form

$$\tilde{\breve{F}}(\theta_g, r_m) = \left(\eta_0 + (1 - \psi) \sum_{i=1}^{m} \frac{r_i^3(r_m) - 1}{k_i} \right) exp \left(\theta_g \right) - \theta_g \sum_{i=1}^{m} \epsilon_i r_i(r_m) = 0. \tag{221}$$

The shape and the position of the slow curve $\tilde{\breve{F}}(\theta_g, r_m) = 0$ in the (θ_g, r_m) phase plane depends on the combination of the values of the parameters $\beta, \psi, \eta_0, k_i, \epsilon_i$.

An arbitrary trajectory, which is the solution of the system 219-220, starts with fast motions at the initial point and at the initial fast part of the process moves parallel to the θ_g-axis (in the zero-approximation). If such trajectory lies above the upper part of the slow curve, it describes conventional explosive regimes with fast increase in the gas temperature, in the present case the chemical reaction tears itself away from the evaporation process and the system blows up (the gas mixture temperature rises sharply). The trajectory reaches the slow curve if the equation $\tilde{\breve{F}}(\theta_g, r_m = 1)$ has at least one non-negative root (because the physical meaning of the temperature variable). This case enable one to determined the region of thermal explosion limit. For this purpose one should solve the system $\tilde{\breve{F}} = 0 = \partial \tilde{\breve{F}} / \partial \theta_g$. The solution of this system is $\theta_g = 1$ (i.e., $\theta_g = 1$ the turning point of the slow curve 221). Substituting $\theta_g = 1, r_m = 1$ into Equation 221 yield the condition for thermal explosion in the form (Bykov et al., 2007)

$$\sum_{i=1}^{m} \epsilon_i \equiv \epsilon_{crit}^{poly} = \eta_0 e. \tag{222}$$

This parameter represent an analogue of the conventional Semenov's heat loss parameter. This new critical parameter $\epsilon_{crit}^{poly} = \eta_0 e$ divides the parameter domain into two sub domains: 1: $\epsilon_{crit}^{poly} < \eta_0 e$ is refer to the fast trajectory which do not hit the slow curve and parallel to the θ_g-axis. 2: $\epsilon_{crit}^{poly} > \eta_0 e$ is refer to the case when the trajectory reach the slow curve and is relevant to the delayed explosive regimes.

The analysis of the full polydisperse system (Equations 219-212) based on the following approximation: The full polydisperse system rewritten for a single droplets' radius i.e., the system 219-212 rewritten for the equivalent monodisperse spray as follow

$$\gamma \frac{d\theta}{d\tau} = \left(\eta_0 - \gamma \theta_g + (1 - \psi) \frac{r^3 - 1}{k^{mono}} \right) exp \left(\theta_g \right) - \theta_g \epsilon^{momo} r, \tag{223}$$

$$\frac{d(r^2)}{d\tau} = -\frac{2}{3} \epsilon^{mono} k^{mono} \theta_g, \tag{224}$$

where

$$\epsilon^{mono} = \frac{4\pi R^{mono} n^{mono} \lambda_g T_{g0} \beta}{A C_{ff} Q_f \mu_f \alpha_g} e^{1/\beta}, \quad k^{mono} = \frac{\alpha_g \mu_g C_{ff}}{\alpha_L^{mono} \rho_L}. \tag{225}$$

In order to compare the dynamics of the full system (describing a truly polydisperse spray) and an approximating one (monodisperse spray), the authors of (Bykov et al., 2007) redefined the conventional definition of the average

radius of the equivalent monodisperse spray i.e., the Sauter Mean Diameter (SMD) in such a way so that the total concentration of the fuel remains the same as it was in the original polydisperse spray, namely

$$R^{mono} = R_{ab} = \left(\frac{\sum_i R_i^a n_i}{\sum_i R_i^b n_i} \right)^{\frac{1}{a-b}} , \quad n^{mono} = \sum_i \frac{R_i^3 n_i}{R_{ab}^3}, \tag{226}$$

which leads to the following relations for ϵ^{mono} and k^{mono} as

$$k^{mono} = \left(\sum_i k_i^{-1} \right)^{-1} , \quad \epsilon^{mono} = (k^{mono})^{-1} \left(\frac{\sum_i \epsilon_i^{(3-a)/2} k_i^{(1-a)/2}}{\sum_i \epsilon_i^{(3-b)/2} k_i^{(1-b)/2}} \right)^{-\frac{2}{a-b}} , \tag{227}$$

where, in order to compare the new definitions of the SMD in Equation 227 to the conventional definition of SMD one should substitute $a = 3$ and $b = 2$.

Using the conventional definition of the SMD, the relative error of the delay time (using direct numerical simulations) is

$$\delta^{mono} = \frac{\left| \tau_{delay} - \tau_{delay}^{mono} \right|}{\tau_{delay}} = 139\%. \tag{228}$$

Whereas, using the modification definition of the SMD the relative error of the delay time is

$$\delta^{mono} = \frac{\left| \tau_{delay} - \tilde{\tau}_{delay}^{mono} \right|}{\tau_{delay}} = 25.12\%. \tag{229}$$

In conclusion this paper (Bykov et al., 2007) presented a model that describes the thermal explosion of a fuel spray which have been extended the monodisperse fuel spray to a polydisperse one. The mathematical formulations involved a SPS system of $(m + 2)$ highly nonlinear ordinary differential equations (where m in the number of different sizes of droplets). By using the energy integral procedure and simple algebraic manipulations the model reduced to only two highly nonlinear ordinary differential equations. By applying the MIM method they obtained the condition for thermal explosion which extended the well known conventional heat loss parameter of Semenov's theory. Analysis of the effect of the delay time on the thermal explosion using the conventional definition of the SMD leads to a significant over-estimate of the ignition time. Hence, the authors (Bykov et al., 2007) suggested an alternative modified definition of the SMD in such a way that the overall liquid fuel volume is also conserved in the averaging process. This new definition of the SMD is significantly influenced on the delay time and hence on the relative error of the delay time. The theoretical predictions are consistent with numerical simulations.

The natural extension of the description of polydisperse fuel spray is to describe the droplet radius by using probability density function i.e., the size distribution of droplets is taken to be continuous and characterized by a probability density function. This extension have been done in the paper (Dombrovskii & Zaichik, 2001). The probability density function P_R is normalized and defines as

$$n_d = \int_0^\infty P_R dR, \quad \alpha_L = \frac{4\pi}{3} \int_0^\infty R^3 P_R dR \equiv \frac{4\pi}{3} \left\langle R^3 \right\rangle n_d. \tag{230}$$

The symbol $\langle \cdot \rangle$ indicates the operation of averaging over the droplet sizes.

The physical assumptions of the continuous model are as follows: the density of liquid fuel is constant, the model take into account the density of convective heat flux and the density of integral flux of thermal radiation to the droplet surface, the temperature of evaporating droplet is taken to be equal to the saturation temperature T_s, the entire heat flux delivered to the droplet surface is fully spent for the evaporation i.e., $q_c + q_r = L j_m$ where j_m is the mass flow of matter from the droplet surface cause by evaporation, the evolution of the size distribution of droplets due to evaporation is described by the kinetic equation for PDF, the expression of the density of convective heat flux to the droplet surface is taken from the so-called film-model (Spalding, 1965), the Reynolds number is assumed to be less than unity $Re \ll 1$. the rate of combustion is described in the approximation of one-stage chemical reaction based on Arrhenius' equation. Under these physical assumptions the continuous physical model presented in (Dombrovskii & Zaichik, 2001) describe the problem of thermal explosion in a two phase polydisperse combustible mixture and has the form

$$c_{pg} \rho_g \alpha_g \frac{dT_g}{dt} = \mu_f \alpha_g A C_f exp \left(-\frac{E}{RT_g} \right) - \int_0^\infty 4\pi R^2 L j_m P_R dR, \tag{231}$$

$$\rho_L \frac{d\alpha_L}{dt} = -\int_0^\infty 4\pi R^2 j_m P_R dR, . \tag{232}$$

$$\frac{dC_f}{dt} = -AC_f exp\left(-\frac{E}{RT_g}\right) + \frac{1}{\mu_f \alpha_g} \int_0^\infty 4\pi R^2 j_m P_R dR, \tag{233}$$

where j_m is the mass flow of matter from the droplet surface, cased by evaporation.
The initial conditions are

$$\alpha_L(0) = \alpha_{L0} = \frac{4\pi}{3} \left\langle R^3 \right\rangle n_{d0}, \ \ C_f(0) = C_{f0}, \ \ T_g(0) = T_{g0}. \tag{234}$$

The system includes an equation of heat balance in the gas phase which includes the heat release due to combustion and the consumption of heat for the evaporation of droplets, an equation for the mass of liquid fuel,and an equation for molar concentration of fuel in gas phase respectively.
The entire heat flux delivered to the droplet surface is fully spent for evaporation i.e.,

$$j_m = \frac{q_c + q_r}{L}. \tag{235}$$

where

$$q_c = \frac{\lambda_g(T_g - T_s)}{R}, q_r = (1 - exp(-2K_a R))\sigma(T_g^4 - T_s^4), \tag{236}$$

and K_a is the spectral absorptivity of fuel.
The evolution of the size distribution of droplets due to the evaporation process is described by the kinetic equation for the PDF presented in (Dombrovskii & Zaichik, 2001). The solution of the kinetic equation is

$$P_R = P_{R0}(R + \Delta), \ \ \Delta = \int_0^t \frac{\int_0^\infty R^2 j_m P_R dR}{\rho_L \int_0^\infty R^2 P_R dR}. \tag{237}$$

Applying the procedure of the energy integral to the system 231-233 and using the approximation $\beta\theta_g \ll 1$ which is valid when solving the problem of thermal and focusing only to the initial stage of the process then the dimensionless form of the system 231-233 is

$$\gamma \frac{d\theta_g}{d\tau} = \left(1 - \gamma\theta_g + \frac{\psi - 1}{\epsilon_2}(1 - \left\langle r^3 \right\rangle N)\right) e^{\theta_g}$$
$$- \epsilon_1 \theta_g \left\langle r \right\rangle N - \epsilon_1 \epsilon_3 \theta_g \left(\left\langle r^2 \right\rangle - \left\langle r^2 exp(-2\varpi_* r) \right\rangle\right) N, \tag{238}$$

$$\frac{d\delta}{d\tau} = \frac{\epsilon_1 \epsilon_2 \theta_g \left\langle r \right\rangle}{3 \left\langle r^2 \right\rangle} + \frac{\epsilon_1 \epsilon_2 \epsilon_3 \theta_g}{3}\left(1 - \frac{\left\langle r^2 exp(-2\varpi r) \right\rangle}{\left\langle r^2 \right\rangle}\right), \tag{239}$$

with the initial conditions

$$\theta_g(0) = 0, \ \ \delta(0) = 0. \tag{240}$$

The following dimensionless parameters are used

$$\tau = \frac{t}{t_{react}}, \ \ t_{react} = A^{-1} exp\left(\frac{E}{RT_{g0}}\right), \ \ \beta = \frac{RT_{g0}}{E}, \ \ \gamma = \frac{c_{pg} T_{g0} \rho_{g0}}{C_{f0} Q_f \mu_f}\beta,$$

$$\theta_g = \frac{E}{RT_{g0}} \frac{T_g - T_{g0}}{T_{g0}}, \ \ R_0 = \left(\frac{\int_0^\infty R^3 P_{R0} dR}{\int_0^\infty P_{R0} dR}\right)^{1/3}, \ \ r = \frac{R}{R_0}, \ \ \psi = \frac{Q_f}{L}, \tag{241}$$

$$\epsilon_1 = \frac{4\pi R_0 \lambda_{g0} T_{g0} n_{d0} \beta}{AC_{f0} Q_f \mu_f \alpha_g} e^{(1/\beta)}, \ \ \epsilon_2 = \frac{Q_f C_{f0} \mu_f \alpha_g}{L \alpha_{L0} \rho_L}, \ \ \epsilon_3 = \frac{4T_{g0}^3 \sigma R_0}{\lambda_{g0}},$$

$$\varpi = K_a^* R_0, \ \ N = \frac{n_d}{n_{d0}}, \ \ \delta = \frac{\Delta}{R_0}, \ \ f_0 = \frac{R_0}{n_{d0}} P_{R0}$$

And the following correlations for average quantities are used

$$
\begin{aligned}
f &= f_0(r + \delta) \\
N &= \int_0^\infty f(r)dr = \int_0^\infty f_0(r + \delta)dr, \\
\int_0^\infty f_0 dr &= \int_0^\infty r^3 f_0 dr = 1, \\
\langle r^n \rangle &= \int_0^\infty r^n f(r)dr = \int_0^\infty r^n f_0(r + \delta)dr \ \ n = 1, 2, 3, \\
\langle r^2 exp(-2\varpi r) \rangle &= \int_0^\infty r^2 exp(-2\varpi r) f_0(r + \delta)dr.
\end{aligned}
\tag{242}
$$

The system 238-239 is in the form of SPS system. Hence, the authors of (Dombrovskii & Zaichik, 2001) applied the MIM method to this system. The condition for thermal explosion of a combustible gas with droplets of fuel can be obtain as a result of investigation of the algebraic equation of the slow curve obtained by substituting $\gamma = 0$ in Equation 238. Hence, the slow curve of the system 238-239 is

$$
\begin{aligned}
\bar{\bar{F}} = \ & \left(1 + \frac{\psi - 1}{\epsilon_2}(1 - \langle r^3 \rangle N)\right)e^{\theta_g} \\
& - \ \epsilon_1 \theta_g \langle r \rangle N - \epsilon_1 \epsilon_3 \theta_g \left(\langle r^2 \rangle - \langle r^2 exp(-2\varpi_* r) \rangle\right)N = 0.
\end{aligned}
\tag{243}
$$

The solution of Equation 243 presented in the phase plane $\theta_g - \delta$ and describes the dynamic of the considered system. In the particular case of monodisperse fuel spray of droplets, when $\delta = 1 - r$, the analysis of the condition of thermal explosion reduced to the calculation of the slow curve in the $\theta_g - r$ phase plane. According to the MIM method, the turning point of the slow curve obtained by the solution of the system $\bar{\bar{F}} = 0 = \partial\bar{\bar{F}}/\partial\theta_g$. The turning point of the slow curve corresponds to the point $\theta_g = 1$. The critical condition of thermal explosion which corresponds to the ignition of combustible medium at the initial moment of time, is determined from the slow curve at $\delta_{maximum} = 0$. This yield the following relations $N = \langle r^3 \rangle = 1$, $\langle r \rangle = \langle r \rangle_0$ and $\langle r^2 \rangle = \langle r^2 \rangle_0$ which determine the condition of thermal explosion defined by the expression

$$
\langle r \rangle_0 + \epsilon_3 \left(\langle r^2 \rangle_0 - \langle r^2 exp(-2\varpi r) \rangle_0\right) = \epsilon_1^{-1}e.
\tag{244}
$$

The paper (Dombrovskii & Zaichik, 2001) deals with the analysis of the effect of polydisperse of fuel droplets and of thermal radiation of the condition of thermal explosion. The size distribution of fuel droplets is assumed to be continuous and found from the solution of the kinetic equation for the probability density function. The mathematical formulations involved a SPS system of highly nonlinear ordinary differential equations. By using the energy integral procedure and simple algebraic manipulations the model reduced to only two highly nonlinear ordinary differential equations. By applying the MIM method they obtained the condition for thermal explosion which extended the well known conventional heat loss parameter of Semenov's theory.

Three initial size distribution of fuel droplet have been applied to the numerical simulation in order to illustrate the qualitative singularities of the effect of polydispersity and radiation on the ignition: gamma distribution, PDF of monodisperse spray system, and exponential distribution. The results of analytical and numerical analysis of the problem have demonstrated that the polydispersity of liquid fuel promotes, and thermal radiation prevents, the ignition of a two-phase combustible mixture. The polydispersity fuel of droplets reduced the time of ignition. The thermal radiation leads to a decrease in the gas temperature during the period of intensive evaporation of fuel and as a result to delay of thermal explosion.

6. Conclusion

This paper includes mathematical and physical modeling of fuel combustion spray self ignition processes. We start from a description of the thermal explosion limit of Semenov's simple model which including one nonlinear ordinary differential equation. The Semenov's model was extended by Melentiev and Todes taking into account the fuel consumption. It includes two nonlinear ordinary differential equation which describes the change in temperature and the change in flammable gas concentration. Then thoroughly a number of modified models was introduced for m multiphase combustion. One of natural generalization for spray combustion takes into account changes within the droplet radii in the case of monodisperse fuel spray. Different papers that deals with monodisperse fuel spray

include the heat flux from the burning gas to the droplets by two processes: convection and radiation fluxes. In reality, the injection of the fuel do not produce monodisperse fuel sprays. It is the polydisperse fuel spray with some special size of droplets dispersion. The main problem of modeling is a compact description of the thermal explosion of polydisperse fuel sprays with different realistic dispersions. Other way it is necessary to write down a large number of equations i.e., each droplet or each group of droplets of close size require an equation that describe the change in the droplet radius in addition to the change of the gas temperature, droplet temperature, change in the concentration etc. Of course it is not economical in terms of power and time computers calculation. Hence, in order to overcome this problem many researchers characterize the the distribution of the droplets diameters by using various distribution function, i.e., describe the droplet radius by using probability density function i.e., the size distribution of droplets is taken to be continuous and characterized by a probability density function. This description of the polydisperse fuel spray using distribution function is done in the last article that we reviewed.

At each reviewed model we presented critical conditions for thermal explosion and estimations of the delay time which are very important from practical point of view. In some cases the approximation of the delay time obtained analytically. Each model was transformed to a dimensionless form that includes small parameters i.e., to a multi-scale system or SPS (singular perturbed system). This form enables the researchers to apply the MIM (the method of integral manifold). In addition to the above analytical method, we applied the well-known the Homotopy Analysis Method (HAM). The advantage of the HAM with compared to other perturbation methods is that the HAM is independent on small/ large physical parameter (no artificial parameter is require). This method provides a simple way to control and hence to ensure the convergence of approximation series. For this purpose, one should choose a proper value of the so called convergence-control parameter. In addition, the HAM provides a great freedom to choose base function that span the solution (linear or nonlinear problem). Another advantage of the HAM is that one can construct a continuous mapping of an initial guess approximation to the exact solution of the given problem through an auxiliary linear operator.

Acknowledgments

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