A Numerical Study of the Time Dependent Combustion of a Gel Fuel Droplet

Arza Hadad and Benveniste Natan
Faculty of Aerospace Engineering
Technion-Israel Institute of Technology, Haifa 32000, Israel

Abstract

The combustion of gel fuels exhibits some distinctive characteristics: it is strongly time dependent and displays a repetitive fluctuations. A model for the combustion of an organic gellant based gel fuel droplet is formulated with the gel considered as a bi-component mixture of fuel and gellant. The conservation laws are written under simplifying assumptions for stages reflecting the stages observed experimentally. The equations are numerically solved for an example case of the evaporation without combustion of a droplet. The effect of the mechanical properties of the gellant on the repetitive stage was also examined.

Nomenclature

$\mathcal{D}_{AB}$	binary diffusivity of species A in species B	$\left[m^2 / s \right]$
$\mathcal{D}_i$	diffusion coefficient of species i in the surroundings	$\left[m^2 / s \right]$
c_p	specific heat capacity	$\left[J / (kg \cdot K) \right]$
k	thermal conductivity	$\left[J / (s \cdot m \cdot K) \right]$
$\mathcal{L}_v$	latent heat of vaporization	$\left[J / kg \right]$
$\dot{\iota}$	mass evaporation rate	$\left[kg / s \right]$
r	radial coordinate	$\left[m \right]$
R	gas constant	$\left[J / (kg \cdot K) \right]$
t	time	$\left[s \right]$
T	temperature	$\left[K \right]$
u_r	radial velocity	$\left[m / s \right]$
$\dot{\iota}$	volumetric heat production rate	$\left[J / \left(s \cdot m^3 \right) \right]$

Greek

γ	surface tension	$\left[N/m \right]$
δ	thickness of the gel layer	$\left[m \right]$
ΔP	pressure drop across the gel layer	$\left[Pa \right]$
ρ	density	$\left[kg / m^3 \right]$
σ	stress in the gel layer	$\left[Pa \right]$
ω_α	mass fraction of species α	
$\dot{\iota}$	volumetric mass production rate of species i,	$\left[kg / \left(s \cdot m^3 \right) \right]$

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Subscripts

b	bubble
f	liquid fuel component of the gel phase
f_vap	vapour of the liquid fuel component
g	gellant component of the gel phase
fg	gel fuel mixture
s	surface of the droplet
surr	surroundings

1. Introduction

Gel fuels are one of the possible answers to the demand for better and safer fuels. Gel fuels are non-Newtonian fluids prepared by adding a gellant to a liquid fuel. Gellants are rheology modifier used to transform liquid fuels into thixotropic shear thinning fluids with a yield stress behaviour [1]. The gelling agent can be either organic or inorganic. Using an organic gellant means that gellant burns with the fuel and contributes to the overall energy content. Therefore, in terms of energy density, an organic gellant is preferable to an inorganic gellant.

Gel fuels and propellants resemble solids in the absence of shear stress. As a result, gel fuels and propellants can be stored almost like solids. Under shear stress, the viscosity of a gel decreases allowing for atomization and combustion in a similar manner to liquid fuels.

Natan and Rahimi [1] have an extensive review of major aspects of gel propellant research. The review presents a background on gel propellants and discusses the advantages they present over liquid and solid propellants. It deals with the rheological characterization and the theoretical evaluation of the performance of gel propellants, and with the preparation, atomization, ignition and combustion of this type of propellant.

Owing to their particular structure, gels inherit properties from both solid and liquid propellants, and as such are advantageous from the point of view of safety, from the point of view of storage and shelf life and from the point of view of performance.

Gels are safer than solids. Gels are insensitive to impact, friction and electrostatic discharge. The combustion of gels is controllable, thus accidental ignition does not pose a serious danger. Gels are fed to the combustion matters in a manner similar to that of liquid fuels; as a result cracks in the gel structure have no effect, as opposed to solid propellant where cracks in the grain increase the burning area and might lead to unwanted effects such as explosions.

Gels are also safer than liquids. The very high viscosity of the gels during storage, and the low storage pressure immensely reduce leakage risks. Gels are much less volatile than liquids. Consequently, the build-up of toxic gases from a spill is very slow.

In addition to increased safety during operation and in storage, gels demonstrate stability in storage with a long shelf life, and a relatively low level of particle sedimentation.

From the performance point of view, the potential of gel fuels lies in the addition of metal particles. The structure of the gel ensures a good dispersion of the metal particles and prevents particle deposition under the effect of gravitational forces. Metalized gel fuels have an increased impulse and increased density specific impulse compared to neat liquid fuels. Moreover, since the feeding process is similar to that of liquid fuels, gels enable total control over fuel flow rate, and procure throttling ability. This is not possible with solid propellants. Throttling ability makes possible the extension of the effective range with proper energy management, control of acceleration levels, and control of terminal velocity. And finally, unlike a solid motor where the grain shape dictates the casing, packing gel fuels is flexible. The fuel tank can have any shape, thus, through appropriate design and efficient use of available space, the size of the vehicle can be reduced.

Much research was done and is still being conducted to fully understand and characterize gel fuels. Important issues are the synthesis of the gels, their flow properties, the effects of long term fuel storage, the atomization, the spray combustion and the combustion of a single droplet. The understanding of the vaporisation and combustion behaviour of a single droplet would be very beneficial for the understanding and prediction of spray combustion behaviour and for the increase of gel fuel combustion efficiency.

A very important aspect of the combustion of gel fuels was observed by Solomon and Natan [2][3] in a study of the combustion of organic-gellant-based non metalized gel fuel droplets. The experimental study revealed the mechanism of combustion of a droplet of such a fuel. The combustion begins with the gel burning like a homogeneous liquid fuel where the only difference is increased viscosity. After a certain amount of fuel has vaporised, an elastic impermeable film of gellant is formed around the droplet. The film prevents fuel vapours from leaving the surface of the droplet. As a result, the vaporised fuel starts building up inside the film producing bubbles in the fuel droplet. The droplet external surface expands to accommodate the swelling of the droplet caused by the growing bubbles. This continues until the fuel bursts through the film, leading later on collapses. Afterward, the process repeats itself until complete depletion

the fuel and gellant. Metal slurry fuels[4] and certain liquid multi-component fuels show similar behaviour[5]. This cyclic time dependent mechanism is analysed in this paper through the non-reactive vaporisation of a droplet in a hot environment.

Earlier work on the subject was done by Kunin et al.[6] who formulated a model which treated two stages of the droplet vaporisation: the formation of the gellant layer and the formation of the fuel vapour bubble up to the point of the rupture of the external envelope. The work presented here includes all the lifecycle of the fuel drop.

2. The formulation of the model

This section details the formulation of the model. It includes the problem statement, the assumptions made, the governing equations and the boundary conditions. The gel fuel taken into consideration is a hydrocarbon liquid fuel gelled with an organic gellant.

2.1 Problem definition

A hydrocarbon gel fuel generally consists of a single or multicomponent liquid hydrocarbon fuel, a gellant and a small amount of solvent. In order to better understand the phenomena involved, the fuel considered in the model is a binary mixture of a single component liquid fuel and organic gellant. The solvent is not included in the model. This is justifiable since the solvent is very volatile and is present is small amounts and as a consequence it has little effect on the overall process.

A model of the combustion of a gel fuel droplet should be quite similar in principle to any model of the combustion of a liquid fuel droplet, such as the model used by Tsukamoto and Niioka [7]; the conservation laws are universal. However, one must take into account the idiosyncrasies of the gel fuel. The viscosity is very high, this reduces the internal mixing. The fuel consists of at least two components, this causes mass diffusion inside the droplet. Most importantly, the model should reflect the different stages of the gel combustion/vaporisation especially the fluctuating phase.

2.2 Assumptions

To avoid an overcomplicated model some assumptions are needed. A single isolated gel droplet in a hot environment is considered. The gel phase is assumed to be an ideal mixture of a liquid hydrocarbon and an organic gellant of very high viscosity. The effects of internal mixing are assumed to be negligible since the gel is a very viscous medium. It is assumed that there is no dissolution of the surrounding gas phase, taken as an ideal gas at constant pressure, in the gel phase. It is assumed that the Soret and Dufour effects are negligible thus eliminating any coupling between mass and energy transport. In addition to the above, the surroundings are assumed to be stagnant and thermal radiation is not included in the model. The combustion of the droplet is a large group of chemical reactions. However, for the sake of simplicity, the chemical processes are represented by a single step global reaction with a rate that follows the Arrhenius equation. The final assumption needed is that of spherical symmetry, meaning that the conservations laws need only be expressed in the radial direction.

2.3 The stages of the droplet combustion

The governing equations and the boundary conditions are formulated for the various stages of the droplet combustion. The stages are defined in a manner to comply with the experimental observations. The first stage is a non-evaporative heating stage. The droplet, initially at uniform temperature and pressure is heated in an elevated ambient temperature. This stage goes on until the surface temperature of the droplet reaches the boiling temperature of the liquid fuel, the more volatile of the two components of the gel. In this stage, there is neither heat generation nor production of species as a result of chemical reaction. There is also no mass diffusion within the droplet because there is no change in the concentration distribution in the droplet. This is a result of the assumption that no vaporization takes place during this stage.

 The second stage begins when the surface temperature reaches the boiling temperature of the more volatile liquid fuel. The heat transfer from the surroundings to the droplet leads to the vaporization of the liquid fuel and to the formation of a gellant layer near the surface of the droplet. This stage goes on until the fuel vapour cannot go through the gellant layer. This occurs when the gellant concentration at the droplet surface reaches a certain critical value. At this point this value is chosen arbitrarily and treated a parameter, as is the initial gel layer thickness. From this stage on, the production of species and energy through chemical reaction takes part in the process. This phase is accompanied by a reduction in the radius of the droplet due to the loss of mass.

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The third stage begins when the surface gel concentrations reaches the critical value mentioned above. With the gellant forming an envelope impermeable to the liquid fuel vapours, and the continuous heat flux into the droplet, the liquid fuel keeps on vaporising, however, the fuel vapours are trapped inside droplet and form an expanding bubble. As the production of fuel vapour continues, the pressure inside the droplet rises until the gellant envelope is ruptured and the vapours burst out.

After the jetting of the fuel vapours, the remaining fuel reforms a spherical droplet, assumed to be homogeneous, and the second and third stages are repeated until all the liquid fuel is depleted. Afterwards, the gellant also vaporises and burns. It is assumed that the gellant begins vaporiing only after all the liquid fuel is depleted.

2.4 The governing equations in the gel phase

The gel phase consists of two species: the liquid fuel, denoted by the subscript **f**, and the gellant denoted by the subscript **g**. The species conservation equation is written in eq.(1) for the liquid fuel. It can also be expressed in terms of the gellant. The energy conservation equation is expressed in eq.(2).

$$\frac{\partial \omega_f}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(\mathscr{D}_{fg} r^2 \frac{\partial \omega_f}{\partial r} \right) \tag{1}$$

$$\rho c_p \frac{\partial T}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 k \frac{\partial T}{\partial r} \right) \tag{2}$$

In Eq.(2), the physical properties ρ, c_p, k are those of the mixture.

2.5 The governing equations in the gas phase

The surrounding gas phase includes the fuel vapour, air (nitrogen and oxygen), and combustion productions (carbon dioxide and water vapour). The conservation laws for mass, energy and species are written in Eqs. (3), (4) and (5) respectively. An equation of state is also required, and for an ideal gas it is given in Eq. (6).

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \rho u_r \right) = 0 \tag{3}$$

$$\rho c_p \left(\frac{\partial T}{\partial t} + u_r \frac{\partial T}{\partial r} \right) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 k \frac{\partial T}{\partial r} \right) + \dot{\iota} \tag{4}$$

$$\frac{\partial \rho \omega_i}{\partial t} + \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \rho u_r \omega_i \right) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \rho \mathscr{D}_i \frac{\partial \omega_i}{\partial r} \right) + \dot{\iota} \tag{5}$$

$$p = \rho R T \tag{6}$$

The subscript i refers to the various species in the surroundings of the droplet. The terms $\dot{\iota}$ and $\dot{\iota}$ are the source terms (heat and mass production rates) as a result of the chemical reaction. In case thermal radiation is taken into account, it will influence the term $\dot{\iota}$.

2.6 Stage characteristics and boundary conditions

At the centre of the droplet, spherical symmetry dictates all gradients be equal to zero. At the far field, the temperature is equal to the ambient temperature, the chemical composition is that of air (oxygen and nitrogen only for simplicity), all the other species have a concentration of zero The boundary conditions at the interface between the gel and the gas phase, remain to be formulated. The subscript **S** is used to denote the surface of the droplet. The boundary conditions and the process behaviour can be determined for each of the combustion stages.

During the first stage, only heating takes place, and thus only the equation of energy need be solved. At the surface the following conditions apply:

$$T\left(r \to r_s^-\right) = T\left(r \to r_s^+\right) \tag{7}$$

$$\left(k_{fg}\frac{\partial T}{\partial r_s}\right)_{r=r_s} = \left(k_{surr}\frac{\partial T}{\partial r_s}\right)_{r=r_s} \tag{8}$$

Here k_{fg} is the thermal conductivity of gel fuel mixture, and k_{surr} is the thermal conductivity of the surrounding gaseous phase. The first stage ends when $T\left(r_s\right)$ reaches the boiling temperature of the liquid fuel.

During the second stage, the liquid fuel evaporates and diffuses into the surrounding gas while a gellant layer forms. The continuous temperature condition, Eq.(7), naturally holds in this stage too. The remaining conditions arise from mass and energy conservation considerations. Keeping in mind the assumption that during this stage only the liquid fuel component evaporates, the heat input into the droplet leading to a mass evaporation rate of $\dot{\iota}$ is:

$$\dot{\iota}\frac{\mathscr{L}}{4\pi r_s^2} - \left(k_{surr}\frac{\partial T}{\partial r}\right)_{r=r_s^+} - \left(k_{fg}\frac{\partial T}{\partial r}\right)_{r=r_s^-} \tag{9}$$

$$u_r\left(r_s\right) = \frac{\dot{\iota}}{4\pi r_s^2 \rho_{f\_vap}} \tag{10}$$

The subscript "f_vap" refers to the gaseous phase. The mass flux out of the droplet at the surface prescribes a concentration gradient at the droplet interface according to Fick's Law:

$$\frac{\dot{\iota}}{4\pi r_s^2} - \nu_{fg}\mathscr{D}_{fg}\frac{\partial \omega_f}{\partial r}\bigg|_{r=r_s^-} \tag{11}$$

$$\omega_{f\_vap}\left(r_s^+\right) = 1, \quad \omega_i\left(r_s^+\right) = 0 \quad i \neq f\_vap \tag{12}$$

The evaporated fuel mass is equal to the integral of $\dot{\iota}$ over time. The second stage ends when the mass fraction of the gellant at the droplet surface reaches the prescribed critical value.

During the third stage, the fuel vapours cannot pass through the gellant layer to the surroundings and form an expanding bubble inside the droplet. The gel fuel mixture concentration distribution is not of much interest and the species conservation equation inside the droplet is not solved for the third stage. No gases leave the droplet during this stage; no diffusion through the droplet surface takes place. Therefore, the gradients of the gas species mass fractions are all zero at the droplet surface as is the velocity of the vapour near the surface:

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$$\left.\frac{\partial \omega_i}{\partial r}\right|_{r=r_s^+} = 0 \tag{13}$$

$$u_r\left(r_s\right) = 0 \tag{14}$$

At this stage, it is safe to assume that the droplet has already been heated to a uniform temperature equal to the boiling temperature of liquid fuel.

$$T\left(r \rightarrow r_s^-\right) = T\left(r \rightarrow r_s^+\right) = T_b \tag{15}$$

Since the temperature gradient inside the bubble is zero, the bubble grows as the fuel evaporates according to:

$$\dot{r} \qquad \pi r_s^2 \left(k_{surr}\frac{\partial T}{\partial r}\right)_{r=r_s^+} \tag{16}$$

The accumulated mass of fuel vapours equal to m_{vap} is a function of time and can be found as a part of the solution process. As the bubble grows and the vapour accumulate inside the droplet, the stress on the gellant envelop grows until it reaches its rupture strength and the bubble bursts through the gellant layer leading to an abrupt rise in the fuel vapour concentration near the droplet surface.

With the mass of fuel evaporated during the second stage known at any time t, the droplet radius and the thickness of the gellant layer described by Kunin et al.[6]. This stage ends when the stress in the gellant envelope reaches the rupture stress. Assuming that the surface tension is the same at the outer surface of the drop and at the outer surface of the layer, the pressure difference between the bubble and the surroundings can be found using the Young-Laplace equation:

$$\Delta P = \gamma\left(\frac{1}{r_s} + \frac{1}{r_b}\right) \tag{17}$$

With the pressure drop across the layer is known, it is possible to calculate the tensile stress acting on the envelope treating it like a thin walled spherical pressure:

$$\sigma = \frac{r_s \Delta P}{\delta} \tag{18}$$

3. Simplified implementation and results

The results in this paper are for vaporisation only. It is assumed that no ignition occurs and no chemical reaction takes place. Looking at the boiling of the droplet separately from the combustion could help understanding the particular nature of the combustion of a gel fuel droplet.

The composition chosen to simulate the gel fuel is a mixture of 85% mass n-octane and 15% mass castor oil.

At $t = 0$ the droplet is inserted into stagnant air at a pressure of $1\,atm$ and temperature of $2000\,K$. The transport properties of all gaseous species are assumed to be equal to those of air at 2000K. In addition The Lewis number in the gas phase is assumed equal to unity.

The gel mixture is assumed to be an ideal mixture. The properties of an ideal mixture are evaluated by weight averaging the properties of the components. The properties are assumed to be independent of temperatures.

3.1 Complete life time for different drop sizes

This section shows the results obtained for droplets of diameters $100\,\mu m$, $150\,\mu m$ and $200\,\mu m$ at an initial temperature of 300K, starting from the introduction into the hot environment at $t = 0$ and up to complete depletion. These results are referred to as set 1. The values of the parameters used to obtain these results are listed Table *1*. The durations of the various stages are shown in Table *2*. It can be verified that all durations are scalable to the total burning time.

The history of the outer radius, the surface temperature and of the concentration of the gellant can be seen in Figure 1. The different stages are marked on the figure. The fluctuating stage can be seen in more details in the next section. The graphs in the figure were obtained for a droplet with an initial radius of 50μm. Graphs for other sizes are not shown because they only differ by the time scale.

Table 1: Parameters used to obtain results set 1

Parameter	Value
Initial droplet radii	50, 75, 100 μm
Initial droplet temperature	300 K
Critical surface gellant concentration	80%
Impermeable gel layer initial thickness	2 μm
Impermeable layer surface tension	10 mN/m
Impermeable layer rupture stress	25 kPa
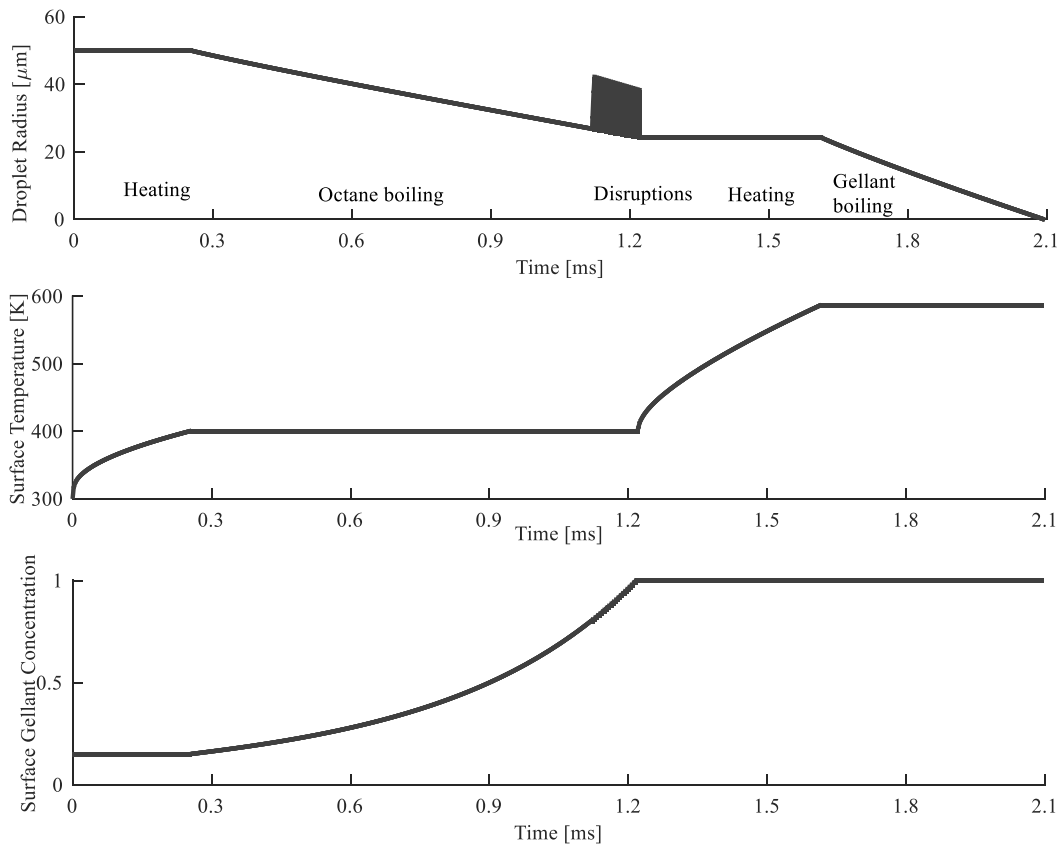
Figure 1: Lifetime of a 100μm diameter droplet (set1)

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3.2 Stages II and III: evaporation of n-octane

The results shown next were obtained for a droplet with a diameter of $100\ \mu m$ at an initial temperature of 400K, the boiling point of n-octane at one atmosphere. Two sets of results are presented: set 2 with the thickness of the gellant envelope, before the swelling, is either 1 or 2 μm, and set 3, where the surface gellant concentration considered impermeable is either 80% or 90%. The other parameters are listed in *Table 3* and *Table 4*

In all four cases, the time required for the depletion of the liquid fuel is about 1.145 *ms*. This is in fact the durations of stages II (conventional boiling) and III (fluctuations and disruptions). This indicates that the properties arbitrarily chosen for the gellant layer, do not affect the whole combustion process much, but only stage III. In Figure 2 and in Figure 3 one can see this influence.

For example, if the gellant layer with thinner than assumed, than the frequency of the fluctuations would be much higher, because the rupture stress would be reached quicker. Stage III for the case of a 2 μm layer consisted of 21 cycles, whereas in the case of a 1 μm layer, it consisted of 160 cycles for the same duration of time.

On the other hand, the gellant concentration at the surface chosen to be critical (above which vapours cannot pass), influences the duration of stage III and not the frequency. When the critical concentration is 80%, stage III consisted of 21 cycles, over a period of about 0.1*ms*. For a critical concentration of 90%, stage III lasted about 0.05 *ms*, with 10 cycles. This shows that the frequency of the fluctuations did not change.

Table 2: Durations of the various stages (set 1)

	50 μm	75 μm	100 μm
Total burning time	2.1 *ms*	4.7 *ms*	8.4 *ms*
Initial heating	0.25 *ms*	0.53 *ms*	1.00 *ms*
Conventional vaporisation	0.9 *ms*	1.9 *ms*	3.5 *ms*
Fluctuating stage	0.11 *ms*	0.24 *ms*	0.40 *ms*
Heating the gellant	0.40 *ms*	0.88 *ms*	1.60 *ms*
Evaporation of the gellant	0.48 *ms*	1.1 *ms*	1.9 *ms*

Table 3: Parameters used to obtain results set 2

Parameter	Value
Initial droplet radius	50μm
Initial droplet temperature	400 K
Critical surface gellant concentration	80%
Impermeable gel layer initial thickness	1, 2 μm
Impermeable layer surface tension	10 *mN/m*
Impermeable layer rupture stress	25 *kPa*

Table 4: Parameters used to obtain results set 3

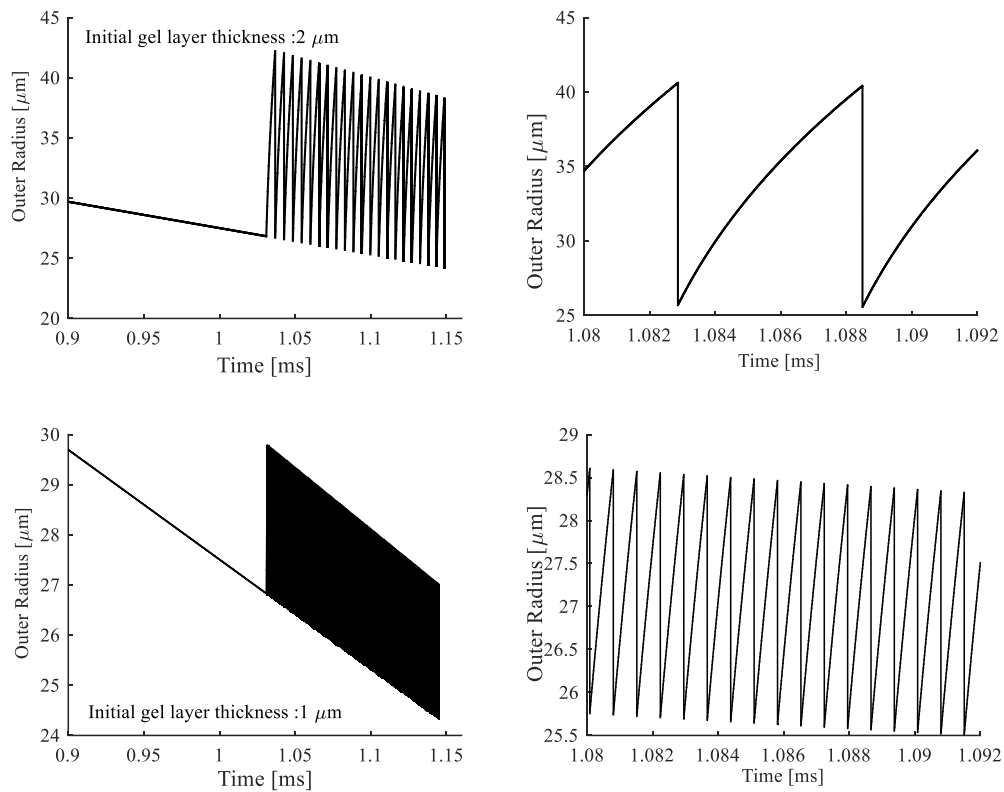| Parameter	Value
Initial droplet radius	50μm
Initial droplet temperature	400 K
Critical surface gellant concentration	80%, 90%
Impermeable gel layer initial thickness	2 μm
Impermeable layer surface tension	10 *mN/m*
Impermeable layer rupture stress	25 *kPa*

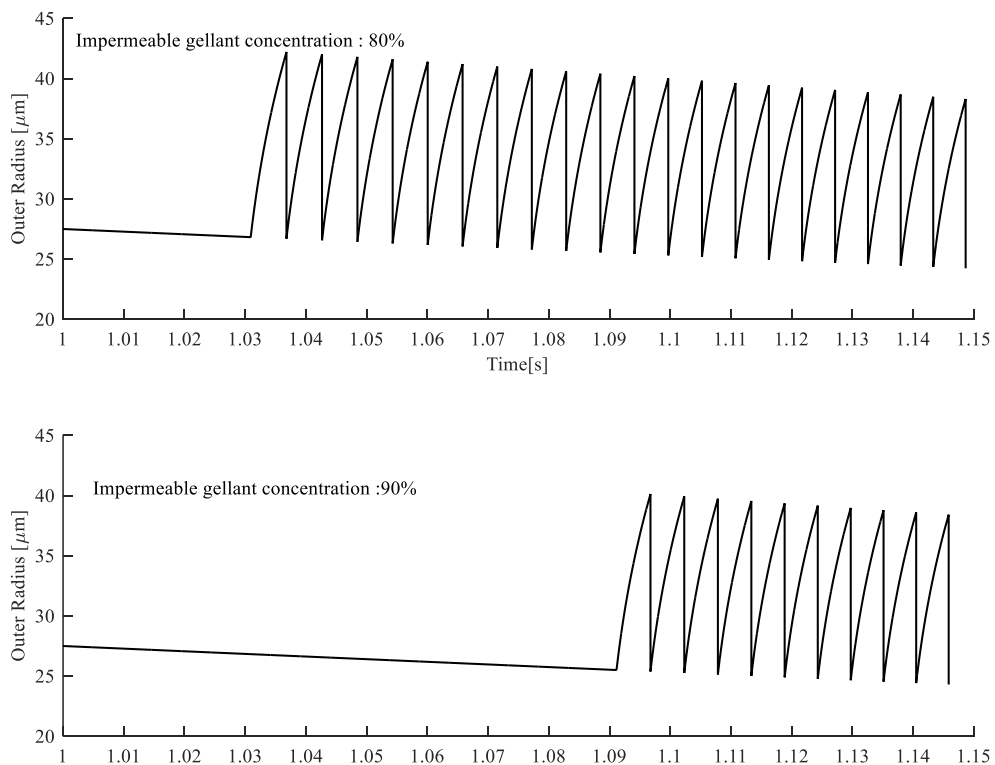Figure 2: Influence of the gel layer thickness (set2)

Figure 3: Influence of the critical suface gellant concentration (set 3)

4. Conclusion

A mathematical model for the combustion of an organic gellant based hydrocarbon gel fuel isolated droplet was presented. The model consists of the conservation laws for the droplet and the surroundings and of stage specific interface conditions. The stages treated correspond to the stages observed experimentally in the combustion of a gel fuel droplet: heating, formation of a gellant layer, formation of a fuel vapour bubble, rupture of the droplet surface causing a rapid expulsion of fuel vapours and the collapse and reformation of the drop. The stages are repeated until the depletion of the fuel. The equations presented were solved for heating without a chemical reaction. The analysis of the influence of different factors showed that the properties of the gellant envelope that forms are d the fuel droplets are only important for the details of the periodic stage, but have little influence on the complete vaporisation process.

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