

Theoretical and Numerical Analysis of Fuel Droplet Combustion Parameters via Different Combustion Models

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Received on: 2/6/2008

Accepted on: 4/9/2008

Abstract

The study introduces a theoretical analysis and numerical solution for the combustion of two kinds of hydrocarbon fuel droplet inside the combustion chamber. The study employs three mathematical models to analyze the combustion process, conventional (classical) model, transient model, and moving droplet model. The combustion process of a stagnant droplet in the steady state was analyzed in the classical model, while, in the transient model, it was assumed that there is a period of time in the stages of the droplet combustion in which the droplet is heated before combustion. For the moving droplet model, the film boundary approximation was incorporated to express the effects of the relative motion on the combustion process parameters. The effect of change in temperature on the thermo-physical properties of the fuel was adopted through the three models. For the classical and moving droplet models, a convenient approximation was adopted for the heat transferred inside the droplet.

Computer programs were created to evaluate the required properties, solving the ordinary differential equations evaluated from heat and mass transfer balances, and then construct systems of non-linear equations.

The three models show that thermo physical properties are strong functions to reference temperature. The transient model shows that the period of droplet heat up is most effective. For the moving droplet combustion model it was shown that the relative movement between droplet and ambient surrounding gas enhanced the mass burning rate and reduced the droplet lifetime. The film theory approach was adopted in moving droplet model.

Key Words : combustion, fuel droplet, models of combustion

Introduction

Droplet burning has relevance to many practical combustion devices, including, rockets, and gas-turbine engines, as well as oil-fired boilers, furnaces, and process heaters. In these devices, spray combustion is the dominant feature [Turns,2000]. The problem of droplet burning includes both the evaporation and the combustion process. Solving problems concerning droplet evaporation and combustion needs the use of mass transfer and thermodynamic laws and equations. In all the above systems, liquid fuels and/or oxidizer are usually injected into the combustion chamber as a spray of droplets, which undergoes process [Lamna, et.al.,2004]. Research on the gasification, oxidation, and dynamics of fuel droplet commands both practical and fundamental interest to energy and combustion science. On the practical aspect one recognizes that petroleum oil constitutes a significant share of the world energy supply [Law, 1982]. According to law, droplet combustion is a problem involving complex chemically reacting multicomponent two-phase flows with phase change, rich in physical and chemical phenomena typically to be studied. Theories and studies concerning the evaporation and combustion fuel droplets took into account a spherical droplet (motionless or moving). It is cold and is placed in a hot stagnant, gravity free environment, [Law,1982]. No forced or natural convection is concerned. Heat is transferred from the ambience towards the cold surface of droplet, where some of it is used to

gasify the droplet and the remaining is transferred to the interior of droplet to heat it up. According to Law, through the above mechanism, a liquid mass can be converted to vapor and eventually dispersed to ambience, with the rate controlling process as heat and mass diffusion. The ignition of the droplet causes a reaction or oxidation of the fuel with heat generated to be transferred both outward and inward. with D^2 -law [Godsave,1953, Spalding,1953, Goldsmith & Penner,1954] with its simple assumptions and some inadequacies. Then different approaches were conducted to develop the D^2 -law. Some included the unsteady droplet heating and combustion [Law & Sirignano,1977]. Others included internal circulation, transient heating, multicomponent fuel, radiation, high pressure, sprays, etc., introducing modern computational models [Williams & Sirignano,1983, Abraham,2001, Dombrovsky & Sazhin,2003, Hohmann & Ranz,2003,Sazhin,et.al.,2004,Sazhin,et.al.,2005,andYan&Aggarwal,2006].

Theories Classical Droplet

Combustion Model: D^2 -law theory for droplet combustion established the basic fundamentals for droplet combustion model. One of the assumptions of that theory is that thermophysical properties are constant for all temperature of droplet surface and it is surrounding, so that its more suitable to consider the dependence of thermophysical properties to a reference temperature which vary with the variation of surface and environmental

temperature. This behavior will be considered later through this work to obtain its effects on the main parameters of combustion process such as mass burning rate. Mass burning rate represents the amount of fuel that is burned during the combustion process. It is dependent on the mass vaporization, rate which is the amount of fuel that evaporates from the surface of the droplet as a result of heat that is transferred to the surface (or droplet) because of the burning fuel in the process. Mass burning rate represents the combustion process and affects other parameters in the process such as flame radius, which is the radius of flame front that is surrounding the burning fuel droplet. The flame radius can be expressed as flame stand off ratio. It is a ratio of the radius of flame to the radius of the individual liquid droplet, and that can show the position of flame front from the surface of the droplet at any time of droplet combustion process. Flame temperature is the temperature of the flame front that is surrounding the fuel droplet. Knowing this temperature can provide primary knowledge to the heat that is transferred inward and outward the fuel droplet, and that heat is dependent on the mass burning rate. In the classical model for combustion, mathematical model will be considered and solved for mass and heat transfer for the gas-phase of droplet combustion process. The solution will provide the basic equations that relates the main characteristic parameters, which will be solved numerically to evaluate their values overall the combustion process. A suitable approach for the heat that is

transferred to the droplet interior will be considered.

Transient Droplet Combustion

Model: The study of transient combustion process is required to understand the effects of heat up period on the combustion parameters. Heat up period is the period of time that the droplet surface is raised from its initial temperature to a steady temperature (boiling temperature) by gaining heat from its surrounding flame. In heat up period, heat that is transferred to the droplet can be divided into two parts, one part used for heating the droplet liquid to its steady temperature, and the other part for vaporizing the liquid fuel, causing dominant effects on the main parameters of combustion process such as mass burning rate. Surface temperature of the droplet vary with time until it reaches to a steady temperature. This variation can affect latent heat of vaporization that can be considered to become slowly –time varying latent heat of vaporization and can be expressed as a function of surface temperature, which, in turns, can be expressed as a function of time, and the numerical substitution can be used to simplify this dependence. Numerical computation will be used to solve the basic equations which relates the basic parameters evaluated from the solution of mass and heat transfer equations for the mathematical model.

Moving Droplet Combustion Model:

The development of spray evaporation and combustion theories requires consideration of the effects of droplet relative motion with respect to the ambient gas on the heat and mass

transfer rates. The results for quiescent flow will no longer hold true and effects of forced convection must be considered. Many investigators [Ranz & Marshall,1962] and [Agoston, et.al.,1957] studied these effects experimentally and predicted empirical correction factors to evaluate mass burning rates of moving droplet as a correction of mass burning rates of a stagnant droplet. For this reason a new approach that describes the behavior of the combustion process parameters under the effects of relative motion of the droplet have been appeared. The mathematical model that will be presented later was constructed to describe the mass and heat transfer equations with appropriate approach to consider the effects of relative motion of the burning droplet. These equations will be solved to obtain the main equations that relate the main characteristic parameters of the combustion process. They will be used to construct the numerical solution to evaluate the values of these parameters overall the combustion process. The effects of temperature on the thermophysical properties will be considered by evaluating these properties under different values of reference temperature, and appropriate approach for the heat that is transferred to the droplet will be analyzed.

Mathematical Work:

Classical Droplet Combustion Model: Problem Statement

Spherical fuel droplet that has the initial radius r_0 is burning and is surrounded by thin flame sheet that has

a radius r_f and is surrounded by infinite medium of oxidizing atmosphere to the radius ∞ .

Liquid fuel is vaporized at the droplet surface, the droplet is the source of vapor in the system, vapor is convecting and diffusing outward toward the flame. The source of convecting species at the droplet surface is the specific volume change associated with phase change at the surface, while the oxidizer diffuses inward from the ambient environment to the flame sheet [Kuo,1986]. The fuel and the oxidizer react stoichiometrically, and the chemical kinetics are assumed to be infinitely fast, so that the fuel vapor mass fraction Y_F is maximum at the droplet surface and monotonically decrease to zero at the flame sheet, where the fuel is totally consumed. The oxidizer mass fraction Y_{ox} mirrors this, being a maximum far from the flame and decrease to zero at the flame sheet. If the fuel is burning at a medium of pure oxygen then the value of mass fraction of the oxidizer at infinity is unity. Most of combustion systems are working in air rather than in pure oxygen, so that the environment will be considered as air in the calculations and Y_{ox} will be calculated. Heat is generated at the reaction on the flame sheet causing the flame temperature T_f to be the highest temperature in the system. Heat is transported via conduction and radiation outward from the flame to infinity and inward back to the droplet surface causing vaporization. The heat deposited at the droplet surface is balanced by the evaporation process at

the vapor-liquid interface. There are three important temperatures in the system, the droplet surface temperature T_s , the flame temperature T_f , and the temperature of the medium at infinity T_∞ . The combustion products have their maximum concentration at the flame sheet (unity) diffusing both inward toward the droplet and outward away from the flame [Turns,2000].

The major assumptions of this model are [Law, 1982]:

1. Spherically symmetric : forced and natural convection are neglected, this reduces the analysis to one dimension.
2. No spray effects : the droplet is an isolated one, immersed in an infinite oxidizing environment.
3. Isobaric process : at 1 atm.
4. Flame-sheet combustion : chemical reaction rates are much faster than gas-phase diffusion rates such that the flame is of infinitesimal thickness and can be treated simply as a sink for the reactants and a source of chemical heat released.
5. Gas-phase is quasi-steady.
6. Simultaneous fuel gasification and consumption : this assumes that the amount of fuel gasified at the surface is instantly consumed at the flame, it neglects the accumulation of fuel vapor between the droplet and the flame.
7. Single fuel species : thus it is unnecessary to analyze liquid-phase mass fraction.

8. Saturation vapor pressure at the droplet surface.
9. No soot, Dufour, sooting, and radiation effects.
10. Thermophysical properties are functions of temperature only.

Conservation of Mass: With the assumption of quasi-steady burning, the mass flow rate $\dot{m}(r)$ is constant, independent of radius; thus:

$$\dot{m} = \dot{m}_F = \rho v_r A = \text{constant}$$

For the inner region bounded between the zone ($r_s < r < r_f$), Fick's law of diffusion can be applied to the inner region :

$$\dot{m}'_A = Y_F(\dot{m}'_A + \dot{m}'_B) - \rho D_{AB} \nabla Y_A$$

Which can be simplified to;

$$\frac{dY_F}{dr} = \frac{-\dot{m}_F}{4\rho\pi D} \frac{1 - Y_F}{r^2} \tag{1}$$

With the boundary conditions;

$$Y_F(r_s) = Y_{F,s} \tag{2.a}$$

$$Y_F(r_f) = 0 \tag{2.b}$$

The outer region is that bounded by the zone ($r_f < r < \infty$), the important diffusing species is the oxidizer, Fick's law of diffusion can be applied to the outer region :

$$\dot{m}'_{ox} = Y_{ox}(\dot{m}'_{ox} + \dot{m}'_{Pr}) - \rho D_{AB} \nabla Y_{ox}$$

It can be written as:

$$\frac{dY_{Ox}}{dr} = \frac{\dot{m}_F}{4\pi\rho D} \frac{(Y_{Ox} + \nu)}{r^2} \quad (3)$$

With the boundary conditions;

$$Y_{Ox}(r_f) = 0 \quad (4.a)$$

$$Y_{Ox}(\infty) = Y_{Ox\infty} \quad (4.b)$$

Conservation of Energy : The Shvab-Zeldovich form of the energy equation is used. Since the chemical reactions occurs at the boundary, i.e., the flame sheet, the reaction rate term is zero both inside the flame and outside the flame [Turns,2000]:

$$\frac{1}{r^2} \frac{d}{dr} \left[r^2 (\rho v r) \int C_p dT - \rho D \frac{d}{dr} \int C_p dT \right] = - \sum h^o f_i \dot{m}_i$$

This equation can be re-arranged and written as:

$$\frac{d_2 T}{dr^2} = \left(\frac{\dot{m}_F C_{p_g}}{4\pi k_g r^2} - \frac{2}{r} \right) \frac{dT}{dr} \quad (5)$$

With the boundary conditions for inner region:

$$T(r_2) = T_s \quad (6.a)$$

$$T(r_f) = T_f \quad (6.b)$$

And for outer region:

$$T(r_f) = T_f \quad (7.a)$$

$$T(\infty) = T_\infty \quad (7.b)$$

Energy Balance at Droplet Surface :

Heat is conducted from the flame through the gas-phase to the droplet surface. Some of this heat is used to vaporize the fuel, while the remaining is

conducted into the droplet interior. Mathematically:

$$Q_{g-i} = \dot{m}_F h_{fg} + Q_{i-i} \quad (8)$$

Where :

$$Q_{g-i} = - \left[4\pi r_s^2 k_g \frac{dT}{dr} \right]_{r_s}$$

The droplet is assumed to be consisting of two zones, an interior zone existing uniformly at its initial temperature T_o , and then surface layer at the surface temperature T_s . For this it is called " onion-skin model ":

$$Q_{i-i} = \dot{m}_F C_{p_i} (T_s - T_o)$$

So that, equation (8) becomes :

$$- \left[- k_g 4\pi r_s^2 \frac{dT}{dr} \right]_{r_s} = \dot{m}_F (h_{fg} + C_{p_i} (T_s - T_o)) \quad (9)$$

Energy Balance at Flame Sheet :

Since the flame temperature is the highest temperature in the system, heat is conducted both toward the droplet, Q_{f-i} , and away to infinity, $Q_{f-\infty}$. The chemical energy released at the flame is taken into account by using absolute enthalpy fluxes for the fuel, oxidizer, and products. A surface energy balance at the flame sheet can be written as:

$$\dot{m}_F \Delta h_c = Q_{f-i} + Q_{f-\infty} \quad (10)$$

Where Q_{f-i} & $Q_{f-\infty}$ can be represented as :

$$Q'_{f-i} = k_g 4\pi r_f^2 \frac{dT}{dr} \Big|_{r_f^-}$$

$$Q'_{f-\infty} = -k_g 4\pi r_f^2 \frac{dT}{dr} \Big|_{r_f^+}$$

Solution : solving equation (1) with the boundary conditions (2.a,b) for \dot{m}'_F gives:

$$\dot{m}'_F = \frac{4 \ln\left(\frac{1}{Y_{Fs} - 1}\right) \pi \rho D r_s}{1 - \frac{r_s}{r_f}} \quad (11)$$

Solving equation (3) with the boundary conditions (4.a,b) for r_f presents:

$$r_f = \frac{-\dot{m}'_F}{\pi \rho D \ln\left(\frac{v}{v + Y_{O_{2max}}}\right)} \quad (12)$$

Solving equation (5) with the boundary conditions (6.a,b) gives the temperature distribution of inner region, which can be derived with respect to r, and the resulted equation can substituted into equation (9) which can be solved for T_s to obtain:

$$T_s = f(\dot{m}'_F, T_f, r_s, r_f) \quad (13)$$

Solving equation (5) with the boundary conditions (7.a,b) gives the temperature distribution of outer region, which can be derived with respect to r, and the resulted equation can substituted into equation (10) which can be solved for T_f to obtain:

$$T_f = f(\dot{m}'_F, T_s, r_s, r_f) \quad (14)$$

Assumption(8) gives the equilibrium between the liquid and vapor-phase of the fuel at the surface, and applying Clausius-Clapeyron equation gives :

$$Y_{Fs} = \frac{A \exp\left(\frac{-B}{T_s}\right) M_{wF}}{A \exp\left(\frac{-B}{T_s}\right) M_{wF} + \left[P - A \exp\left(\frac{-B}{T_s}\right)\right] M_{wO_2}} \quad (15)$$

The droplet life time was obtained using the mass balance, which states that the rate at which the mass of the droplet decreases is equal to the rate at which the liquid is vaporized [Williams, 1965] :

$$\frac{dm_d}{dt} = -\dot{m}'_F \quad (16)$$

Where :

$$m_d = \rho_l V = \frac{4}{3} \pi r_s^3 \rho_l$$

And \dot{m}'_F can be expressed as a function of r_s :

$$\dot{m}'_F = 4 \pi \rho D r_s \ln\left(\frac{1}{\frac{v}{v + Y_{O_{2max}}}}\right)$$

Equation (16) can be written as :

$$\frac{dr_s}{dt} = \frac{-3\rho D}{r_s \rho_l} \ln\left(\frac{1}{\frac{v}{v + Y_{O_{2max}}}}\right) \quad (17)$$

Transient Droplet Combustion Model

Problem Statement : In order to formulate the model that describes the droplet heating and combustion, the major assumptions will be [Chigier,1981]:

1. Constant, stagnant, unbounded atmosphere.
2. Combustion process is spherically symmetric and isobaric.

3. The combustion process is following the double-film theory.
4. Fuel and oxidizer meets in a stoichiometric ratio at the flame front.
5. The reaction kinetics is fast compared with gas-phase transfer.
6. Physical properties will be calculated at reference temperature.
7. Single component droplet with no liquid-phase flows.
8. No soot formation, negligible radiation.

The problem is analyzed as follows. At time $t = 0$, the droplet with radius $r_s = r_{s0}$ and temperature $T = T_{s0}$ is igniting in constant, unbounded atmosphere characterized by its temperature T_∞ , pressure P_∞ , and oxidizer mass fraction $Y_{ox\infty}$. The outwardly diffusing fuel vapor reacting stoichiometrically and completely with the inwardly diffusing oxidizer gas at a thin flame front located at r_f . For analyzing the inner and outer regions, mass and heat balance will be obtained considering the non-dimensional quasi-steady phase equations [Law,1976].

Conservation of Mass : Inner region is expressed by non-dimensional equation [Law,1976]:

$$\dot{m}_F Y_F - \dot{r}^2 \frac{dY_F}{d\hat{r}} = \dot{m}_F \tag{18}$$

Where :

$$\dot{m} = \frac{\dot{m}'}{4\pi\rho D r_s}, \hat{r} = \frac{r}{r_s}$$

With the boundary conditions:

$$Y_F(1) = Y_{F_s} \tag{19, a}$$

$$Y_F(\hat{r}_f) = 0 \tag{19, b}$$

Outer region is represented by the non-dimensional equation[Law,1976]:

$$\dot{m}_F Y_{ox} - \dot{r}^2 \frac{dY_{ox}}{d\hat{r}} = -\dot{m}_F v \tag{20}$$

With the boundary conditions:

$$Y_{ox}(\hat{r}_f) = 0 \tag{21, a}$$

$$Y_{ox}(\infty) = Y_{ox\infty} \tag{21, b}$$

Conservation of Energy :for the inner region:

$$\dot{m}_F (\hat{T} - \hat{T}_s) - \dot{r}^2 \frac{d\hat{T}}{d\hat{r}} = -\dot{m}_F \bar{Q} \tag{22}$$

Where :

$$\bar{Q} = \frac{Q}{h_{fg}}, \hat{T} = \frac{C_p T}{h_{fg}}$$

With the boundary conditions :

$$\hat{T}(1) = \hat{T}_s \tag{23, a}$$

$$\hat{T}(\hat{r}_f) = \hat{T}_f \tag{23, b}$$

For the outer region :

$$\dot{m}_F (\hat{T} - \hat{T}_s) - \dot{r}^2 \frac{d\hat{T}}{d\hat{r}} = -\dot{m}_F (\bar{Q} - \bar{H}) \tag{24}$$

Where :

$$\tilde{H} = \frac{\Delta h_c}{h_{fg}}$$

And the boundary conditions :

$$\tilde{T}(\tilde{r}_f) = \tilde{T}_f \tag{25, a}$$

$$\tilde{T}(\infty) = \tilde{T}_\infty \tag{25, b}$$

Solving equation (18) with the boundary conditions (19.a,b) for \tilde{m}_F and expressing with dimensional form:

$$\dot{m}_F = \frac{4 \ln(1 - Y_{F_s}) \pi \rho D r_s}{\frac{r_s}{r_f} - 1} \tag{26}$$

Solution After solving equation (20) for r_f and applying boundary conditions, equation (21,a,b), expressing with dimensional form:

$$r_f = \frac{-\dot{m}_F}{4 \ln\left(\frac{v}{v + Y_{O_{xxx}}}\right) \pi \rho D} \tag{27}$$

T_f can be expressed in dimensional form after solving equation (22) with boundary conditions (23,a,b) as :

$$T_f = \frac{Cp_g T_s - Q + \exp\left(\frac{-\dot{m}_F}{4\pi\rho D r_f}\right) Q \exp\left(\frac{\dot{m}_F}{4\pi\rho D r_s}\right)}{h_{fg}} \tag{28}$$

Where, Q expressed after solving equation (24) with the boundary conditions (25,a,b), in dimensional form :

$$Q = \frac{Cp_g(T_s - T_s) - \Delta h_c + (\Delta h_c + Cp_g(T_s - T_f)) \exp\left(\frac{\dot{m}_F}{4\pi\rho D r_f}\right)}{\exp\left(\frac{\dot{m}_F}{4\pi\rho D r_f}\right) - 1} \tag{29}$$

The relation of surface temperature with droplet radius can be found using the expression of time varying latent heat of vaporization as :

$$\tilde{Q} = 1 + \frac{\dot{Q}_{sen}}{h_{fg} \dot{m}} \tag{30}$$

Where :

$$\frac{\dot{Q}_{sen}}{\dot{m}} = \frac{\frac{4}{3} \pi r_s^3 \rho_l Cp \frac{dT}{dt}}{-4\pi \rho_l r_s^2 \frac{dr_s}{dt}}$$

Chain rule can be used to reduce one of the derivatives as :

$$\frac{dT_s}{dt} = \frac{dT_s}{d\sigma} \frac{d\sigma}{dr_s} \frac{dr_s}{dt}$$

Where :

$$\sigma = \frac{r_s^2}{r_{so}^2}$$

Substituting into equation (30), and simplifying :

$$\frac{d\tilde{T}_s}{d\sigma} = \frac{3(1 - Q)}{2\sigma} \tag{31}$$

In order to solve this equation to obtain \tilde{T}_s as function of σ (or r_s), the term \tilde{Q} which is function of $(\tilde{T}_s, \tilde{m}_F, \tilde{T}_f, \text{and } \tilde{r}_f)$ must be expressed as function of \tilde{T}_s only, the vapor is saturated at the droplet surface, an independent relation

between Y_{F_s} and \hat{T}_s was given by [Law,1976]:

$$Y_{F_s}(T_s) = P_{\infty}^{-1} \exp\left[\frac{C_p}{R} (\hat{T}_b^{-1} - \hat{T}_s^{-1})\right]$$

Using computational substituting is necessary obtain \hat{Q} as function of \hat{T}_s , then substituting the resulted equation into (31) gives :

$$\frac{d\hat{T}_s}{d\sigma} = \frac{3}{2\sigma} (1 - f(\hat{T}_s))$$

With boundary condition :

$$\hat{T}_s(1) = \hat{T}_o$$

Solving this equation presents $\hat{T}_s = f(\sigma)$, which can be expressed as dimensional form as :

$$T_s = f(r_s) \tag{32}$$

The droplet lifetime could be evaluated as follows:

$$\hat{m}_F = \frac{m}{4\pi\rho_g D r_s}$$

Which can be expressed as :

$$\hat{m}_F = -\frac{4u\rho_l r_s^2 \frac{dr_s}{dt}}{4\pi\rho_g D r_s} \tag{33}$$

Where dt can be expressed as dimensionless form as :

$$\hat{t} = \frac{2\rho_g D}{\rho_l r_{so}^2} t$$

Differentiating :

$$dt = \frac{\rho_l r_{so}^2}{2\rho_g D} d\hat{t}$$

This equation can substituting into equation (33) and r_s can be expressed as dimensional from σ , rearranging the resulted equation gives:

$$d\hat{t} = -\frac{d\sigma}{\hat{m}_F} \tag{34}$$

Moving droplet combustion model

Problem Statement : The essence of film-theory is the replacement of the heat and mass transfer boundary conditions at infinity with the same conditions moved inward to the so-called film radius, δ_m for species and δ_T for energy. The film radii were defined in terms of Nusselt number, Nu , for heat transfer, and Sherwood number, Sh , for mass transfer. Physically, the Nusselt number is dimensionless temperature gradient at the droplet surface, and the Sherwood number is the dimensionless concentration (or mass fraction) gradient at the surface. The film radii are given by [Turns,2000] :

$$\frac{\delta_T}{r_s} = \frac{Nu}{Nu - 2}, \quad \frac{\delta_m}{r_s} = \frac{Sh}{Sh - 2} \tag{35}$$

Conservation of Mass : for inner region mf can be expressed as that for the classical model:

$$\dot{m}_F = \frac{4 \ln\left(\frac{1}{1 - Y_{F_s}}\right) \pi \rho D r_s}{1 - \frac{r_s}{r_f}} \tag{36}$$

Outer region can be expressed as :

$$\frac{dY_{Ox}}{dr} = \frac{m'_F}{4\pi\rho D} \frac{(Y_{Ox} + \nu)}{r^2} \quad (37)$$

With boundary conditions :

$$Y_{Ox}(\delta_m) = Y_{Ox\infty} \quad (38, a)$$

$$Y_{Ox}(r_f) = 0 \quad (38, b)$$

Conservation of Energy : For inner region the surface temperature can be expressed as that of classical model , while for outer region equation (5) can applied with boundary conditions :

$$T(\delta_T) = T_\infty \quad (39)$$

$$T(r_f) = T_f \quad (7. a)$$

Energy Balance at the Flame Sheet : this balance can expressed as equation (10).

Solution : solving equation (37) with the boundary conditions (38,a,b) for rf ,and substituting equation (35) :

$$r_f = \frac{m'_F r_s Nu}{(Nu - 2) \left[\frac{4 \ln \left(\frac{\nu}{\nu + Y_{Ox\infty}} \right) \pi \rho D r_s Nu}{Nu - 2} - m'_F \right]} \quad (40)$$

Solving equation (5) with the boundary conditions (7.a)and (39) gives the temperature distribution of outer region, which can be derived with respect to r, and the resulted equation can substituted into equation (10) which can be solved for T_f , then substitute equation (35) to obtain:

$$T_f = f(m'_F, T_s, r_s, r_f, Nu) \quad (41)$$

The droplet lifetime can be obtained from equation (16), Where m'_F can expressed as a function of r_s :

$$\dot{m}_F = 2 Nu \pi \rho D r_s \left(\ln \left(\frac{1}{1 - Y_{FS}} \right) - \ln \left(\frac{\nu}{\nu + Y_{Ox\infty}} \right) \right) \quad (42)$$

Expressing Nu as :

$$Nu = 2 + \frac{0.555 Re^{0.5} Pr^{0.333}}{[1 + 1.232 / (Re Pr^{1/3})]}$$

An Re as :

$$Re = \frac{2\rho u r_s}{\mu}$$

Substituting these two parameters into equation (42), then substituted in equation (16) gives :

$$\frac{dr_s}{dt} = f(r_s) \quad (43)$$

Calculations

For the three model, the following relations were used for calculate the terms and thermo-physical properties as; for Cp, k, and μ [Andrews & Biblarz,1981]:

$$Cp = \sum_1^{\gamma} a_i T^{i-1}$$

$$k = \sum_1^{\gamma} b_i T^{i-1}$$

$$\mu = \sum_1^{\gamma} c_i T^{i-1}$$

and:

$$k_g = 0.4k_F(T) + 0.6k_{ox}(T)$$

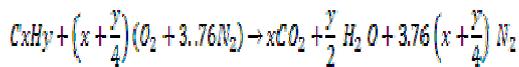
Where k_x for air, For binary diffusion coefficient [Raid, et.al.,1987] :

$$D_{AB} = \frac{3}{16} \frac{(4\pi k_B T / MW_{AB})^{\frac{1}{2}}}{(P/RuT)\pi \sigma_{AB}^2 \Omega_D} f_D$$

The parameters of this equation are listed in reference above, Mass fraction of the oxidizer (Oxygen) at the infinite medium (air) was suggested as followed:

$$Y_{O_{xxx}} = \frac{\text{mol oxidizer} \times MW_{ox}}{\text{mol air} \times MW_{air}}$$

The molecular weights of the fuel and the products that used in the analyses, MW_F and MW_{Pr} , were calculated as:



So :

$$MW_F = 12x + y$$

$$MW_{Pr} = 44x + 9y + 105.28(x + \frac{y}{4})$$

The above relations were obtained at reference temperature as[Sparrow & Gregg,1958]:

$$T_r = T_s + \frac{1}{3} (T_{\infty} - T_s)$$

Numerical Analyses

Computer programs were created to evaluate the required properties, solving the ordinary differential equations evaluated from heat and mass Transfer balances, then constructs systems of non-linear equations as follows; for the classical

model, the program fixed the value of surface temperature as T_{boil} , This is a reasonable assumption when the droplet is burning vigorously after its initial heat-up transient.[Turns,2000, Kuo,1986, kotake & Okazaki,1969, Law, 1982]. The program substituted equation (13) into equation (14) and resolving for T_f , then used the resulted equation with equations (11)and(12) to construct system of non-linear equation, calculating the Jacobian matrix for the system, then solving the system with Newton-Raphson method using the Jacobian. The droplet lifetime was obtained by solving equation (17) using Range-Kutta 4 method with appropriate time interval. For transient model, the program solves dimensionless equations for mass and heat balances, then made numerical substitution to obtain $T_s = f(r_s)$, constructing system of non-linear equations using equations (26),(27),(28),(29),(32) and the equation that related $Y_{F_s} = f(T_s)$, then solving the system with Newton-Raphson method using the Jacobian. Droplet lifetime can be obtained using equation (34). For moving model, the program fixed the value of surface temperature as T_{boil} , The program substituted equation (13) into equation (41) and resolving for T_f , then used the resulted equation with equations (11)and(40) to construct system of non-linear equation, then solving the system with Newton-Raphson method using the Jacobian. For droplet lifetime, Range-Kutta 4 method was used with suitable time interval to solve equation (43).

Results and discussion

The droplet size used in calculations are; $d=100\mu m$ as an initial diameter, and $d=0$ as

a final diameter. The environment conditions are taken as 1500K, and pressure 1 atm., while For the moving droplet model, the used initial Reynolds number have been selected as 100, 200, 300, respectively.

Figures (1) to (3), show the behavior of mass burning rate with the size ratio of the two fuels and for three models. The droplet size changes from r_{so} to zero. It is expressed in terms of a size ratio so it changes from 1 to zero. It is evident from these figures, that the burning rate for the moving droplet model is higher than that for the classical model, which in turns, is higher than that for the transient model. This can be attributed to the dependence of the burning rate in the moving droplet model on the Nusselt number, the values of burning rate shown in figure (3) increased with the increase in the assumed initial Reynolds number, The moving fuel droplet enhances the burning rate. For the classical model, the burning rates greater than that for the transient model due to the classical theory, which assumes that all the heat gain to the droplet is used in the vaporization of the fuel droplet at the surface. This will lead to an increase in mass vaporization rate, which in turn, will increase the mass burning rate. Actually, some of the heat gained to the droplet is used for heating the droplet in early stages of its lifetime. This decreases the amount of fuel vaporized from the droplet surface, and this will lead to a decrease in the mass burning rate.

Figure (4) to (6) represent the variation of flame radius in terms of flame stand off ratio for the two fuels and three

models as a function of size ratio. It can be seen that the values of stand off ratio for the transient model is higher than that for the other two models. The lowest values of stand off ratio are that for the moving droplet model. The assumption of quasi-steady burning of the fuel in the stagnant case resulted in raising the values of flame stand off ratios much more than its original values. Thus, the values of the flame stand off ratio of the moving droplet model are closer to the real ones.

Figures (7) to (9) show the variation of flame temperature with size ratio, the flame temperature increases with the decrease in the size of droplet for the transient model. This can be attributed to the assumption of variable surface temperature. For the moving droplet model, the decrease in the size of the droplet causes a decrease in Reynolds number. This led to a decrease in Nusselt number, which in turns, caused the flame radius to increase and a decrease in flame temperature. The flame temperature values for the classical and moving droplet models are higher than that of the transient model for the same condition. The burning rate of these two models is higher than that of the transient model. This will lead to the burning a larger amount of fuel. The values of flame temperature increase with the increase in the initial Reynolds number, which causes the burning rate to increase.

Figures (10) to (12) show the relationship between the time of the combustion process with the size ratio for the three models and for the same

condition. From these figures, it can be seen that the droplet size decreases with the increases in time. This is attributed to the consumption of the liquid fuel during the combustion process. This behavior continues through the hole process and the complete consumption of the droplet. The final time of the process is reached when the droplet radius diminishes completely. In the case of moving droplet model, the effect of movement enhanced the mass burning rate and this led to the reduce in the lifetime. This could be seen clearly in the figures of moving droplet model with the increase in the initial Reynolds number. For the transient model, the lifetime is observed to be shorter than that of the classical model. This is because the final time depends only on the values of the final burning time.

Regarding and referring to the results expressed in the figures, two fuels were considered, namely: n-heptane and n-dodecane. The difference encountered between the two fuels can be attributed to the fact that the two fuels have different boiling point. The boiling point for n-heptane and n-dodecane are (371.4) and (489.3) respectively. For the transient model, the amount of heat that is used to reach the boiling point of n-dodecane is larger than that for n-heptane, and the fraction of heat used to heat up the droplet for n-dodecane is larger than that of n-heptane. As a result, the heat required to complete the vaporization will be less. Consequently, the vaporization rate will be less. The reduction in the burning rate causes a reduction in the flame conditions, which are position and the temperature. the

position of the flame or radius of the flame. The flame temperature may increase as the burning rate becomes larger, since large amount of fuel is burning. Referring to the figure (11), it can be seen that the fuel of the largest burning rate has the shortest lifetime. Increase the burning rate causes the fuel to consume more rapidly. For that reason the figures of transient model is exactly opposite to the arrangements of fuel in the figures of other two models.

Conclusion

The three models show that thermophysical properties are strong functions to reference temperature even when the droplet surface temperature are assumed constant. For classical model shows that the variation of surface temperature can be neglected and this temperature can be assumed constant. For transient model shows that the period of droplet heat up is dominant in the process and caused the mass burning rate at the early stages to be less than that expected in classical theory droplet combustion, and for moving droplet combustion model shows that the values of the main characteristic parameters are considered to be close to the real state, and relative movement between droplet and ambient surrounding gas enhanced the mass burning rate which, in turns, enhanced the other parameters and reduced the droplet lifetime. The film theory approach that was adopted in moving droplet model caused that the radius of the flame to approach closely from the outer film that is bounded by the zone $r_f < r < \delta_T$ for all times of the combustion

process. This behavior neglects the effects of forced convection.

References

- [1] Abraham, J., 2001, **"Improved Modeling of Drop Vaporization and Combustion in Sprays"**, Purdue University, Lafayette School of Mech. Eng.
- [2] Agoston, G.A., Wise, H., Rosser, W.A., 1957, Sixth Symposium (International) on Combustion, Reinhold, New York, pp. 708.
- [3] Andrews, J.R., Biblarz, O., 1981, **"Temperature Dependence of Gas Properties in polynomial Form"**, Naval Postgraduate School, NPS67-81-001, January.
- [4] Chigier, N., 1981, **"Energy, Combustion, and Environment"**, McGraw-Hill, Inc..
- [5] Dombrovsky, L.A., Sazhin, S.S., 2003, **"A Simplified Non-isothermal Model for Droplet Heating and Evaporation"**, Int. Comm. Heat Mass Transfer, Vol. 30, No. 6, pp. 787-796.
- [6] Godsave, G.A.E., 1953, **"Studies of the combustion of Drops in a Fuel Spray : The Burning of Single Drops of Fuel"** Fourth Symposium (International) on Combustion, Williams and Wilkins, Baltimore, pp. 813-839.
- [7] Goldsmith, M., Penner, S.S., 1954, **"On the Burning of Single Drops of Fuel in an Oxidizing Atmosphere"**, Jet propulsion, Vol. 24, pp. 245.
- [8] Hohmann, S., Renz, U., 2003 **"Numerical Simulation of Fuel Spray at High Ambient Pressure: The Influence of Real Gas Effects and Gas Solubility on Droplet Vaporization"**, Int. Journal of Heat and Mass Transfer, Vol. 46, pp. 3017-3028.
- [9] Kotake, S., Okazaki, T., 1969, **"Evaporation and Combustion of Fuel Droplet"**, Int. J. Heat and Mass Transfer, Vol. 12, pp. 595-610.
- [10] Kuo, K.K., 1986, **"Principles of Combustion"**, John Wiley and Sons Inc..
- [11] Lamna, G., et.al., 2004, **"On the Evaporation of a Monodisperse Droplet stream at High Pressure"**, XXI. ICTAM, 15-21 August, Warsaw, Poland.
- [12] Law, C.K., 1976, **"Unsteady Droplet Combustion with Droplet Heating"**, Combustion and Flame, Vol. 26, pp. 17-22.
- [13] Law, C.K., 1982, **"Recent Advances in Droplet Vaporization and Combustion"**, Prog. Energy Combust. Sci., Vol. 8, pp.171-201.
- [14] Law, C.K., Sirignano, W.A., 1977 **"Unsteady Droplet Combustion with Droplet Heating II : Conduction Limit"**, Combustion and Flame, Vol. 28, pp.175-186.
- [15] Ranz, W.E., Marshall, W.R., 1962, **"Evaporation from drops"**, Chem. Engng. Prog., Vol. 48, pp. 173-180.
- [16] Ried, R.C., Prausnitz, J.M., Poling, B.E., 1987, **"The Properties of Gases and Liquids"**, 4th edition, McGraw-Hill, Inc..
- [17] Sazhin, S.S., 2005, **"New Approach to Numerical Modeling of Droplet Transient Heating and Evaporation"**, Int. Journal of Heat and Mass Transfer, Vol. 48, pp. 4215-4228.
- [18] Sazhin, S.S., et. al., 2004, **"Numerical Modeling of Droplet**

"Transient Heating and Evaporation", School of Engineering, University of Brighton

[19]Spalding, D.B., 1953, **"The combustion of Liquid Fuels"**, 4th Symposium on Combustion, pp. 864-874.

[20]Sparrow, E.M., Gregg, J.L., 1958, **"Similar Solutions for Free convection From A Non-isothermal vertical Plate"**, Trans. Of the ASME, Vol. 80, pp. 379-386.

[21]Turns, S.R., 2000, **"An Introduction to Combustion Concepts and Applications"**, Second Edition, McGraw-Hill International Editions.

[22]Williams, A., Sirignano, 1983, **"Fuel Droplet Vaporization and Spray Combustion Theory"**, Prog. Energy Combust. Sci. , Vol. 9, pp. 291-322.

[23]Williams, F.A., 1965, **"Combustion Theory"**, Addison-Wesley Publishing Company, Inc.

[24]Yan, C., Aggarwal, S.K.,2006, **"A high-Pressure Droplet Model for Spray Simulations"**, Transaction of ASME, Vol. 128, pp. 482-492.

Nomenclatures

A : Clausius-Clapeyron constant, atm
 B : Clausius-Clapeyron constant, K
 C_p : Specific heat, J/kgK
 D : Binary mass Diffusivity coefficient, m²/s
 h : Enthalpy, J/kg
 h_{fg} : Latent heat of vaporization, J/kg
 k : Thermal conductivity, W/mK
 m : Mass, kg
 \dot{m} : Mass flow rate, kg/s
 \dot{m}'' : Mass flux, kg/m²s
 M_W : Molecular Weight, kg/kgmol
 Nu : Nusselt number
 P : Pressure, atm

Pr : Prandtl number

Q : Heat transfer rate, W

Q : Time varying latent heat of vaporization per unit mass, J/kg

r : Radius, m

Re : Reynolds number

Sh : Sherwood number

t : Time, s

u : Relative velocity, m/s

v_r : Radial velocity, m/s

x : Number of carbon atoms in fuel molecule

Y : Mass fraction, kg/kg

y : Number of hydrogen atoms in fuel molecule

Greek Symbols

μ : Viscosity, Ns/m²

δ_m, δ_T : Film thickness based on heat or mass transfer, m

Δh_c : Heat of combustion, J/kg

σ : Size ratio

v : Oxidizer to fuel stoichiometric ratio, kg/kg

Subscripts and abbreviations

b : Boiling, d : Droplet, F : Fuel, f : Flame,

g : gas, $g - i$: Gas-phase to interface region,

$i - L$: Interface region to liquid-phase,

ox : Oxidizer, Pr : Products, ref : reference,

s : Droplet surface, sen : Sensible, θ : initial,

∞ : Environment

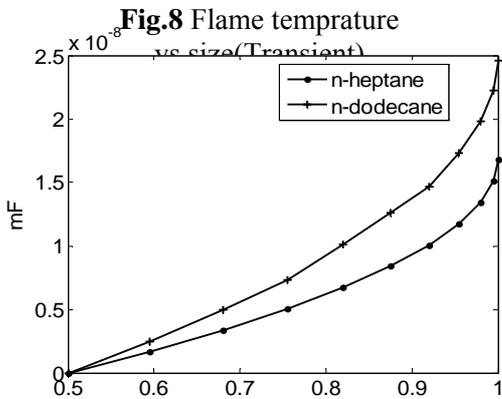


Fig.8 Flame temperature vs size (Transient)

Fig.1 Burining rate vs.size ratio (Classical)

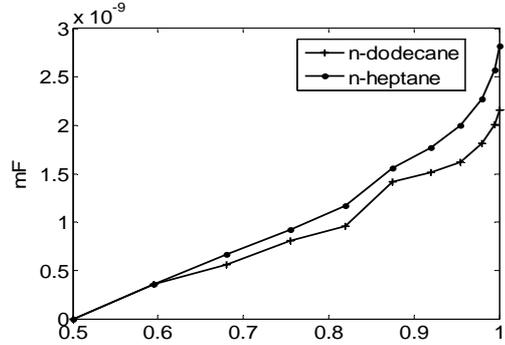


Fig.2 Burining rate vs.size ratio (Transient)

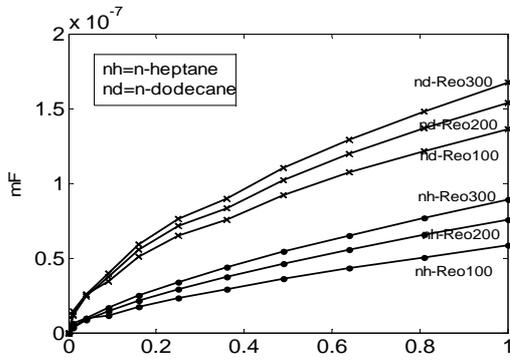


Fig.3 Burining rate vs.size ratio (Moving)

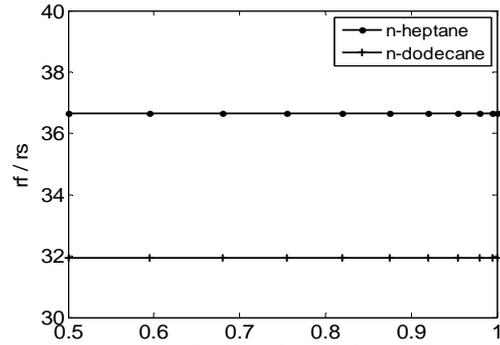


Fig.4 Stand off ratio vs.size ratio (Classical)

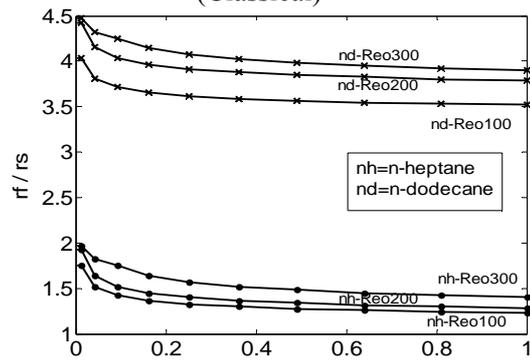
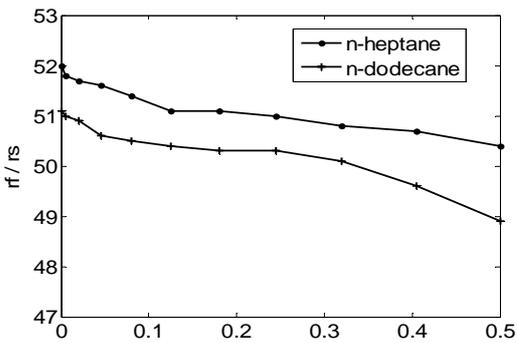


Fig.6 Stand off ratio vs.size ratio (Moving)

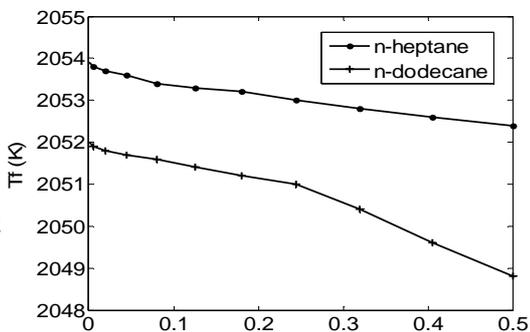


Fig.14 comparison of present moving model with correction equation of Ranz & Marshal

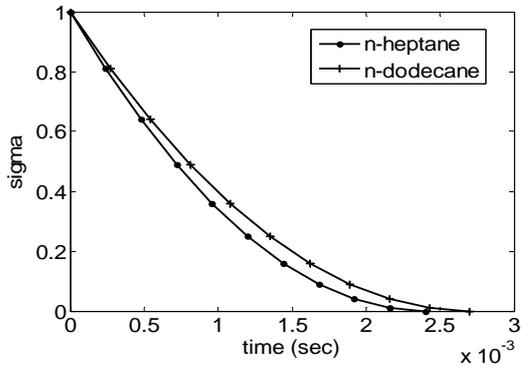


Fig.9 Flame temperature vs.size(Moving)

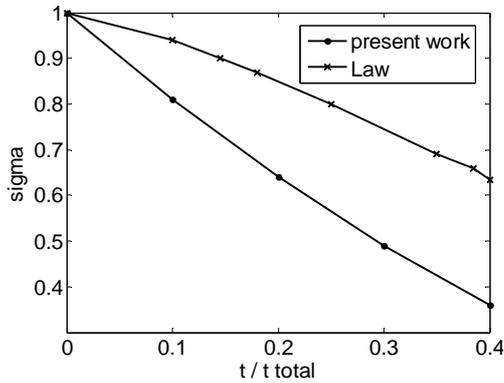


Fig.11 size ratio vs. time (Transient)

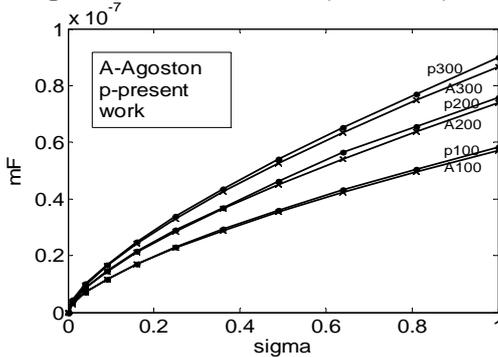


Fig.5 Stand off ratio vs.size ratio (Transient)

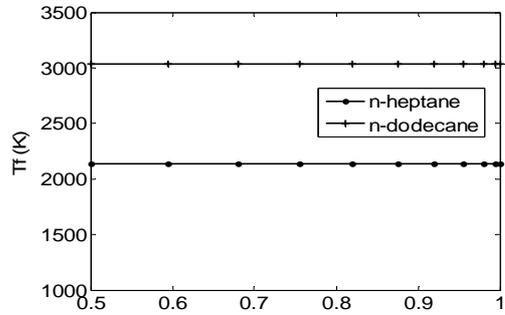


Fig.7 Flame temperature vs.size(Classical)

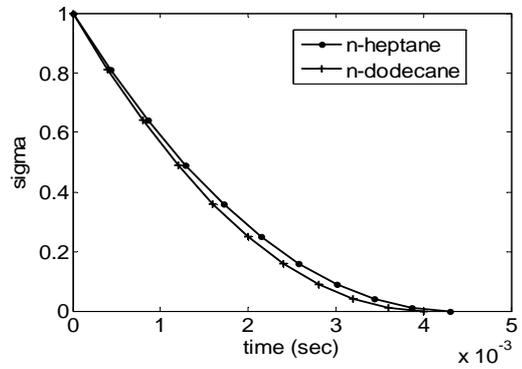


Fig.10 size ratio vs. time (Classical)

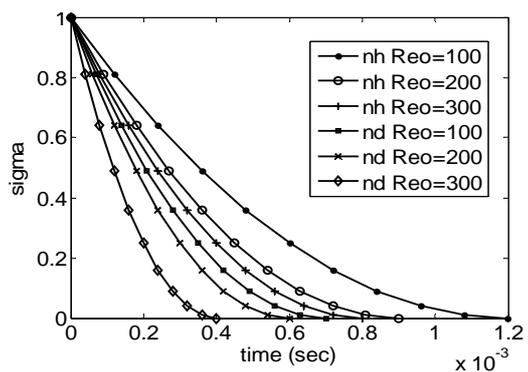


Fig.12 size ratio vs. time (Moving)

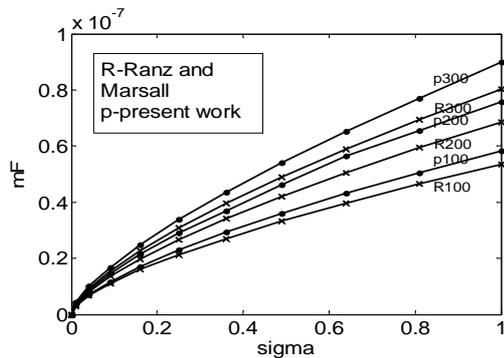


Fig.13 comparison of present Transient model with model of Law

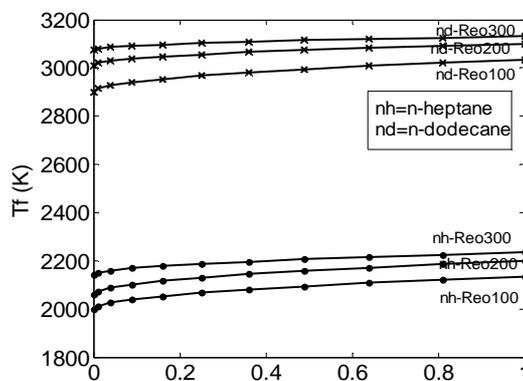


Fig.15 comparison of present moving model with correction equation of Agoston, et.al.