WKBJ approximation for thermally radiating and chemically reactive fluid

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Abstract

This paper investigates steady state solutions to thermally radiating and chemically reactive fluid in a channel. The reaction is assumed to be strongly exothermic under generalized Arrhenius kinetics, neglecting the consumption of the material. Approximate analytical solutions are constructed for the governing nonlinear boundary value problem using WKBJ approximation. Results pertaining to 4 categories of mass species propagation parameter are derived. Two special reactions are used in the validation of the results by numerical solutions, which demonstrated a high level of agreement. Also important features of the problem are discussed.

Key Words: Reactive fluid, thermal radiation; WKBJ approximation

Introduction

The prediction of the factors that control the thermal ignition of combustible materials is of fundamental importance in many industrial processes (see, for example Bowes, 1984; Schmidt, 1998; Okoya, 2004; Makinde et al., 2005; Makinde, 2008). Combustion processes are very fast and exothermic in nature. Therefore, once the reaction is ignited the process proceeds very quickly and tends to be very non-isothermal. Hence, combustion processes (for example, fires, furnaces, and IC engines) release large amounts of energy, and they have many applications in the production of power, heat, and in incineration processes. Generally, combustion processes are complex because of the combination of complex kinetics, mass transfer control, and large temperature variations. In effect, it is seen that high temperature phenomena or high-power radiation sources are common features of these processes just like as in geophysical and astrophysical applications. Other examples where high temperature variations are encountered are found in nuclear reactions, such as in the sun or in nuclear explosions (Ghoshdastidar, 2004); in compressors in ships and gas flares in the petroleum industries (Abowei and Sikoki, 2005). Peterson et al. (2007) stated that where considerations of safety from waste-gases and emissions are concerned in petroleum industries, one of the performance parameters of interest is thermal radiation generated by the flare. This implies that thermal radiation is very important in the study of combustion processes.

For non-isothermal chemical reactors, Schmidt (1998) stated that they have nonlinearities that never occur in non-reacting systems. This explains the fact that in modeling chemically reactive combustible materials, the evolving equations are highly nonlinear. One feature of such equations as provided in Chung (2002) is that the sensible enthalpy is coupled with the chemical species, which contributes to the heat source and diffusion of species interacting with temperature. Obviously, therefore, a realistic mathematical description of the governing reactive-diffusive equation of thermal explosion needs to include the effects of thermal radiation and generalized Arrhenius temperature dependent kinetics.

The reactive-diffusive temperature-dependent equation is not easily amenable to exact analytical solution except for some very simplified physically reasonable assumptions, if not it is an impractical proposition to even think of an exact solution. At best or for the sake of practical interest and for the purpose of gaining insights, one has to settle for numerical result or an approximate solution. This, indeed, provides one route to the knowledge and understanding of physical problems. To this end, several methods of approximation have been devised for tackling various types of problems in Mathematical Physics and Quantum Mechanics. It is the objective of this paper, therefore, to construct approximate solutions to the reactive-diffusive problem of thermally radiating and chemically reactive fluid in a channel. These approximate solutions give a wider applicability in understanding the basic physics and chemistry of the problem, which are particularly important in industrial and technological fields.

The sections followed hereafter respectively are: the mathematical formulation of the problem and dimensionless forms of the governing equations; solution to the concentration equation via WKBJ approximation; concentration solution for a turning point region and connection formulae; numerical validation, and general concluding remarks of the results of the previous sections.

Mathematical Formulation

The mathematical investigation is based upon a thermally radiating and chemically reactive fluid bounded by two horizontal impermeable parallel walls. The lower wall which is on $y = -d/2$ is maintained at a temperature $T = T_1$ and mass concentration $C = C_1$ and the upper wall, which is on $y = d/2$ is maintained at a temperature $T = T_2$ and mass concentration $C = C_2$, where d is the distance between the upper and lower wall. A chemical reaction takes place with a temperature-dependent reaction rate coefficient $k_{f_i}(T)$ and a generalized Arrhenius activation energy is invoked in the mass concentration. For the energy distribution, it is considered that radiative heat transfer plays a significant role in the chemically reactive fluid in the channel. Therefore, the governing mass concentration and energy equations for an optically thin fluid are the followings:

$$\alpha_d \frac{d^2 T}{dy^2} - \frac{1}{\rho_0 c_p} \frac{dq}{dy} = 0, \tag{1a}$$

$$D \frac{d^2 C}{dy^2} - k_{f_i}(T)\, C = 0, \tag{1b}$$

$$\frac{dq}{dy} = 4\,\alpha\sigma\left(T^4 - T_0^4\right), \tag{1c}$$

$$k_{f_i}(T) = k_{r_i}^2\, T^{n_i}\, e^{-\frac{E_{A_i}}{RT}}, \tag{1d}$$

where T, C, y, α_d, D, α, σ, $k_{f_i}(T)$, k_r, n_i, E_{A_i} and R represents temperature, concentration, transverse coordinate, thermal diffusivity, mass diffusivity, absorption coefficient or penetration depth, the Stefan-Boltzmann

constant, temperature-dependent reaction rate coefficient, pre-exponential or frequency factor, an exponential constant, activation energy, and universal or ideal gas constant. Here, the i accounts for the reaction step.

The governing boundary conditions associated to equations (1) are

$$T = T_1 \,, C = C_1 \quad \text{for} \quad y = -\frac{d}{2}, \tag{2a}$$

$$T = T_2 \,, C = C_2 \quad \text{for} \quad y = \frac{d}{2}. \tag{2b}$$

The radiative flux equation (1c) is highly nonlinear in T. However, when it is assumed that the temperature differences within the fluid are sufficiently small, then the linear differential approximation of Cogley-Vincenti-Gilles equilibrium model (Cogley *et al.*, 1968) of the radiation flux becomes significant. In this case T^4 can be expressed as a linear function of temperature in Taylor series about the centre temperature (T_0) of the channel and neglecting higher order terms. This results in the following approximation:

$$T^4 \cong 4T_0^3 T - 3T_0^4. \tag{3}$$

Therefore, equation (1c) is now written as

$$\frac{dq}{dy} = 16 \, \alpha \, \sigma \, T_0^3 \left(T - T_0 \right). \tag{4}$$

The functional form (1d) of the reaction-rate coefficient predicts a very strong dependence of reaction rates on temperature, and this fact is central in describing the complexities of chemical reactions. The factor $\exp(-E_{A_i}/RT)$ describes the probability of crossing a potential energy barrier between reactant and product molecules. In other words, E_{A_i} is defined as this energy barrier (or threshold) that must be surmounted to enable the occurrence of the bond redistribution steps required to convert reactants into products.

In order to facilitate the analysis, the following dimensionless variables and parameters are employed:

$$Y = \frac{y}{d}, \quad \Theta = \frac{T}{T_0}, \quad \Phi = \frac{C}{C_0}, \quad E_i = \frac{E_{A_i}}{RT_0},$$

$$r_i^2 = \frac{k_{r_i}^2 d^2 T_0^{n_i}}{D}, \quad N = \frac{16\alpha\sigma T_0^3 d^2}{\alpha_d}. \tag{5}$$

Therefore, the dimensionless governing equations are

$$\frac{d^2\Theta}{dY^2} - N\left(\Theta - 1\right) = 0, \tag{6a}$$

$$\frac{d^2\Phi}{dY^2} - r_i^2 Q_i(Y)\,\Phi = 0, \tag{6b}$$

where

$$Q_i(Y) = \Theta^{n_i} e^{-E_i/\Theta}. \tag{7}$$

The boundary conditions are now

$$\Theta = \Theta_1 \,, \Phi = \Phi_1 \quad \text{for} \quad Y = -1/2 \tag{8a}$$

$$\Theta = \Theta_2 \,, \Phi = \Phi_2 \quad \text{for} \quad Y = 1/2. \tag{8b}$$

The parameters entering the problem are N, radiation parameter; E_i, activation energy parameter; n_i, exponential constant and r_i^2, modified frequency factor. The mathematical statement of the problem embodies the solution of equations (6) subject to equations (8).

Exact analytical result for the energy equation (6a) and approximate solution for the concentration equation (6b) subject to the equations (8) are herein deduced. The energy equation (6a) is uncoupled from the concentration equation (6b). Therefore, one can advance solution for the temperature variable $\Theta(Y)$ whereupon the solution of the concentration $\Phi(Y)$ is then derived. The solution for the temperature is given as follows:

$$
\Theta(Y) = \frac{1}{2\cosh\left(\frac{1}{2}\sqrt{N}\right)\sinh\left(\frac{1}{2}\sqrt{N}\right)}\left[\left(\Theta_2 + \Theta_1\right)\sinh\left(\frac{1}{2}\sqrt{N}\right)\cosh\left(\sqrt{N}Y\right)\right.
$$

$$
-2\sinh\left(\frac{1}{2}\sqrt{N}\right)\cosh\left(\sqrt{N}Y\right) + \left(\Theta_2 - \Theta_1\right)\cosh\left(\frac{1}{2}\sqrt{N}\right)\sinh\left(\sqrt{N}Y\right)
$$

$$
\left. +2\cosh\left(\frac{1}{2}\sqrt{N}\right)\sinh\left(\frac{1}{2}\sqrt{N}\right)\right]. \tag{9}
$$

Concentration Solution via WKBJ Appoximation

The WKBJ approximation, is a simple asymptotic method for proffering approximate analytical solutions that pave the way for an approximate description of the mechanisms underlying some second-order ordinary differential equations that model physical phenomena. The WKBJ is derived from Wentzel-Kramers-Brillouin-Jeffreys (Hinch, 1991), who somewhat independently discovered this method.

The concentration equation (6b) is highly nonlinear. In most of combustion calculations, there are several hundreds of reactions that could be considered. However, due to limited computational resources, it is customary to select only important reaction mechanisms, neglecting those that are less important (i.e. those reactions whose rates cannot be measured). For example, a simple prototype of combustion reactions is hydrogen oxidation:

$$
2H_2 + O_2 \rightarrow 2H_2O
$$
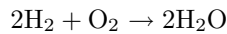
This reaction is extremely complex, and the standard model describing it consists of 38 reaction steps among 8 species (Schmidth, 1998; Chung, 2002).

In what follows, we envisage and seek mathematically tractable scenarios of reaction rates of the elementary steps in the hydrogen oxidation reaction that may lead to 3 categories of the potential function as displayed in the Figure 1: (a) $Q_i(Y) = Q_0 = 1$ (a constant potential), in which there is no variation of the potential throughout the computational domain, (b) $Q_i(Y) > 0$, denoted as $Q_{>0}(Y)$ depicts that the potential slowly varies, but it is either above or below the constant potential and equals Q_0, from where it grows or decreases, and (c) $Q_i(Y) = 0$, denoted as $Q_{=0}(Y)$. This exhibits a turning point, and gives a wrong behavior to the concentration solution. A 4th category out of curiosity and for the purpose of sharpening our intuition about the solution of the concentration is considered. This is the situation where the potential is still considered slowly varying, but $Q_i(Y) < 0$, denoted as $Q_{<0}(Y)$.

For the 1st category, we consider that the exponential constant n_i and the activation energy E_i are small, such that $n_i = E_i = 0$. In this case, the potential function (7) becomes a constant: $Q_i(Y) = Q_0 = 1$. Therefore,
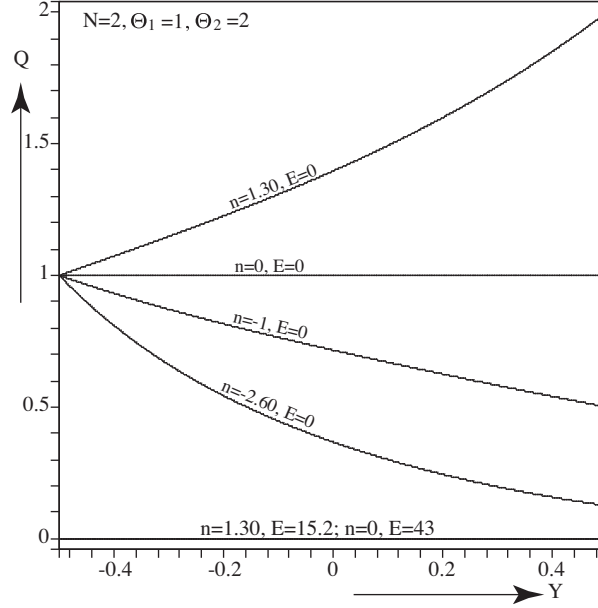
Figure 1. Potential profiles as a function of Y.

the solution to equation (6b) with the aid of the boundary conditions (8) becomes

$$\Phi(Y) = \frac{1}{2\cosh\left(\frac{1}{2}r_i\right)\sinh\left(\frac{1}{2}r_i\right)}\left[\left(\Phi_2 + \Phi_1\right)\sinh\left(\frac{1}{2}r_i\right)\cosh\left(r_iY\right)\right.$$

$$\left. + \left(\Phi_2 - \Phi_1\right)\cosh\left(\frac{1}{2}r_i\right)\sinh\left(r_iY\right)\right]. \tag{10}$$

The WKBJ approximation is used to derive the 2nd and the 4th categories of the potential function. Here, the derivation presented by Oyewumi et al. (2005) is followed closely. Suppose that the constant exponent n_i and the activation energy parameter E_i are not necessarily small, then $Q_i(Y)$ is no longer a constant, and hence the ad hoc solution (10) is unacceptable. On the alternative, we assume that the chemical reaction rate r_i is large and define it as

$$r_i = \frac{1}{\epsilon_i}, \tag{11}$$

where ϵ_i is considered to be a small parameter. Equation (6b) now becomes

$$\epsilon_i^2 \frac{d^2\Phi}{dY^2} - Q_{>0}(Y)\Phi = 0, \tag{12}$$

specifically for the potential $Q_i(Y) > 0$.

Now, up to an arbitrary multiplicative constant, the solution (10) may alternatively be written as

$$\Phi(Y) = \exp(\pm r_i Y) \tag{13}$$

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Equation (13) suggests that if $Q_{>0}(Y)$ is no longer a constant, but varies slowly with Y, then slow variation of $Q_{>0}(Y)$ with Y means that it varies appreciably only over a small distance and it does approximate a constant potential function, where $|dQ_{>0}/dY|$ is small, and provided Y is not near turning points for $Q_{=0}(Y)$. We may try a solution of the nonlinear concentration equation (6b) in the form

$$\Phi(Y) = \exp[\Psi(Y)], \tag{14}$$

which converts equation (6b) to

$$\epsilon_i^2 \frac{d^2\Psi}{dY^2} + \epsilon_i^2 \left(\frac{d\Psi}{dY}\right)^2 - Q_{>0}(Y) = 0. \tag{15}$$

Equation(15) is a second-order nonlinear ordinary differential equation. The nonlinearity in the equation is used to develop an iteration procedure to obtain the zeroth-order approximate solution,

$$\Psi(Y) = \pm\frac{1}{\epsilon_i} \int_{b-}^{Y} Q_{>0}(s)^{1/2} ds + C_0, \tag{16}$$

where C_0 is an integration constant. For nth-order approximation, we then write

$$\Psi_{n+1}(Y) = \pm \int_{b-}^{Y} \left[\frac{1}{\epsilon_i^2} Q_{>0}(s) - \frac{d^2\Psi_n}{dY^2}\right]^{1/2} ds + C_{n+1}. \tag{17}$$

For $n = 0$, equation (17) becomes

$$\Psi_1(Y) = \pm \int_{b-}^{Y} \left[\frac{1}{\epsilon_i^2} Q_{>0}(s) \mp \frac{1}{2} Q_{>0}(s)^{-1/2} \frac{dQ_{>0}}{dY}\right]^{1/2} ds + C_1. \tag{18}$$

As a corrective measure of the procedure, $\Psi(Y)$ demands that $\Psi_1(Y)$ be close to $\Psi_0(Y)$. This can only be achieved if

$$\left|\frac{1}{2} Q_{>0}(s)^{-1/2} \frac{dQ_{>0}}{dY}\right| << \left|\frac{1}{\epsilon_i^2} Q_{>0}(s)\right|. \tag{19}$$

If condition (19) holds, then, an approximate value consideration of Binomial expansion (Abramowitz and Stegun, 1970) reduces equation (18) to

$$\Psi_1(Y) \approx \pm\frac{1}{\epsilon_i} \int_{b-}^{Y} Q_{>0}(s)^{1/2} ds - \frac{1}{4} \ln Q_{>0}(Y), \tag{20}$$

where the integration constant C_1 has been absorbed into the normalization of $\Phi(Y)$. This first order iteration equation (20) constitutes the WKBJ approximation for $Q_{>0}(Y)$. Therefore, by using equation (20) on equation (14), the general solution to the nonlinear concentration equation(6b) becomes

$$\Phi(Y) = Q_{>0}(Y)^{-1/4} \left[A^+ \exp\left(\frac{1}{\epsilon_i} \int_{b-}^{Y} Q_{>0}(s)^{1/2} ds\right) + A^- \exp\left(-\frac{1}{\epsilon_i} \int_{b-}^{Y} Q_{>0}(s)^{1/2} ds\right)\right], \tag{21}$$

where A^+ and A^- are integration constants to be evaluated using the boundary conditions (8). The concentration solution (21) for $Q_{>0}(Y)$ indicates that it increases or decreases exponentially as one goes away from the turning point $Q_{=0}(Y)$. The application of the boundary conditions permits the general solution (21) to be rewritten:

$$\Phi(Y) = Q_{>0}(Y)^{-1/4}\left[\left\{\Phi_2\, Q_{>0}(1/2)^{1/4} - \Phi_1\, Q_{>0}(-1/2)^{1/4}\exp\left(-\frac{1}{\epsilon_i}\int_{-1/2}^{1/2}Q_{>0}(s)^{1/2}\,ds\right)\right\} \times\right.$$

$$\left.\times\frac{\sinh\left(\frac{1}{\epsilon_i}\int_{-1/2}^{Y}Q_{>0}(s)^{1/2}\,ds\right)}{\sinh\left(\frac{1}{\epsilon_i}\int_{-1/2}^{1/2}Q_{>0}(s)^{1/2}\,ds\right)} + \Phi_1\, Q_{>0}(-1/2)^{1/4}\exp\left(-\frac{1}{\epsilon_i}\int_{-1/2}^{Y}Q_{>0}(s)^{1/2}\,ds\right)\right]. \tag{22}$$

It is pertinent to remark here that the solution (22) will differ from the exact solution (if any) by terms of order ϵ_i.

The concentration solution for the 4th category, where the potential function is negative (i.e. $Q_i(Y) = -Q_{<0}(Y)$), is given by

$$\Phi(Y) = -Q_{<0}(Y)^{-1/4}\left[B^+\exp\left(\frac{\iota}{\epsilon_i}\int_{b^-}^{Y}Q_{<0}(s)^{1/2}ds\right) + B^-\exp\left(-\frac{\iota}{\epsilon_i}\int_{b^-}^{Y}Q_{<0}(s)^{1/2}ds\right)\right], \tag{23}$$

where B^+ and B^- are integration constants to be evaluated using the boundary conditions (8). Hence, the equivalent general solution for the case $Q_{<0}(Y)$ becomes

$$\Phi(Y) = Q_{<0}(Y)^{-1/4}\left[\left\{\Phi_2\, Q_{<0}(1/2)^{1/4} - \Phi_1\, Q_{<0}(-1/2)^{1/4}\exp\left(-\frac{\iota}{\epsilon_i}\int_{-1/2}^{1/2}Q_{<0}(s)^{1/2}\,ds\right)\right\} \times\right.$$

$$\left.\times\frac{\sin\left(\frac{1}{\epsilon_i}\int_{-1/2}^{Y}Q_{<0}(s)^{1/2}\,ds\right)}{\sin\left(\frac{1}{\epsilon_i}\int_{-1/2}^{1/2}Q_{<0}(s)^{1/2}\,ds\right)} + \Phi_1\, Q_{<0}(-1/2)^{1/4}\exp\left(-\frac{\iota}{\epsilon_i}\int_{-1/2}^{Y}Q_{<0}(s)^{1/2}\,ds\right)\right], \tag{24}$$

where $\iota = \sqrt{-1}$. The concentration solution for $Q_{<0}(Y)$ oscillates and behaves in the form of plane waves that travel toward $\pm Y$ and whose propagation constants gradually change from one region to another. The factor $Q_{<0}(Y)^{-1/4}$ is used to ensure that the probability of finding the concentration at a point in space is inversely proportional to the speed of the mass species at that point. Hence, on physical grounds, the concentration solution (24) is expected to be suitable for a sufficiently slowly varying potential function $Q_{<0}(Y)$. We note that the expressions (22) and (24) are singular at $Y = 0$ since both contains the factor $Q_{>0}(Y)^{-1/4}$ and $Q_{<0}(Y)^{-1/4}$, respectively.

Concentration Solution for the Region $Q_{=0}(Y)$

Approximate analytical solutions for the concentration equation (6b) have been derived via the WKBJ approximation for the regions of $Q_{>0}(Y)$ and $Q_{<0}(Y)$, where the potential function changes slowly. The condition for the application of WKBJ approximation is not satisfied at the region of $Q_{=0}(Y)$, at which the mass species propagation constant vanishes. However, a suitable solution can be determined by approximating the actual

variation of the potential function $Q_i(Y)$ around $Q_{=0}(Y)$ by a linear variation:

$$Q_{la_i}(Y) \approx A(Y - Y_0) = A'(Y_0 - Y), \tag{25}$$

where $A' = |A|$ and the WKBJ approximation is invalid in the interval $a < Y < b$. This interval is the region in which the linear approximation (25) to the potential function is assumed valid, where a and b are respectively placed on the left and right to the turning point Y_0. The use of equation (25) in equation (6b) gives

$$\frac{d^2\Phi}{dY^2} - r_i^2 A'(Y_0 - Y)\,\Phi = 0. \tag{26}$$

The substitution $\zeta = (r_i^2 A')^{1/3}(Y_0 - Y)$, transforms equation (26) into Airy differential equation

$$\frac{d^2\Phi}{d\zeta^2} - \zeta\,\Phi = 0, \tag{27}$$

for $a < Y < Y_0$.

Similarly, for $Y_0 < Y < b$ and the substitution $\eta = (r_i^2 A')^{1/3}(Y - Y_0)$ transforms equation (26) into the modified Airy differential equation

$$\frac{d^2\Phi}{d\eta^2} + \eta\,\Phi = 0. \tag{28}$$

The equation (28) is exactly solvable (Abramowitz and Stegun, 1970), and its solution is

$$\Phi(\eta) = A_1\,\eta^{1/2} J_{1/3}\left(\frac{2}{3}\eta^{3/2}\right) + A_2\,\eta^{1/2} J_{-1/3}\left(\frac{2}{3}\eta^{3/2}\right), \tag{29}$$

where $J_{\pm 1/3}$ are the independent solutions of Bessel's differential equation of order $1/3$ with A_1 and A_2 representing the integration constants.

The differential equations (27) and (28) are related to each other through the substitution $\eta = -\zeta$, and hence the solution of the Airy differential equation (27) becomes

$$\Phi(\zeta) = \zeta^{1/2}\left[B_1\,I_{1/3}\left(\frac{2}{3}\zeta^{3/2}\right) + B_2\,I_{-1/3}\left(\frac{2}{3}\zeta^{3/2}\right)\right], \tag{30}$$

where $I_{\pm 1/3}$ satisfies the Modified Bessel's differential equation of order $1/3$ with B_1 and B_2 being integration constants.

The solutions (29) and (30) are asymptotically extendable to the regions $Q_{>0}(Y)$ and $Q_{<0}(Y)$, where the WKBJ method is valid. Consequently, the next section deals with the connection formulae.

Asymptotic Expansions and Connection Formulae

With the use of asymptotic expansions of $J_{\pm 1/3}$ and $I_{\pm 1/3}$ (Abramowitz and Stegun, 1970; Dicke and Wittke, 1980; Mei, 1995) and by normalizing $\Phi(\zeta)$ and $\Phi(\eta)$ respectively, we obtain the following relations:

$$\Phi(\zeta) = B_0\,\zeta^{-1/4}\exp\left(-\frac{2}{3}\zeta^{3/2}\right), \tag{31a}$$

$$\Phi(\eta) = 2B_0\,\eta^{-1/4}\cos\left(\frac{2}{3}\eta^{3/2} - \pi/4\right), \tag{31b}$$

where $A_1 = A_2$, $B_1 = B_2$, and $B_0 = \frac{3B_2}{2\sqrt{\pi}}$ is an arbitrary constant. The joining condition or connection formula is given by the 2 equations (31a, b) from the region $Y < Y_0$ to the region $Y_0 < Y$, and this is written:

$$\zeta^{-1/4}\exp\left(-\frac{2}{3}\zeta^{3/2}\right)\Bigg|_{Y<Y_0} \rightarrow 2\,\eta^{-1/4}\cos\left(\frac{2}{3}\eta^{3/2} - \pi/4\right)\Bigg|_{Y_0<Y} \tag{32}$$

for $B_0 = 1$. By virtue of the relations for ζ and η, and the respective scenarios for $Q_{>0}(Y)$ and $Q_{<0}(Y)$, from equation (32) we obtain the expected connection formulae

$$Q_{<0}(Y)^{-1/4}\exp\left(-\frac{\iota}{\epsilon_i}\int_Y^{Y_0}Q(s)^{1/2}ds\right) \rightarrow 2\,Q_{>0}(Y)^{-1/4}\,\times$$
$$\times\cos\left(\frac{1}{\epsilon_i}\int_Y^{Y_0}Q(s)^{1/2}ds - \pi/4\right), \tag{33a}$$

$$-Q_{<0}(Y)^{-1/4}\exp\left(\frac{\iota}{\epsilon_i}\int_{Y_0}^Y Q(s)^{1/2}ds\right) \leftarrow 2\,Q_{>0}(Y)^{-1/4}\,\times$$
$$\times\cos\left(\frac{1}{\epsilon_i}\int_{Y_0}^Y Q(s)^{1/2}ds - \pi/4\right) \tag{33b}$$

respectively for the regions $Y < Y_0$ and $Y_0 < Y$. The arrows in equations (32) and (33a, b) indicate that the connection should be made in the direction of the increasing exponential. Therefore, we are now in a position to construct the concentration solution decaying in $Y < Y_0$ as

$$\Phi(Y) = \left(\frac{3B_2}{2\sqrt{\pi}}\right)Q_{<0}(Y)^{-1/4}\exp\left(-\frac{1}{\epsilon_i}\int_Y^{Y_0}Q(s)^{1/2}ds\right). \tag{34}$$

For $Y > Y_0$, the WKBJ concentration connection formula gives

$$\Phi(Y) = 2\left(\frac{3B_2}{2\sqrt{\pi}}\right)Q_{>0}(Y)^{-1/4}\cos\left(\frac{1}{\epsilon_i}\int_{Y_0}^Y Q(s)^{1/2}ds - \pi/4\right). \tag{35}$$

Validation of WKBJ Approximation

Here we restrict our attention to the concentration solutions for $Q_i(Y) = $ a constant and $Q_i(Y) > 0$, which are validated by numerical solutions. It is important to note here that the numerical experiments were conducted using a Computer Symbolic Algebra Package (**MAPLE**) general ODE solver in a Macintosh Pentium 4 Machine.

First, we consider the case for $Q_i(Y) = $ a constant, where $n_i = 0 = E_i$ which resulted the exact concentration solution (10). Table 1 displays this exact solution together with the WKBJ approximate solution (22) versus numerical evaluation of the governing dimensionless equations (6 - 8) for $n_i = 0 = E_i$ and $r = 1$. It is observed that the WKBJ solution replicates the exact solution, and evidently there is little or no difference between the exact solution and the numerical evaluation. The results showed such high level of agreement in that the maximum relative error was 8.06×10^{-10}.

Table 1. Exact concentration solution (10), WKBJ approximation (22) and numerical.

Y	Exact	WKBJ	Numerical	Relative Error
-0.50	1.000000000	1.000000000	1.000000000	0.000000000
-0.40	1.043949098	1.043949098	1.043949098	0.000000000
-0.30	1.098346389	1.098346389	1.098346389	0.000000000
-0.20	1.163736300	1.163736300	1.163736300	0.000000000
-0.10	1.240773276	1.240773276	1.240773275	8.06×10^{-10}
0.00	1.330228326	1.330228326	1.330228326	0.000000000
0.10	1.432996750	1.432996750	1.432996749	6.98×10^{-10}
0.20	1.550107086	1.550107086	1.550107085	6.45×10^{-10}
0.30	1.682731414	1.682731414	1.682731414	0.000000000
0.40	1.832197086	1.832197086	1.832197085	5.46×10^{-10}
0.50	2.000000000	2.000000000	2.000000000	0.000000000

Okoya (2004) evaluated transitional values of r and E for the reactions of Sensitized ($n = -2$, $r = 1/2$, $E = 8$) and Bimolecular ($n = 1/2$, $r = 1$, $E = 3$). These reactions are herein considered for the computations of $Q_i(Y) > 0$.

The results displayed in Table 2 and Table 3 respectively, show comparison of the WKBJ approximate concentration solution to that of the numerical computation for sensitized and bimolecular reaction for different values of N. It is evident that the WKBJ approximate solution reveals the characteristics of the problem and compares favorably well with the numerical computation. It is seen that $N = 0$, $N = 5$, and $N = 10$ respectively gives an average relative error of 0.09738120764, 0.03413250574, and 0.01356787374 for the sensitized reaction, and 0.052518721, 0.001170115, and 0.032581937 for bimolecular reaction. In general, it is observed that increase in the radiation parameter, N, increases the concentration.

Concluding Remarks

In this paper, the study of a steadily thermally radiating and chemically reactive fluid in a channel is presented by the use of WKBJ approximation, which is validated by numerical solution. It is confined to 4 categories of the mass species propagation parameter $Q_i(Y)$: $Q_i(Y) = $ a constant, $Q_i(Y) > 0$, $Q_i(Y) = 0$, and $Q_i(Y) < 0$. The concentration solutions for $Q_i(Y) = $ a constant and $Q_i(Y) > 0$ were validated by numerical solutions. The

Table 2. Sensitized reaction concentration solution: WKBJ approximation (22) versus numerical for variations of N.

Y	$N = 0$			$N = 5$			$N = 10$		
	WKBJ	Numerical	Relative Error	WKBJ	Numerical	Relative Error	WKBJ	Numerical	Relative Error
-0.50	0.9999999999	1.000000000	1 00 × 10⁻¹⁰	1.000000000	1.000000000	0.000000000	0.9999999999	1.000000000	1 00 × 10⁻¹⁰
-0.40	0.990514885	1.099972505	0.099509415	1.070327842	1.099981870	0.026958652	1.113261114	1.099985892	0.011924626
-0.30	1.021553761	1.199946616	0.148667326	1.149942980	1.199964968	0.041686207	1.226877539	1.199972871	0.021929383
-0.20	1.082694010	1.299923408	0.167109383	1.235930584	1.299949801	0.049247453	1.337300209	1.299961247	0.027921152
-0.10	1.167477904	1.399904318	0.166030214	1.326483153	1.399937058	0.052469434	1.441435891	1.399951441	0.028779948
0.00	1.271618282	1.499891147	0.152192954	1.420834518	1.499927686	0.052731321	1.537207193	1.499944054	0.024240805
0.10	1.392101563	1.599886049	0.129874553	1.519305722	1.599923004	0.050388226	1.624461406	1.599939988	0.015095107
0.20	1.526708268	1.699891502	0.101878993	1.623362661	1.699924852	0.045038574	1.706021749	1.699940645	0.00364494
0.30	1.673741385	1.799910271	0.070097320	1.735610509	1.799935787	0.035737540	1.788458682	1.799948245	0.006383274
0.40	1.831864385	1.899945367	0.035833126	1.859679866	1.899959300	0.021200156	1.882091729	1.899966273	0.009407822
0.50	1.999999999	2.000000000	1 00 × 10⁻¹⁰	1.999999999	2.000000000	1 00 × 10⁻¹⁰	2.000000000	2.000000000	0.000000000

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Table 3. Bimolecular reaction concentration solution: WKBJ approximation (22) versus numerical for variations of N

Y	$N = 0$			$N = 5$			$N = 10$		
	WKBJ	Numerical	Relative Error	WKBJ	Numerical	Relative Error	WKBJ	Numerical	Relative Error
-0.50	1.000000000	1.000000000	0.000000000	1.000000000	1.000000000	0.000000000	1.000000000	1.000000000	0.000000000
-0.40	1.036683412	1.091307933	0.050054178	1.090521910	1.093531872	0.002752514	1.118288515	1.094533533	0.021242266
-0.30	1.092572261	1.183369796	0.076727947	1.185099004	1.187702541	0.002192078	1.236591122	1.189666665	0.037946623
-0.20	1.164242159	1.276501433	0.087942928	1.282124663	1.282700623	0.000449021	1.352639075	1.285518712	0.049621783
-0.10	1.249500620	1.371087019	0.088678835	1.380412616	1.378728585	0.001219948	1.464135514	1.382238441	0.055935446
0.00	1.346948169	1.467582014	0.089560866	1.479232292	1.476066356	0.002140256	1.568977793	1.480021123	0.056697214
0.10	1.455734636	1.566515927	0.070718267	1.578400723	1.575071195	0.002109431	1.665704663	1.579135315	0.051971607
0.20	1.575417910	1.668495229	0.057785187	1.678397489	1.676215237	0.001300200	1.754141216	1.679965185	0.042286237
0.30	1.705879668	1.774206702	0.038511315	1.780469283	1.780130920	0.000190041	1.836091913	1.783077226	0.028873656
0.40	1.847274554	1.884421476	0.019712640	1.886695417	1.887672802	0.000517772	1.915812852	1.889323924	0.013826470
0.50	2.000000002	2.000000000	$1\ 00 \times 10^{-9}$	2.000000001	2.000000000	$5\ 00 \times 10^{-10}$	2.000000001	2.000000000	$5\ 00 \times 10^{-10}$

WKBJ approximate results showed a close agreement with the computational results. For $n_i = 0 = E_i$ the results make no discernible difference, whereas for sensitized and bimolecular reactions, the mean relative errors were about $1\% - 10\%$. It is hoped that the present investigations may further serve as toolkits for numerical experimentations. It is noted here that the efficient computation of thermal radiation effect with strongly exothermic reaction under generalized Arrhenius kinetics is essential for the design and analysis of industrial thermal systems, such as furnaces, boilers, burners, nuclear power plants, combustion products (such as, H_2O and CO_2), and gas turbines.

Symbols

T	temperature;
C	concentration;
y	transverse coordinate;
d	distance between the upper and lower walls of the channel;
α_d	thermal diffusivity;
D	mass diffusivity;
α	absorption coefficient or penetration depth;
σ	Stefan-Boltzmann constant;
T_0	centre temperature;
$k_{f_i}(T)$	temperature-dependent reaction rate coefficient;
k_r	pre-exponential or frequency factor;
n_i	an exponential constant;
r_i^2	modified frequency factor $(= \frac{k_{r_i}^2 d^2 T_0^{n_i}}{D})$;
ϵ_i	small parameter;
E_{A_i}	activation energy;
Y	non-dimensional transverse coordinate $(= \frac{y}{d})$;
Θ	non-dimensional temperature $(= \frac{T}{T_0})$;
Φ	non-dimensional concentration $(= \frac{C}{C_0})$;
E_i	non-dimensional activation energy $(= \frac{E_{A_i}}{RT_0})$;
N	radiation parameter $(= \frac{16\alpha\sigma T_0^3 d^2}{\alpha_d})$;
R	universal or ideal gas constant;
i	reaction step.

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