The study of combustion associated phenomena in internal combustion engines is important for reasons that include pollutant formation control, and the heat transfer between the hot gases, the piston and combustion chamber walls. The main objective of the present paper is presenting a reliable and precise algorithm based on mollification and marching methods to determine the energy absorption coefficient. The stability and convergence of numerical solutions are investigated and the efficiency of the proposed algorithm is tested with two numerical examples.

Keywords: Combustion Engines; Nonlinear Cauchy problem; marching scheme; mollification method

1. Introduction

Heat transfer to the combustion chamber walls of internal combustion engines is recognized as one of the most important factors having a great influence both in engine design and operation ([1],[2],[3],[4]), which has attracted many scientists and engineers from different field of studies. Some of the most important applications of this phenomenon can be applied to industries in which designing and developing of internal combustion (IC) engines are assets, as cases in point, automotive industry, missile industries and those industries related to thermal furnaces.

Nowadays, technology changes in the field of the internal combustion engines (mainly the diesel ones) are happening extremely fast. New demands are added towards the areas of controlled ignition of new and alternative fuels ([5]), reduction of tailpipe emissions ([6]) and improved engine construction that would ensure operation under extreme combustion chamber pressures (well above 200 bar) [7].

Furthermore, in recent years, highly laboratory costs of the designing and manufacturing of combustion engines and furnaces, especially when conditions are variable, demand for mathematical models in analyzing issues and accurate simulation of mathematical models in the field of combustion.

Based on the physical conditions of the phenomena, generating a suitable mathematical model is also a difficult task to do. For instance, combustion gases such as CH4 need to check 53 components and 325 chemical interaction [8].

Many studies in the field of numerical simulation of the combustion chamber have been done. For instance, in 2005, Merkle et al. ([9]) studied cold flow into and

The accurate solution of combustion processes in terms of mathematical models requires a fully understanding of all the basic phenomena involved and their detailed description, in general, in terms of ordinary or partial differential equations. Such models are formulated in terms of physical properties or constants that, in general, contain some level of uncertainties.

Mathematical models proposed in the field of partial differential equations are often the most important of which can be mass conservation equations and the momentum and energy conservation equations pointed out [12–14]. One of the most highly regarded models that energy equation is applied in order to simplify assumptions can be expressed as follows [12–14],

\[\rho (x, t) u_t (x, t) - u_{xx} (x, t) = f (x, t), \quad (x, t) \in Z \equiv \Omega \times [0, T], \quad (1)\]
\[u (x, 0) = \gamma (x), \quad x \in \Omega, \quad (2)\]
\[u (x, t) = s (t), \quad x \in \partial \Omega, \quad t \in [0, T], \quad (3)\]
\[u (x, T) = r (x), \quad x \in \partial \Omega. \quad (4)\]

The conditions (2), (3) and (4) are respectively called the initial condition, the boundary condition and the overdetermination condition. Furthermore, \(\gamma\) represents the gravitational force, and \(f\) represents the energy semester. This term can be written as follows

\[f (x, t) = \eta (x) g (x, t) + h (x, t). \quad (5)\]

In equation (5), \(\eta (x) g (x, t)\) is the energy absorbed by the fluid in the combustion chamber and \(h (x, t)\) describes that the energy generated from chemical reactions. This study aimed to estimate the unknown function \(\eta (x)\) as energy absorption coefficient is fluid and it is assumed that the function \(g (x, t)\) in the following conditions applies. Under these assumptions, the problem (1) - (4) can be considered as a parabolic inverse problem of estimating the heat source.

In this article, we consider the problem in the case that its domain is limited to \(Z \equiv \{(x, t)| (x, t) \in [0, 1] \times [0, T]\}. Therefore, relations (2) and (3) to be rewritten as follows.

\[u (x, 0) = \gamma (x), \quad x \in [0, 1], \quad (6)\]
\[u (0, t) = \psi (t), \quad t \in [0, T]. \quad (7)\]

Temperature and heat flux at \(x = 0\) and also the initial value of the \(f\) as additional conditions for determining the solutions to be considered are as follows.

\[u_x (0, t) = \varphi (t), \quad t \in [0, T], \quad (8)\]
\[f (0, t) = f_0 (t), \quad t \in [0, T]. \quad (9)\]

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In sequence we will introduce a numerical marching scheme based on the mollification method (see [17]) to find the solution of the problem (1)-(9) under the assumption that $\gamma$, $\varphi$, $\psi$ and $f_0$ are only known approximately as $\gamma^\varepsilon(x)$, $\varphi^\varepsilon(t)$, $\psi^\varepsilon(t)$ and $f_0^\varepsilon(t)$ such that

\begin{align}
\|\gamma(x) - \gamma^\varepsilon(x)\|_\infty & \leq \varepsilon, \\
\|\varphi(t) - \varphi^\varepsilon(t)\|_\infty & \leq \varepsilon, \\
\|\psi(t) - \psi^\varepsilon(t)\|_\infty & \leq \varepsilon, \\
\|f_0(t) - f_0^\varepsilon(t)\|_\infty & \leq \varepsilon.
\end{align}

Because of the presence of the noise in the problem’s data, we first stabilize the problem using the mollification method.

2. Regularized problem and the marching scheme

The regularized form of the problem (1)-(9) may be written as follows

\begin{align}
\rho(x, t)v_t(x, t) - v_{xx}(x, t) & = f(x, t), & (x, t) \in [0, 1] \times [0, T], \\
v(x, 0) & = J_\delta \psi(x), & x \in [0, 1], \\
v(0, t) & = J_\delta \psi(t), & t \in [0, T], \\
v_x(0, t) & = J_{\delta_x} \varphi(t), & t \in [0, T], \\
f(0, t) & = J_{\delta_f} f_0(t), & x \in [0, 1],
\end{align}

Determining $v(x, t), f(x, t) \in [0, 1]$ and $r(x) \in [0, 1]$ from the problem (14)-(18) is our initial object and $\eta(x)$ will be obtained from $f(x, t) = \eta(x)g(x, t) + h(x, t)$ automatically. Notice that the radii of mollification, $\delta_1$, $\delta_2$, $\delta_3$ and $\delta_4$, are chosen automatically using general cross validation (GCV) methods [15]. Here without loss of generality, we set $T = 1$.

Establishing a numerical algorithm, assume $M$ and $N$ are positive integers and then the finite differences parameters discretization of $I = [0, 1]$ and $J = [0, 1]$ will be $h = \Delta x = 1/M$ and $k = \Delta t = 1/N$. Let $U_{i,n}, Q_{i,n}, W_{i,n}, Q_{i,n}$ and $F_{i,n}$ denote the discrete computed approximations of $v(ih, nk)$, $v_x(ih, nk)$, $v_t(ih, nk)$ and $f(ih, nk)$ respectively, and then the space marching algorithm may be written as follows:

The algorithm of space marching scheme may be written as follows

1. Select $\delta_0$, $\delta^0_1$, $\delta^0_2$ and $\delta^0_3$.
2. Perform mollification of $\psi^\varepsilon, \varphi^\varepsilon, \gamma^\varepsilon$ and $f_0^\varepsilon$ in the interval $[0, 1]$. Let

\begin{align}
U_{0,n} & = J_{\delta_0} \psi^\varepsilon(nk) \quad (n \neq 0), & U_{i,0} & = J_{\delta_i} \gamma^\varepsilon(ih), & i \in \{0, 1, \ldots, M\} \\
Q_{0,n} & = K(0)J_{\delta_0} \varphi^\varepsilon(nk), & F_{0,n} & = J_{\delta_0} f_0^\varepsilon(nk).
\end{align}

3. Perform mollified differentiation in time (see the first chapter of [17]) of $J_{\delta_0} \psi^\varepsilon(nk)$. Set

\begin{align}
W_{0,n} & = D_t(J_{\delta_0} \psi^\varepsilon(nk)) \quad (n \neq 0), & W_{0,0} & = D_t(J_{\delta_0} \gamma^\varepsilon(0)),
\end{align}

where $D$ denotes the centered difference operator, i.e., $D\eta(x) = \frac{\eta(x+\Delta x) - \eta(x-\Delta x)}{2\Delta x}$. 

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(4) Initialize \( i = 0 \). Do while \( i \leq M - 1 \),

\[
U_{i+1,n} = U_{i,n} + hQ_{i,n}, \quad n \neq 0, \tag{19}
\]
\[
Q_{i+1,n} = Q_{i,n} + h [\rho(\delta, nk)W_{i,n} - F_{i,n}], \tag{20}
\]
\[
W_{i+1,n} = W_{i,n} + hD_{t}(J\delta Q_{i,n}), \tag{21}
\]
\[
F_{i+1,n} = \rho((i + 1)h, nk)W_{i+1,n} - D_{x}(J\delta' Q_{i,n}). \tag{22}
\]

3. Stability and Convergence Analysis

In this section, we analyze the stability and convergence of the proposed marching scheme in (19)-(22).

Without loss of generality, from now on, we assume \( |\delta|_{-\infty} = \min(\delta, \delta', \delta'', \delta^*) \) and denote \( |Y|_{i} = \max_{n} |Y_{i,n}| \). To discuss the stability and convergence, two smoothing assumptions are also considered as follows,

\[
u(x, t) \in C^{2}(I \times I), \tag{23}
\]
\[
f(x, t) \in C(I \times I). \tag{24}
\]

**Theorem 3.1 (Stability of the Algorithm)** If Assumptions (23)-(24) holds, there exists a constant \( \Lambda \), such that

\[
\max\{|U_{M}|, |Q_{M}|, |W_{M}|, |F_{M}|\} \leq \Lambda \max\{|U_{0}|, |Q_{0}|, |W_{0}|, |F_{0}|\} \tag{25}
\]

**Proof.** For the operator \( D_{t} \), one can conclude that there exist a constant such as \( C \) where (theorem 3 in [16])

\[
|D_{t}(Q_{i,n})| \leq \frac{C}{|\delta|_{-\infty}}|Q_{i,n}|, \tag{26}
\]
\[
|D_{x}(Q_{i,n})| \leq \frac{C}{|\delta|_{-\infty}}|Q_{i,n}|. \tag{27}
\]

From (19) and (20), we also have

\[
|U_{i+1,n}| \leq (1 + h) \max\{|U_{i,n}|, |Q_{i,n}|\}, \tag{28}
\]
\[
|Q_{i+1,n}| \leq |Q_{i,n}| + h(M|W_{i,n}| + |F_{i,n}|) \leq (1 + Mh) \max\{|Q_{i,n}|, |W_{i,n}|, |F_{i,n}|\}, \tag{29}
\]

where \( M = \max_{(x,t)\in[0,1] \times [0,1]} \{\rho(x, t)\} \). Similarly, using (21) and (26), we have

\[
|W_{i+1,n}| \leq |W_{i,n}| + h \frac{C}{|\delta|_{-\infty}}|Q_{i,n}| \leq \left(1 + h \frac{C}{|\delta|_{-\infty}}\right) \max\{|Q_{i,n}|, |W_{i,n}|\}. \tag{30}
\]

Finally, we have from (22) and (27)

\[
|F_{i,n}| \leq M|W_{i,n}| + \leq \frac{C}{|\delta|_{-\infty}}|Q_{i,n}| \leq \left(M + \frac{C}{|\delta|_{-\infty}}\right) \max\{|W_{i,n}|, |Q_{i,n}|\}. \tag{31}
\]
Let $C_\delta = \max \left\{ 1 + h, 1 + Mh, 1 + h \frac{C}{\| \cdot \|_{-\infty}}, M + \frac{C}{\| \cdot \|_{-\infty}} \right\}$, then from (28)-(31) we obtain
\[ \max\{|U_{i+1}|, |Q_{i+1}|, |W_{i+1}|\} \leq (1 + hC_\delta) \max\{|U_i|, |Q_i|, |W_i|\}. \tag{32} \]

Now by applying (31), we have
\[ \max\{|U_{i+1}|, |Q_{i+1}|, |W_{i+1}|, |F_{i+1}|\} \leq (1 + hC_\delta) \max\{|U_i|, |Q_i|, |W_i|, |F_i|\} \leq (1 + hC_\delta) \max\{|U_i|, |Q_i|, |W_i|, |F_i|\}. \tag{33} \]

by iterating this last inequality $M$ times
\[ \max\{|U_M|, |Q_M|, |W_M|, |F_M|\} \leq (1 + hC_\delta)^M \max\{|U_0|, |Q_0|, |W_0|, |F_0|\}. \tag{34} \]

which means
\[ \max\{|U_M|, |Q_M|, |W_M|, |F_M|\} \leq (\exp C_\delta) \max\{|U_0|, |Q_0|, |W_0|, |F_0|\}. \tag{35} \]

Letting $\Lambda = \exp C_\delta$ completed the proof of this statement. \hfill \blacksquare

**Theorem 3.2 (The convergence of the algorithm)** For fixed $\delta$ as $h$, $k$ and $\varepsilon$ tend to zero, the discrete mollified solution converges to the mollified exact solution restricted to the grid points.

**Proof.** From the definitions of discrete error functions,

\begin{align*}
\Delta U_{i,n} &= U_{i,n} - v(ih, nk), & \Delta Q_{i,n} &= Q_{i,n} - v_x(ih, nk), \tag{36} \\
\Delta W_{i,n} &= W_{i,n} - v_t(ih, nk), & \Delta F_{i,n} &= F_{i,n} - f(ih, nk). \tag{37}
\end{align*}

Using Taylor series, we obtain some useful equations satisfied by the mollified solution $v$, namely,

\begin{align*}
v((i+1)h, nk) &= v(ih, nk) + hv_x(ih, nk) + O(h^2), \tag{38} \\
v_x((i+1)h, nk) &= v_x(ih, nk) + h(\rho(ih, nk)v_t(ih, nk) + f(ih, nk)) + O(h^2), \tag{39} \\
v_t((i+1)h, nk) &= v_t(ih, nk) + h \frac{d}{dt} v_x(ih, nk) + O(h^2). \tag{40}
\end{align*}

Furthermore
\begin{align*}
\Delta U_{i+1,n} &= \Delta U_{i,n} + (U_{i+1,n} - U_{i,n}) - (v((i+1)h, nk) - v(ih, nk)) \\
&= \Delta U_{i,n} + h(Q_{i,n} - v_x(ih, nk)) + O(h^2) \\
&= \Delta U_{i,n} + h \Delta Q_{i,n} + O(h^2). \tag{41}
\end{align*}
\[ \Delta Q_{i+1,n} = \Delta Q_{i,n} + (Q_{i+1,n} - Q_{i,n}) - (v_x((i+1)h, nk) - v_x(ih, nk)) \]
\[ = \Delta Q_{i,n} + h(\rho(ih, nk)W_{i,n} - F_{i,n}) \]
\[ - h(\rho(ih, nk)v_t(ih, nk) - f(ih, nk)) + O(h^2) \]
\[ = \Delta Q_{i,n} + h(\rho(ih, nk)\Delta W_{i,n} - \Delta F_{i,n}) + O(h^2). \]  
(42)

\[ \Delta W_{i+1,n} = \Delta W_{i,n} + (W_{i+1,n} - W_{i,n}) - (v_t((i+1)h, nk) - v_t(ih, nk)) \]
\[ = \Delta W_{i,n} + hD_t(J_{\delta}; Q_{i,n}) - hv_{st}(ih, nk) + O(h^2) \]
\[ = \Delta W_{i,n} + h(D_t(J_{\delta}; Q_{i,n}) - v_{st}(ih, nk)) + O(h^2). \]  
(43)

Since
\[ \Delta F_{i,n} = \rho(ih, nk)\Delta W_{i,n} + (D_x(J_{\delta}; Q_{i,n}) - v_{xx}(ih, nk)), \]  
(44)
we have
\[ \Delta Q_{i+1,n} = \Delta Q_{i,n} + h(D_x(J_{\delta}; Q_{i,n}) - v_{xx}(ih, nk)) + O(h^2). \]  
(45)

Now from equalities (41), (43) and (45), and using the error estimates of discrete mollification (Proposition 1 in [16]), we have
\[ |U_{i+1,n}| \leq |U_{i,n}| + h|\Delta Q_{i,n}| + O(h^2), \]  
(46)
\[ |\Delta Q_{i+1,n}| \leq |\Delta Q_{i,n}| + h|D_x(J_{\delta}; Q_{i,n}) - v_{xx}(ih, nk)| + O(h^2) \]
\[ \leq |\Delta Q_{i,n}| + h\left( C\frac{|\Delta Q_{i,n}|}{|\delta|_{-\infty}} + C_{\delta}h^2 \right) + O(h^2), \]  
(47)
\[ |\Delta W_{i+1,n}| \leq |\Delta W_{i,n}| + h|D_t(J_{\delta}; Q_{i,n}) - v_{st}(ih, nk)| + O(h^2) \]
\[ \leq |\Delta W_{i,n}| + h\left( C\frac{|\Delta Q_{i,n}|}{|\delta|_{-\infty}} + kC_{\delta}h^2 \right) + O(h^2). \]  
(48)

Suppose
\[ \Delta_i = \max\{|\Delta U_{i,n}|, |\Delta W_{i,n}|, |\Delta Q_{i,n}|\}, \]  
(49)
\[ C_0 = \max\left\{ 1, \frac{C}{|\delta|_{-\infty}} \right\}, \]  
(50)
\[ C_1 = \left\{ \frac{Ch}{|\delta|_{-\infty}} + C_{\delta}h^2, \frac{Ck}{|\delta|_{-\infty}} + C_{\delta}h^2 \right\}. \]  
(51)

Then we obtain
\[ \Delta_{i+1} \leq (1 + hC_0)\Delta_i + hC_1 + O(h^2) \]
\[ \leq (1 + hC_0)(\Delta_i + C_1) + O(h^2), \]  
(52)
and after \( L \) iterations
\[ \Delta_L \leq \exp(C_0)(\Delta_0 + C_1). \]  
(53)
Moreover from
\[ |\Delta U_{0,n}| = |U_{0,n} - v(0,nk)| = |J_{\delta_{0}}\psi^{\varepsilon}(nk) - v(0,nk)| \leq C(\varepsilon + k), \]
\[ |\Delta Q_{0,n}| = |Q_{0,n} - q(0,nk)| = |K(0)J_{\delta_{0}}\varphi^{\varepsilon}(nk) - K(0)v_x(0,nk)| \]
\[ = |K(0)||J_{\delta_{0}}\varphi^{\varepsilon}(nk) - v_x(0,nk)| \leq MC(\varepsilon + k), \]
\[ |\Delta W_{0,n}| = |D_t(J_{\delta_{0}}\psi^{\varepsilon}(nk)) - v_t(0,nk)| \leq \frac{C}{\delta_{0}}(\varepsilon + k) + C_{\delta}k^2, \]
we see that when \( \varepsilon, h, \) and \( k \) tend to 0, then \( \Delta_0 \) and \( C_1 \) tend to 0 too. Consequently \( (\Delta_0 + C_1) \) tends to 0 and so does \( \Delta_L \) and this complete the proof of this theorem. ■

4. Numerical experiments

In this section to show the efficiency of the proposed mollified marching scheme we discuss the implementation of our numerical method to solve two standard test problems. For the experiments we use MATLAB 10 under Windows 7 Professional X64. The radii of mollification are always chosen automatically using the mollification and GCV methods and in all cases, without loss of generality, we set \( p = 3 \) (see [15, 17]).

Discretized measured approximations of boundary data are modeled by adding random errors to the exact data functions. For example, for the boundary data function \( h(x,t) \), its discrete noisy version is generated by
\[ h_{\varepsilon,j,n} = h(x_j, t_n) + \varepsilon_{j,n}, \quad j = 0, 1, \ldots, N, n = 0, 1, \ldots, T, \]
where the \( \varepsilon_{j,n} \)'s are Gaussian random variables with variance \( \varepsilon^2 \).

The errors between the exact and approximate solutions are measured by the absolute error norm and the relative weighted \( l^2 \) error norm given by
\[
\text{Norm}(v,U) = \left\{ \frac{(1/(M+1)(N+1))\sum_{i=0}^{M}\sum_{j=0}^{N}|v(ih,jl) - U_{i,j}|^2}{(1/(M+1)(N+1))\sum_{i=0}^{M}\sum_{j=0}^{N}|v(ih,jl)|^2} \right\}^{1/2}.
\]

Solving the solution, first \( v(x,t) \), \( f(x,t) \) are determined from (14)-(18) by the proposed marching method and then \( \eta \) will be determined by introducing \( A_n \) as follows.
\[
A_n = \frac{f(ih,jk) - h(ih,nk)}{g(ih,nk)},
\]
\[
\text{Computed } \eta = \min_{0 \leq n \leq N} \{ A_n \text{ Norm}(A_n, \text{Exact } \eta) \}.
\]

Example 4.1 As the first test case, in equations (14)-(18) consider
\[
\rho(x,t) = 1, \quad g(x,t) = e^t + 2, \quad h(x,t) = \frac{3e^t - 3e^{t+4x} + 6}{e^{2x}},
\]
\[
\gamma(x) = e^{2x}, \quad \psi(t) = e^t, \quad \varphi(t) = 2e^t.
\]
The exact analytical solution of this problem can be derived as

\[ u(x,t) = 2e^{t+2x}, \quad \eta(x) = -\frac{3}{e^{2x}}. \]

Table 1 illustrates the relative $l_2$ errors between the exact and computed $v$ and its derivatives in three different noise levels for $M = N = 64, 128, 256, 512$ and 1024.

<table>
<thead>
<tr>
<th>$M = N$</th>
<th>$\varepsilon$</th>
<th>$v$</th>
<th>$v_t$</th>
<th>$v_x$</th>
<th>$\eta$</th>
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<td>0.0001</td>
<td>0.051216</td>
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</table>

Figure 1 illustrates the difference between computed and exact $\eta$ for $M = N = 512$ in three noise levels.

**Example 4.2** As the first test case, in equations (6)-(9) consider

\[ \rho(x,t) = 1, \quad g(x,t) = e^t + 2, \]
\[ h(x,t) = -\sinh(x^2 + t + 2) - \cosh(x^2 + 2) \ (e^t + 2) - 4x^2 \cosh(x^2 + t + 2), \]
\[ \gamma(x) = \cosh(x^2 + 2), \quad \psi(t) = \cosh(t + 2), \quad \varphi(t) = 0. \]
The exact analytical solution of this problem can be derived as

\[ u(x,t) = \cosh(x^2 + t + 2), \quad \eta(x) = \cosh(x^2 + 2). \]

Table 2 illustrates the relative \( l_2 \) errors between the exact and computed \( v \) and its derivatives in three different noise levels for \( M = N = 64, 128, 256, 512 \) and 1024.

<table>
<thead>
<tr>
<th>( M = N )</th>
<th>( \varepsilon )</th>
<th>( v )</th>
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Figure 2 illustrates the difference between computed and exact \( \eta \) for \( M = N = 512 \) in three noise levels.

![Figure 2](image.png)

Figure 2. \( v \)'s relative \( l_2 \) error norm for example 4.2.

5. Conclusion

The physical problem considered in this paper consists of predicting the energy absorption coefficient of an internal combustion engine considering some noises in the initial, boundary and overdetermination conditions. A regularization approach based on the mollification method and the space marching scheme is developed to solve the proposed inverse problem numerically and the missing terms. The stability and convergence of the solution of the proposed numerical approach are
proved and some examples are investigated to support the main results of this work.

References


