Optimizing electro-thermo fields for soot oxidation using microwave heating and metal

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Abstract. Soot is produced by incomplete combustion of various carbon-containing compounds. Soot is one of the main environmental pollutants and has become an important environmental and specific objective. To reduce soot from exhaust emission of diesel engine, a new technique is proposed and implemented by using metal inserted in the soot exposed to electromagnetic radiation. This paper presents a simulation to obtain optimum metal length and shape that give optimum electric field for attaining temperature enough for soot oxidation using microwave heating and a thin metal rod. Four cases were numerically examined to investigate the electric field and temperature distributions in a mono-mode TE$_{10}$ microwave cavity having closed surfaces of perfect electric conductors. The operating frequency is 2.45 GHz, and power supply is 1500 W. The simulation methodology is coupling the absorbed electromagnetic energy with heat transfer energy. The absorbed electromagnetic energy is found from the electric field within the soot. The simulation was run using ANSYS based on finite element method. The results of the four simulation cases show that the optimum simulation is represented by case 2 where the value of electric field is 39000 V/m and heating time to arrive at the oxidation temperature (873 K) is 35 s using cylindrical metal rod of 8 mm length. It is revealed that the concept of achieving high temperature for soot oxidation by using thin metal rod inside a microwave cavity can be applied.

1. Introduction
Soot is elemental, amorphous, and black carbon. Soot consists of spherical particles with primary diameter between 10 to 500 nm [1]. It is agglomerated to form chainlike spherical particles with 100 to 800 nm [2]. Production of soot represents incomplete combustion; therefore it is usually undesirable because it causes air contamination and pollution, absorption of solar radiation and health hazard. After-treatment devices are used in diesel engines to filter and trap the soot particles in the exhaust gas with efficiency among 50% to 90% [3]. But the increasing of trapped soot in the filter leads to close the filter after a period of time and increases the back pressure. The higher back-pressure causes temperatures and pressures rise in the intake and exhaust lines, that resulting in some fuel penalty and changing the engine working conditions [4]. So periodically, a controlled regeneration process is required to oxidize the soot particulates at ignition temperature (600°C). In order to obtain a high temperature, a microwave heating was used and simulated in the literature to determine the electric
field and temperature distribution on dielectric materials. Tada et al. [5] solved Maxwell equations employing two-dimensional finite difference time domain (FDTD) to investigate the electromagnetic field in a microwave applicator filled partially with a dielectric material, operating in the dominant TE10 mode at a frequency of 2.45 GHz. The electric field and power distributions were predicted for a lossy material and the results showed the electric field varies with dielectric material properties and position in a microwave cavity. Huang et al. [6] solved the coupled electromagnetic field equations, reaction equation and heat transport equation by using FDTD method to predict temperature rising and transmitted power through the electromagnetic cell and the findings indicated that electromagnetic energy is absorbed by the dielectric material and dissipated as heat energy leading to increase in the material temperature. Makul et al. [7] analyzed heat generation by microwave energy inside hardened cement paste. Electromagnetic distribution inside a rectangular wave guide and thermal models were taken into account. The compressive strength of the hardened cement paste increases and then slightly decreases from 14-18 days. Ciacci et al. [8] proposed two-dimensional mathematical model for the microwave-induced pyrolysis of wood block, based on a close combination of the propagation and absorption of electromagnetic waves into the material and heat/mass transfer with chemical reactions using a quasi-steady approximation for the electromagnetic field. The comparison with external heating showed that the differences are not only for the spatial temperature distribution, conversion rates and species densities but also for the weight loss characteristics. Salvi et al. [9] simulated numerically temperature profile in Newtonian fluids during continuous flow microwave heating by one way coupling electromagnetism, fluid flow, and heat transport in ANSYS and COMSOL Multiphysics softwares. They reported that the simulation of power loss distributions and temperature profiles are in close agreement by both softwares. Theoretical and experimental researches were conducted on materials mixed with metal powder for material sintering [10]. Experimentally proved there is no temperature rise for solid metal bar exposed to electric and magnetic fields in a microwave heating [11]. The numerical model of susceptor-assisted microwave heating reveals that the maximum temperature increase by using susceptor and the efficiency of the microwave heating depends on the sample size and thermal conductivity [12]. The theoretically and experimentally finding of thick metal objects post in a microwave oven reflect the microwave, while thin metal forms electric current on the metal surface [13].

In order to obtain high temperature in short time for soot microwave heating and oxidation with lower power consumption, a new technique is presented in this paper. This technique is inserting metal in the soot exposed to electromagnetic radiation. The formed electric field and temperature distribution were optimized numerically by conducting four simulation cases using ANSYS based on finite element method (FEM).

2. Problem formulation
The geometry of the analysis includes a microwave cavity WR430 [14] with dimensions (a= 0.10922 m on x-axis, b= 0.05461 m on y-axis and λg/2 = 0.07386 m on z-axis). Where λg/2 is half waveguide wavelength on z-axis. The cavity contains cylindrical sample of soot and cylindrical aluminum rod (the dimensions as mentioned in Table 1). The center of the soot is located in the center of x and y axes and 0.4λg in z-axis. The rod is posted vertically in the center of the sample as depicted in figure 1.
3. Methods
The governing equations of the electric field, absorbed electromagnetic energy and heat transfer equations in a microwave cavity are described in the following.

3.1. Electric field in a microwave
Maxwell’s equations represent the coupling of unsteady electric, $E$ and magnetic $H$ field components. The wave has only one component of electric field and one component of magnetic field that are transverse to the direction of propagation. Therefore Maxwell’s equations can be presented in terms of a transverse electric field (TE) or transverse magnetic field (TM) wave equation. To study the microwave heating, it is useful to present Maxwell’s equations as one equation in terms of a steady transverse electric field equation called Helmholtz equation (1) for inhomogeneous vector wave [16].

$$\nabla \times \nabla \times E = \left( \omega^2 \mu_0 \mu_r \varepsilon_0 \left( \varepsilon'_r - j \varepsilon''_r \right) - j \omega \mu_0 \mu_r \sigma \right) E$$

(1)

Complex permittivity $\varepsilon_r$ is equal to:

$$\varepsilon_r = \varepsilon'_r - j \varepsilon''_r$$

(2)

Let:

$$\gamma^2 = -\omega^2 \mu_0 \mu_r \varepsilon_0 \varepsilon'_r \left[ 1 - j \left( \frac{\varepsilon''_r}{\varepsilon'_r} + \frac{\sigma}{\omega \varepsilon_0 \varepsilon'_r} \right) \right]$$

(3)

Replacing equation (3) into equation (1) gives:

$$\nabla \times \left( \nabla (\nabla E) \right) + \gamma^2 2E = 0$$

(4)

The solution of Laplace’s equation (4) is:

$$E = E_0 e^{-\gamma^2 x y z}$$

(5)

3.2. Electric field at the surfaces boundaries
The boundary conditions (BC) of the cavity are perfect electric conductor (PEC), so the tangential component of the electric field is equal to zero on the cavity surfaces. At incident port, a continuous transverse electric field mode $10$ (TE$_{10}$) is implemented in a rectangular waveguide WR430 and shorting port at end of the waveguide in propagation direction ($z$-axis). Then the components of $E$ are:

$$E_x = 0, \ E_z = 0$$

(6)
\[ E_y = E_0 e^{-y^2xz} \]  

### 3.3. Electric field at the incident port

The following mathematical model was formed to apply boundary condition at incident port of waveguide and represent the electric field in relation to source power.

\[ E_y = \sqrt{2P_0/\beta_0 \cdot (a \cdot b)} \ e^{-y^2xz} \]  

Where \( P_0 \) is input power at waveguide incident port.

\[ \beta_0 = \sqrt{(1 - (f_c/f)^2)/(\mu/\varepsilon)} \]  

Where:

\[ f_c = \left( \frac{1}{2\pi\sqrt{\mu\varepsilon}} \right) \sqrt{(m\pi/a)^2 + (n\pi/b)^2} \]  

\( m \) and \( n \) are integers numbers of sinusoidal half wavelength variation in x and y axes. \( a \) and \( b \) are dimensions of wave incident plane in x and y axes.

### 3.4. Absorbed electromagnetic energy

The absorbed electromagnetic energy is dissipated as thermal energy within the material inside a closed surfaces microwave cavity as in following equation

\[ P_{abs} = J_{HEAT} = \left( \frac{1}{2} \right) \omega \varepsilon_0 \left( \epsilon_r'' + \sigma/\omega\varepsilon_0 \right) |E|^2 \]  

\( P_{abs} \) is the average volumetric absorbed power dissipated into heat \( (J_{HEAT}) \)

### 3.5. General Transient Heat Transfer

Heat transfer equation is given by [17]:

\[ -\iiint \left[ \frac{\partial}{\partial x} \left( k_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( k_y \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( k_z \frac{\partial T}{\partial z} \right) - J_{HEAT} + \rho c_p \frac{\partial \theta}{\partial \tau} \right] dv = 0 \]  

The boundary conditions (BC) are:

a. Heat convection BC

\[ k_x \frac{\partial T}{\partial x} \cos \theta_x + k_y \frac{\partial T}{\partial y} \cos \theta_y + k_z \frac{\partial T}{\partial z} \cos \theta_z = -h(T - T_a) \]  

b. Heat flux BC

\[ k_x \frac{\partial T}{\partial x} \cos \theta_x + k_y \frac{\partial T}{\partial y} \cos \theta_y + k_z \frac{\partial T}{\partial z} \cos \theta_z = -q \]  

Where, \( \cos \theta \) is the direction normal to the surface of heat transfer \( (ds) \)

The initial condition is:

\[ T = T_i \ at \ time = 0 \]

After the substitution of equation (13) and equation (14) in equation (12), the general heat transfer equation in FEM will be obtained [18]:

\[ -\iiint \left[ \frac{\partial}{\partial x} \left( k_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( k_y \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( k_z \frac{\partial T}{\partial z} \right) - J_{HEAT} + \rho c_p \frac{\partial \theta}{\partial \tau} \right] dv - \iint q ds \]

\[ -\iint h(T - T_a) ds = 0 \]
4. Numerical analysis
The simulation was conducted by using finite element method of ANSYS software. The simulation couples the harmonic high frequency electromagnetic analysis with transient thermal analysis to find the electric field distribution in the microwave cavity and dissipated heat and temperature distribution in the soot contains metal object and posts inside a mono-mode TE\(_{10}\) microwave cavity WR430, working under a frequency of 2.45 GHz and 1500 W power supply. Investigation of the temperature distribution during a microwave heating process is obtained by coupling the equations of absorbed electromagnetic energy (dissipated heat) with heat transfer energy. The absorbed energy is found from the electric field formed from the interaction of electromagnetic wave with metal and dielectric material. The dissipated heat was applied as elements body load in thermal analysis.

The inputs of High Frequency Electromagnetic code are dielectric properties of air \((\mu_r = 1, \varepsilon_r' = 1)\), soot \((\mu_r = 1, \varepsilon_r' = 8.6, \varepsilon_r'' = 7.4)\) [18] and metal rods \((\mu_r = 1, \varepsilon_r' = 1, \tan \delta = \sigma / 2\pi f \varepsilon_0 \varepsilon_r')\). The boundary conditions for the cavity are perfect electric conductor surfaces on \(x\) and \(y\) axes and mono-mode incident port (TE\(_{10}\)) and shorter port with distances equal to \(+\lambda_g/2\) and \(-\lambda_g/2\) on \(z\)-axis respectively. Element type for high frequency electromagnetic code is tetrahedral solid (HF119).

The inputs of Transient Thermal code are thermal properties (density, specific heat and thermal conductivity) of the soot and the metal object. The thermal boundary condition is 9 W/m\(^2\)K heat transfer coefficient for soot. Conduction heat transfer was used between the soot and metal object (aluminum). The initial condition is 25°C. The soot reduction was presented by “killing” each element upon attaining the oxidation temperature of 600°C. The analysis is nonlinear so the solution process requires some intermediate equilibrium steps to correct the heat flow. This is accomplished by step-by-step incremental analysis to reach applied heat at time \(n\) and performing Newton-Raphson iteration at each step. Auto time step was selected by program according to Newton-Raphson method for nonlinear equations controlled between (0.001-0.25) s. Element type is tetrahedral (Solid87).

The simulation is based on mesh independency test using 10 elements per each dimension for the cavity, 20 elements per each dimension for soot, and 0.0002 m element size for metal.

In order to apply the simulation, some reasonable assumptions were made, these are: The simulation work did not deal with chemical reaction. KILL command was used to remove soot elements of temperature more than 600°C. The working substance is soot powder which was treated as a packed bed in the simulation work.

5. Results and discussion
For the purpose of soot oxidation strategy many simulation cases were conducted to obtain optimum electric field to control the temperature distribution by using high frequency electromagnetic radiation and metal objects inside a microwave cavity. Table 1 explains the results of four simulation cases that were conducted to compare and discuss the effect of length and shape of metal rod on the formed electric field and temperature inside the soot.

| Case No. | Metal Rod | Max. \(E_{\text{sum}}\) inside the soot | Time of Oxidation |
|----------|-----------|--------------------------------------|-------------------|
|          | Length (mm) | Diameter (mm) | Shape | (v/m) | (873 K) | (s) |
| 1        | 2          | 1          | cylinder | 15,000 |         | 78.5 |
| 2        | 8          | 1          | cylinder | 39,000 |         | 35  |
| 3        | 2          | 1          | cone    | 61,000 |         | 48  |
| 4        | 8          | 1          | cone    | 610,000|         | not limited |
5.1. Effect of metal rod length on electric field and temperature distribution

Case 1 reveals the maximum value of $E$ formed at rod tips (2 mm length) posted inside a soot sample located in a microwave cavity is 15 kV/m as depicted in figure 2. Where the rod tips represent the positive and negative terminals and the rod middle is neutral. The difference in the temperatures are about 2 K due to small sample dimensions and the temperature at sample tips are higher than the middle section (as shown in figure 6) due to the effect of $E$ on dissipated heat according to equation 11. The heating time for whole soot oxidation is 78.5 s as reported in Table 1.

Case 2 implies the value of maximum $E$ is 39 kV/m as displayed in figure 3. The difference in the temperatures between sample middle and tips are more than 10 K as modeled in figure 7. The increase in the value of maximum E resulted from the increase in rod length from 2 mm to 8 mm according to equation 5 and the increased $E$ led to increase the temperature close to rod terminals while the temperature at the sample middle stay close to initial temperature as shown in figure 7a. The time of heating for whole soot oxidation is 35 s as recorded in Table 1. The comparison between cases 1 and 2 shows there is a reduction in oxidation time in case 2 due to the higher temperature resulted from higher formed $E$ in case 2.

5.1. Effect of metal rod shape on electric field and temperature distribution

Case 3 shows the maximum amount of $E$ is 61 kV/m formed at the head of the metal cone where the cone have a 2 mm length and a point head as presented in figure 4. This means the energy is focused in one direction by tapered rod (cone), so it is increased. Also as in case 1 there is small difference in temperature between tips and middle as shown in figure 8a. The time for whole soot oxidation is 48 s heating. The comparison between cases 1 and 3 show about 40% of the oxidation time is reduced due to the energy focusing by using the short conical rod.

Case 4 indicates that the higher $E$ is obtained by using conical shape metal with 8 mm length, where the value of $E$ attained 610 kV/m at cone head as simulated in figure 5. The increasing in cone length leads to increase the focusing of $E$ as mentioned in case 2. The predicted difference in the temperatures between the sample bottom tip and middle are more than 100 K (as shown in figure 9a) due to the very high $E$ formed at cone tip. The soot oxidation at sample tips achieved after 18 s heating as shown in figure 9b, but the noticed there is no oxidation for the whole soot where the same quantity of soot still not oxidized during the time from the 20th second to 60th second due to the reduction in temperature in spite of continuous microwave heating as shown in figures 9c and 9d. The reason of this unexpected phenomenon belongs to the rapid oxidation of elements at the high temperature (the sample tips). The rapid oxidation did not give enough time to increase the temperature of middle elements due to the heat flow by conduction from high to low temperature. Consequently the remaining soot temperature was decreased with time progress due to the generated heat at middle of the sample is less than the lost heat by convection.
Figure 2. Electric field distribution of case 1

Figure 3. Electric field distribution of case 2
Figure 4. Electric field distribution of case 3

Figure 5. Electric field distribution of case 4
Figure 6a. Temperature distribution of the sample at 1s, case 1

Figure 6b. Temperature distribution of the sample at 78s, case 1

Figure 7a. Temperature distribution of the sample at 1s, case 2

Figure 7b. Temperature distribution of the sample at 34s, case 2
Figure 8a. Temperature distribution of the sample at 1s, case 3

Figure 8b. Temperature distribution of the sample at 47s, case 3

Figure 9a. Temperature distribution of the sample at 1s, case 4

Figure 9b. Temperature distribution of the sample at 18s, case 4
6. Conclusions

This work presents a new technique to get locally high electric field to obtain rapidly high temperature for soot oxidation by using microwave heating and thin metal objects inside a microwave cavity. Four cases were examined numerically to simulate the electric field and temperature distribution. The methodology of simulation was implemented using ANSYS based on FEM. The findings from the results are:

- The increasing of electric field leads to increase dissipated heat and consequently increase material temperature.
- The metals inside a sample redistribute the electric fields with high and low values.
- Case 2 represents the optimum simulation for the value of electric field is 39000 V/m, and heating time to arrive oxidation temperature (873 K) is 35 s using cylindrical metal rod 8 mm length.
- The technique of achieving high temperature for soot oxidation by using metal object inside a microwave cavity can be applied. The temperature distribution can be controlled by size and shape of metal object.

Nomenclature

- $C_p$: Specific heat
- $D$: Electric flux vector
- $ds$: Surface integral
- $dv$: Volume integral
- $E_0$: Amplitude of electric field intensity
- $f$: Operating frequency
- $f_c$: Cutoff frequency
- $h$: Heat transfer coefficient
- $k$: Thermal conductivity
- $I$: Current
\( j \)  Imaginary part of a complex number
\( T \)  Temperature
\( t_a \)  Ambient temperature
\( t_i \)  Initial temperature
\( Z_0 \)  Intrinsic impedance for medium
\( Z_{xy} \)  Transverse wave impedance
\( \gamma \)  Complex propagation constant
\( \varepsilon \)  Complex Permittivity
\( \varepsilon_0 \)  Permittivity of vacuum or air (8.854x10^{-12} \text{ F/m})
\( \varepsilon_r' \)  Relative dielectric constant
\( \varepsilon_r'' \)  Relative dielectric loss factor
\( \lambda_c \)  cutoff wavelength
\( \lambda_g \)  waveguide wavelength on z-axis
\( \lambda_f \)  Free space wavelength
\( \mu \)  Magnetic permeability
\( \mu_0 \)  permeability of vacuum or air (1.257x10^{-6} \text{ H/m})
\( \mu_r \)  Relative permeability
\( \rho \)  Density
\( \sigma \)  Electric conductivity
\( \omega \)  Angular frequency

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