Modelling radiative properties of participating species in a microwave plasma reactor for diamond deposition

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Abstract. The paper details the modelling of radiation in a microwave assisted plasma reactor used to deposit synthetic diamond over a substrate. The main radiatively active constituents in the reactor are atomic and molecular hydrogen, acetylene, methane and soot (if produced). Radiation from hydrogen occurs in ultraviolet (UV) whereas the hydrocarbons are active in the infrared region. Soot absorb and scatter in the UV but only absorption is important in the infrared-visible (IR-V) region. Hence, the two spectral regions have been treated independently. A two temperature model has been adopted for hydrogen thermodynamic state where $T_g$ represents rotational, vibrational and translational temperature and $T_e$ represents electronic excitation temperature. As scattering is significant in UV, the radiative transfer equation is solved using Discrete Ordinate Method (DOM) with cumulative-k narrow-band model for molecular hydrogen. Radiation from atomic hydrogen has been found to be negligibly small compared to molecular hydrogen. In the IR-V, radiative transfer equation is solved using ray tracing method with gas properties represented by statistical narrow-band models. Preliminary simulations for reactor conditions indicate that soot significantly increase the radiative transfer in the reactor and presence of soot can disrupt the operation of the plasma reactor.

1. Introduction

Low pressure hydrogen methane plasmas generated using microwave resonating cavities can be used to deposit synthetic diamond on a substrate. A comprehensive review of the modelling diamond deposition process in plasma reactors is provided by Hassouni et al \cite{1}. Understanding different mechanisms in the deposition is critical to produce diamonds of high quality. The number of parameters affecting the deposition process is large and it is desired to develop numerical models that take into account the different mechanisms in the medium. Such a development would assist in understanding and optimizing the process.

In line with the objective, it is intended to model radiative transfer in the plasma reactor which may effect temperature levels, composition, and flow fields. This work concerns modelling the radiative properties of the main participating species in the plasma reactor and solving the radiative transfer equation (RTE) in a two dimensional axi-symmetric domain. The present model will be coupled with plasma and flow multi-physics models in the future. Owing to simulated plasma composition \cite{1}, the main radiatively active constituents of the plasma reactor are molecular and atomic hydrogen, hydrocarbons such as methane, acetylene, and soot. Table
1 summarizes the radiative model developed for Ultraviolet (UV) and Infrared-Visible (IR-V) regions respectively. The following sections discuss the details of modelling of radiative properties of different constituents in the plasma reactor and present some preliminary results of radiative transfer for representative reactor conditions.

### Table 1. Description of radiative transfer model in UV and IR-V spectrum.

|        | UV                  | IR-V                |
|--------|---------------------|---------------------|
| \( \nu \text{ cm}^{-1} \) | 60000 to 120000     | 25 to 30000         |
| Soot   | Absorption and scattering | Absorption only     |
| Gas    | Molecular Hydrogen under NLTE | Acetylene and methane |
| Narrow band model | Cumulative-k distribution | Statistical narrow-band |
| RTE    | Discrete ordinate method | Ray tracing         |

2. Radiative properties of participating species

A medium can interact with radiation either by emission, absorption or scattering. The Radiative Transfer Equation (RTE) accounts for the change in the spectral intensity \( I_\nu (s, \Omega) \) along abscissa \( s \), at wavenumber \( \nu \) and direction \( \Omega \), resulting from these mechanisms

\[
\frac{\partial}{\partial s} I_\nu (s, \Omega) = \eta_\nu + \frac{\sigma_\nu}{4\pi} \int_{4\pi} \Phi_\nu(\Omega', \Omega) I_\nu (s, \Omega') d\Omega' - (\kappa_\nu + \sigma_\nu) I_\nu (s, \Omega),
\]

where \( \eta_\nu, \kappa_\nu \), and \( \sigma_\nu \) are respectively emission, absorption and scattering coefficients and \( \Phi \) is the scattering phase function. Molecular spectra of hydrogen and hydrocarbons display large number of lines and line-by-line computation is expensive. Rather, narrow-band models are used to approximate the radiative properties. The choice of the computational model used for RTE solution depends on the narrow-band model of the gas as well as radiative properties of soot. Hydrogen is active in the UV whereas hydrocarbons are mainly active in the IR-V region. Concerning soot, their albedo in the Rayleigh limit scales as \( \nu^3 \). Therefore, scattering can be neglected in the IR-V but must be taken into account in addition to emission and absorption in the UV region. Both molecular and atomic hydrogen in the plasma zone of the reactor are at non-equilibrium and a two temperature model is adopted in this study, i.e., an electronic temperature \( T_e \) and vibration-rotation-translation temperature \( T_g \) for heavy particles. The typical conditions in the plasma reactor are given in table 2 (adapted from collisional-radiative calculations of Hassouni et al [2]). Other constituents are assumed to be at local thermal equilibrium at \( T_g \). Hence, to simplify RTE solving, the two spectral regions are considered separately. In the IR-V region, statistical narrow-band (SNB) model [3] has been chosen for modelling the radiative properties of the hydrocarbons due to its ability to treat arbitrary mixture of absorbing gases. The RTE in the IR-V is solved using a ray tracing method. As soot scatters in the UV region and since SNB models are not compatible with scattering and deterministic ray tracing, the RTE in UV region is solved using Discrete Ordinates Method (DOM) [4] coupled with cumulative-k (CK) narrow band model [3] for hydrogen.

2.1. Molecular hydrogen

Line data in UV spectrum (Lyman and Werner bands) for molecular hydrogen have been taken from Abgrall et al [5]. The database provides for each line \( i \) lower and upper rotational \( (J) \) and vibrational \( (v) \) quantum numbers, Einstein coefficient \( A_{ul} (s^{-1}) \) and the transitional wavenumber \( \nu_i (cm^{-1}) \) for \( B^1\Sigma_u^+ \rightarrow X^1\Sigma_g^+ \) (19585 transitions) and \( C^1\Pi_u \rightarrow X^1\Sigma_g^+ \) (8881 transitions) band systems. The energy levels of \( B^1\Sigma_u \) and \( C^1\Pi_u \) states with respect to \( v = 0, J = 0 \) of \( X^1\Sigma_g^+ \)
Table 2. Typical conditions inside the plasma reactor (adapted from Hassouni et al [2]).

| Microwave power density (W cm⁻³) | p (Pa) | T_g (K) | T_e (K) |
|----------------------------------|--------|---------|---------|
| 4.5                              | 1400   | 1585    | 5763    |
| 9                                | 2500   | 2059    | 5670    |
| 15                               | 5200   | 2702    | 5462    |
| 22                               | 8400   | 3204    | 5328    |
| 30                               | 11000  | 3410    | 5217    |

state have been calculated from ground state level energies provided by Dabrowski [6]. Spectral emissive power and absorption coefficient are calculated as

\[ \eta_i(\nu) = \frac{N_u A_u l h \nu c f(\nu - \nu_i)}{(W m^{-3} sr^{-1} cm)}, \]
\[ \kappa_i(\nu) = N_u A_u \frac{l}{8 \pi r^2 c} \left( \frac{N_i}{N_u} - 1 \right) f(\nu - \nu_i) \ (m^{-1}). \]  

where \( g_u/l \) is the level degeneracy given by \( 2J + 1 \), \( N_u \) and \( N_i \) are the number densities of the two levels and \( f(\nu - \nu_i) \) is the normalized profile of the line. Voigt profile is used for the line shape with collision broadening width, roughly estimated as \( \gamma_c = 0.1 (273/T_g)^{0.7} \) [7], and Doppler broadened line width \( \gamma_d = \frac{\nu}{c} \sqrt{2kT_d/n2/m} \). The number density of an energy level \((n, v, J)\) is given by

\[ N_{n,v,J} = \frac{g_s(2J + 1) \exp \left( -\frac{E_n}{kT_e} \right) \exp \left( -\frac{E_{vr,n}}{kT_g} \right)}{Q(T_g, T_e)} \]  

where \( E_n \) and \( E_{vr,n} \) are the electronic and vibrational-rotational energies respectively, \( g_s \) is the nuclear statistical weight and \( N \) is the number density of hydrogen molecules which can be calculated using ideal gas law \((N = x p / kT)\). The molecular partition function for the two temperature non-equilibrium model can be written as

\[ Q(T_g, T_e) = \sum_n \sum_{v,J} \exp \left( -\frac{E_n}{kT_e} \right) g_s(2J + 1) \exp \left( -\frac{E_{vr,n}}{kT_g} \right). \]  

Solution of RTE under non-equilibrium conditions requires modelling of both absorption and emission coefficients. Integrating the RTE over a ray between 0 and \( s \) gives

\[ I_\nu(s) = \tau_\nu(0, 0) I_\nu(0) + \int_0^s \frac{\eta_\nu(s') \partial \tau_\nu(s', s)}{\kappa_\nu(s')} ds' \]  

where \( \tau_\nu(s', s) \) is the spectral transmissivity of the path \( s' \rightarrow s \). Averaging the above equation over a narrow spectral band gives

\[ \bar{I}^{\Delta \nu}(s) = \frac{\tau_\nu(0, 0) I_\nu(0)^{\Delta \nu}}{\tau_\nu(s', s)^{\Delta \nu}} + \int_0^s \frac{\eta_\nu(s') \partial \tau_\nu(s', s)}{\kappa_\nu(s')} ds' \]  

Thus, for accurate approximation of spectrally averaged emission, the narrow band model has to accurately predict the spectrally averaged kernel of Eq. 6. \( \eta_\nu \) and \( \tau_\nu \) are strongly correlated for molecular band systems. This can be confirmed from figure 1 where the comparison between \( \eta_\nu \tau_\nu \) and \( \bar{I}^{\Delta \nu} \) for \( B \rightarrow X \) band systems is poor. However Lamet et al [8] have shown that

\[ \frac{\eta \partial \tau(s, s')^{\Delta \nu}}{\kappa} \approx \frac{\bar{I}^{\Delta \nu}}{\kappa} \frac{\partial \tau(s, s')^{\Delta \nu}}{\partial s'} \]  

(7)
Figure 1. Correlation between emission and transmission for pure molecular hydrogen over path length 1 cm and pressure $p = 0.1$ bar for $B^1\Sigma_u^+ \rightarrow X^1\Sigma_g^+$ at $T_e = 5500$ K and $\Delta \nu = 1000$ cm$^{-1}$ for two values of gas temperature.

is a good approximation over the narrow band for a given electronic system. Hence, $\bar{\eta}/\kappa$ can be tabulated and the transmissivities can be evaluated using the CK model [3]. For overlapping electronic systems like $B \rightarrow X$ and $C \rightarrow X$ in our case, the two systems must be treated as belonging to two different gases, for the above decorrelation approximation (Eq. 7) to remain accurate. Moreover, the mixture transmissivity can be accurately calculated as the product of single transmissivities.

In the CK model, knowledge of line positions is unnecessary for computation of transmissivities and absorption coefficient distribution function is sufficient. Further, the spectrally averaged intensities are calculated using the smooth cumulative distribution functions and quadratures. CK narrow band parameters for $B \rightarrow X$ and $C \rightarrow X$ systems at gas temperatures between $500 - 3500$ K and electronic temperatures varying between $500 - 6000$ K have been generated. The entire spectrum has been divided into bands of equal width 1000 cm$^{-1}$. 7 quadrature points have been used for each system. Thus the RTE for hydrogen molecule becomes for each narrow band and each couple of quadrature points ($i$ for system $B$ and $j$ for system $C$)

$$\frac{\partial}{\partial s} I^{ij} = \kappa^i_B \left( \frac{\eta}{\kappa} \right)_B + \kappa^j_C \left( \frac{\eta}{\kappa} \right)_C + \kappa_{soot} I_{b,\nu}(T_g) + \frac{\sigma}{4 \pi} \int_{\Omega'} \Phi I^{ij}(\Omega') d\Omega'$$

$$- (\kappa^i_B + \kappa^j_C + \kappa_{soot} + \sigma) I^{ij}$$

where $\kappa_{soot}$ is the spectral absorption coefficient of soot and $I_{b,\nu}$ is the spectral black body intensity. The average spectral intensity over the narrow band is $\bar{I}^{\Delta \nu} = \sum_i \sum_j w_{B,i} w_{C,j} I^{ij}$ where $w_{B,i}$ and $w_{C,j}$ are the Gauss like quadrature weights of CK for $B \rightarrow X$ and $C \rightarrow X$ band systems respectively. Figure 2 shows that the transmissivities obtained using line-by-line calculations and the CK model for a column of 1 cm of pure molecular hydrogen are in good agreement. Figure 3 compares the averaged emission coefficient computed from line-by-line and from the CK model according to

$$\bar{\eta}^{\Delta \nu} = \sum_i \sum_j w_{B,i} w_{C,j} \left( \kappa^i_{\nu,B} \left( \frac{\eta}{\kappa} \right)_B + \kappa^j_{\nu,C} \left( \frac{\eta}{\kappa} \right)_C \right)$$

The CK model underestimates the emission with a relative error on the integrated emission of about 10%. This underprediction is due to the 7-point quadrature which is not sufficient to capture steep distribution functions due to almost Doppler lines in the optically thin limit.
Figure 2. Comparison of transmissivity of a 1 cm column of pure hydrogen computed using line by line and CK model for $T_g = 3000 \, K$, $T_e = 5500 \, K$, $p = 0.1 \, \text{bar}$ and $\Delta \nu = 1000 \, \text{cm}^{-1}$.

Figure 3. Comparison of emissive power of pure H$_2$ computed using line by line and CK model for $T_e = 5500 \, K$, $p = 0.1 \, \text{bar}$ and $\Delta \nu = 1000 \, \text{cm}^{-1}$ for two values of gas temperature.

The accuracy of the model is however increased when a finite optical thickness is considered as shown in table 3.

Table 3. Relative error of total net emission coefficient of CK model with line-by-line model for pure hydrogen at $T_g = 3000 \, K$, $T_e = 5500 \, K$ and $p = 0.1 \, \text{bar}$

| Plasma radius (cm) | Relative error % |
|--------------------|------------------|
| 0                  | 5.60             |
| 1                  | 2.54             |
| 5                  | 0.36             |

2.2. Atomic hydrogen

Lyman (emission to $n = 1$) and Balmer series ($n = 2$) are the dominant lines for atomic hydrogen. Lyman series occur in UV whereas Balmer series are found in the visible part of the spectrum. NIST database [9] has been used for spectral calculations of atomic hydrogen. Spectral emissive power and absorption coefficient are evaluated in the same way as for molecular hydrogen (equation 2) but with Doppler line shape. Atomic hydrogen is assumed to be at
electronic excitation temperature $T_e$ as for molecular hydrogen. The number density of a given electronic level is given by

$$n_u = \frac{x_p}{kT_g} g_u \exp \left( \frac{-E_u}{kT_g} \right) Q(T_e)$$ \hspace{1cm} (10)

The first 40 states have been considered to evaluate the partition function. In order to evaluate the relative contribution of atomic hydrogen and molecular hydrogen to radiative transfer, we have compared the products $4\pi \eta\nu \tau\nu(R)$ which represent the radiative power at the centre of a sphere of radius $R$. Figure 4 shows the cumulative net emission coefficient $\int_{\nu}^{\nu'} 4\pi \eta\nu' \tau\nu' d\nu'$ for a mixture containing 90% molecular hydrogen and 10% atomic hydrogen with radius $R = 1$ cm at $T_g = 3000$ K and $T_e = 5500$ K. Although the optically thin total emission coefficients are comparable, the atomic contribution becomes much smaller than molecular contribution due to self absorption. Hence atomic hydrogen may be neglected in radiative transfer calculations.

Figure 4. Cumulative spectral net emission coefficient for plasma radius $R = 1$ cm containing 90% hydrogen molecule and 10% hydrogen atom at $T_g = 3000$ K, $T_e = 5500$ K and $p = 0.1$ bar.

2.3. Hydrocarbons

Methane and acetylene are the two main constituents of the plasma reactor active in the IR-V. Radiative properties for methane (CH$_4$) is taken from high temperature database provided in Refs. [10, 11]. No high temperature database is available for Acetylene (C$_2$H$_2$). HITRAN 2008 [12, 13] has been used to evaluate C$_2$H$_2$ radiative properties. HITRAN provides line by line data of transition wavenumber $\nu_i$, line strength $S_i$ at 296 K, self and air broadened line widths $\gamma_i$, temperature exponent for air line broadening $n$, lower level energy $E_i$ and also, the partition functions $Q(T_g)$ up to 3000 K. Assuming Lorentz broadening, the transmissivity of a layer calculated using SNB model with inverse-exponential tailed distribution satisfies [3]

$$- \ln (\bar{\tau}) = \frac{\bar{\beta}}{\pi} \left( \sqrt{1 + \frac{2\pi x_p \bar{k}}{\bar{\beta}}} - 1 \right),$$ \hspace{1cm} (11)

where $\bar{k}$ is the mean absorption coefficient in the weak absorption limit and $\bar{\beta}$ is the line overlapping parameter. Parameter $\bar{k}$ is determined by integrating absorption coefficient over the narrow band $\Delta\nu$. Parameter $\bar{\beta}$ is estimated by least squares adjustment to the transmissivities over path lengths ranging between $10^{-6}$ to $10^{3}$ cm. The parameters have been determined for temperatures in the range 300 to 3000 K and band widths 25 cm$^{-1}$. Figure 5 indicates that the transmissivity of SNB model compares well with line by line calculations for acetylene gas.
**Figure 5.** Comparison between exact (full lines) and SNB (Dots) transmissivities for 5\% \(C_2H_2\), \(\Delta \nu = 25\ \text{cm}^{-1}\), pressure 0.2 \(\text{bar}\), and path length 10 \(\text{cm}\) at 1000 \(\text{K}\) (black curves) and 2000 \(\text{K}\) (blue curves) for two different spectral bands.

### 2.4. Soot

Soot is active both in UV and IR-V regions. Experimental studies [1] on the microwave reactor suggest that formation of soot extinguishes the plasma. Hence, modelling soot properties for both regions of the spectrum is important. However, there is lack of knowledge regarding the structure as well as properties such as complex refractive index \(m\) of the soot. For the present study, refractive index model described by Lee and Tien [14] has been adopted. The structure of soot particles can be assumed to be composed of large number of connected spheres. The structure is defined by fractal law [15] which relates the radius of gyration \(R_g\) of the aggregate, the number of mono-dispersed spheres \(N\) and their radius \(R_p\) according to

\[
N = k_f (R_g/R_p)^{D_f},
\]

where \(k_f\) is known as the fractal prefactor and \(D_f\) is the fractal dimension of the aggregate. The radius of each monomer particle is usually less than 25 \(\text{nm}\), which is much smaller than the wavelength of radiation \(\lambda\). Rayleigh Debye Gans [16] approximation is commonly used to model the radiative properties of soot. RDG assumes the soot to be composed of particles whose complex permittivity is close to that of vacuum. The scattering cross section and phase functions are modelled based on the structure of the soot, while absorption cross sections is the same as that of \(N\) independent Rayleigh scatterers. According to RDG for fractal structures [17], the cross-sections, absorption \(C_{abs}\) and scattering \(C_{sca}\) for fractal aggregates are given by

\[
C_{abs} = N \frac{4\pi x_p^3}{k^2} \text{Im} \left( \frac{m^2 - 1}{m^2 + 2} \right)
\]

\[
C_{sca} = N^2 \frac{8\pi x_p^6}{3k^2} \left| \frac{m^2 - 1}{m^2 + 2} \right|^2 \left( 1 + \frac{4}{3D_f} \frac{2}{2} (N/k_f)^{2D_f} \right)^{-D_f/2}
\]

where \(x_p = 2\pi R_p/\lambda\) and \(k = 2\pi/\lambda\). For computational simplicity, it is assumed here that soot particles are isotropic scatterers. Farias et al [18] have evaluated the range of validity of
RDG approximation and concluded that application of RDG for optical diagnostics of soot in the visible and UV regions is satisfactory. However, both imaginary and real parts of $m$ are relatively high in the infrared region. We have shown in Ref. [19] that RDG approximation underpredicts absorption in the infrared region and a model for absorption in the IR-V as a function of refractive index, optical size parameter and fractal parameters has been developed and is used in present calculations. The model for absorption cross-sections is based on rigorous solutions of Maxwell’s equations using Multi-Sphere T-Matrix method [20].

2.5. Solution of radiative transfer equations

Radiative transfer equations are solved using Discrete Ordinate Method [4] in the UV while direct ray tracing method is used in the IR-V region. The inputs to the RTE solver are electronic and gas temperatures, species concentrations and pressure distribution inside the reactor. The 2-D spatial domain is discretized into large number of finite volumes using structured grids (figure 6) and can have non-uniform spacings. It is assumed that temperature, pressure and concentrations are uniform within a finite volume. The RTE has to be solved over several discrete directions. For both DOM and ray tracing methods, the octant of the sphere at each spatial node is discretized into $N_\theta \times N_\phi$ directions with an assumption that the radiation intensity is constant within the discrete solid angle. Symmetry of the domain means that equations have to be solved only for half the directions according to $\phi$. The output from the solver is the volumetric radiative source $\nabla \cdot q_{rad}$ at all internal spatial nodes and radiative flux $q_{rad}$ at the walls of the reactor. The radiative solvers have been extensively validated against benchmark solutions.

3. Sample radiation calculations

Simulations have been performed for the simple geometry and conditions shown in figure 7. The plasma reactor is represented by two zones - hot and cold zones. The hot zone represents the plasma where Hydrogen is characterized by its gas and electronic excitation temperatures. Other constituent gases are assumed at gas temperature. Hydrogen in the cold zone is assumed to be at thermal equilibrium. Volumetric concentration of soot is assumed to be uniform throughout the domain. Radiative properties of soot have been calculated using RDG approximation in the UV region and the model developed in Ref. [19] in IR-V region with soot clusters having fractal parameters $D_f = 1.8$, $k_f = 1.3$ and $N = 100$ mono-dispersed particles of radius $R_p = 15$ nm.

Figure 8 shows the radiative power distribution along the axis of the reactor for different soot concentrations. While the hot zone strongly emits radiation, the cold zone absorbs radiation. Addition of soot to the mixture greatly changes the radiative power of the medium. Soot is important for both IR-V and visible-UV spectrum. In the UV spectrum, soot absorbs radiation and the increase in absorption in the cold region is several orders of magnitude compared to
Table 1: Reactor conditions for full simulation.

| Parameter | Hot zone | Cold zone |
|-----------|----------|-----------|
| $T_g$ (K) | 3000     | 500       |
| $T_e$ (K) | 5500     | 500       |
| $p$ (atm) | 0.1      | 0.1       |
| $X_{H_2}$ | 0.967    | 0.967     |
| $X_{CH_4}$| 0.003    | 0.03      |
| $X_{C_2H_2}$| 0.03 | 0.003     |

All walls are at 500 K

Figure 7. Reactor conditions for full simulation.

Figure 8. Radiative power distribution along the axis of the reactor with uniform soot distribution. Full lines correspond to IR region and Dashed lines with circles correspond to UV region. The colors indicate the soot volume fraction. Calculations are carried out with $20 \times 20$ spatial mesh and $N_\theta = N_\phi = 40$.

no-soot condition. The amount of radiative power emitted in the hot region and absorbed in the cold region is a strong function of soot concentration. The orders of magnitude of radiative power can become comparable to that of input microwave energy discharge (see table 2). This indicates that microwave energy may not be sufficient to sustain the plasma in the presence of high volume fractions of soot.
4. Conclusion
Radiative property models for hydrogen molecule, hydrocarbons and soot in plasma reactor conditions have been developed. Two different approaches have been adopted for treating IR-V and UV spectra regions. In the UV region, molecular hydrogen is found to be more significant compared to atomic hydrogen. Hence, atomic hydrogen has been neglected for radiative transfer calculations. Molecular hydrogen radiation has been modelled by CK narrow-band model, in the framework of two-temperatures representation of thermodynamic state, which is compatible with scattering by soot particles. In the IR-V region where scattering can be neglected, CH$_4$ and C$_2$H$_2$ properties have been modelled using SNB. Preliminary calculations for synthetic reactor conditions indicate that soot can be the most critical constituent affecting the radiative transfer in the reactor. Presence of small amounts of soot can yield local radiative powers of the same orders of magnitude as microwave power and can extinguish the plasma. Coupling of the radiative transfer model with other multiphysics models would enable full simulation of the plasma reactor and improve the predictions of the deposition process.

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