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Uniform Magnetic Fields and Equilibrium Flame Temperatures

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The impact of a constant uniform magnetic field on equilibrium flame temperature under constant volume conditions was examined. The equilibrium combustion compositions were found using an expression for Helmholtz free energy that included a magnetic-field contribution. Changes in the Helmholtz free energy for a mixture of paramagnetic and diamagnetic ideal gases were minimized using the method of Lagrange multipliers. The magnetic susceptibility for the paramagnetic gases was calculated using the Curie law. Equilibrium flame temperatures were obtained from the first law of thermodynamics for a closed adiabatic system with no work interactions. A model reaction of methane in air was used to quantitatively examine changes in the equilibrium flame temperature and product mole fractions as a function of volume and magnetic induction. Equilibrium flame temperature and product mole fractions were plotted as a function of magnetic-field strength and volume for all product species. The results indicate that with the increase in magnetic-field strength, the equilibrium flame temperature increases for all volumes considered.

Nomenclature

g_L = Lande's g factor
h = enthalpy
k = Boltzmann constant
m_i = molecular weight of species i
N_A = Avogadro's number
n = number of moles
R_u = universal gas constant
S_i = total electron spin of species i
T = absolute temperature
y = mole fraction
ε_u = internal energy residual
μ_B = Bohr magneton
μ_0 = magnetic permeability of vacuum
χ_i = magnetic susceptibility per unit mass of species i

Subscripts

equil = equilibrium flame temperature
f = formation
i = species i
p = products
r = reactants

Superscript

o = reference conditions

Introduction

RECENT increases in the cost of oil and the increasing debate over anthropogenic global warming highlights the fact that combustion processes are critical to our civilization. As such, it is imperative that a fundamental understanding of combustion processes and the phenomena that can be used to intelligently control such processes be developed. Magnetic fields have long been known to influence flame behavior through the paramagnetic and diamagnetic properties of the constituent species. A review of the literature associated with this interaction can be found in Baker and Calvert [1]. Application of a magnetic field has previously been shown to change flame shape, emission intensities, and temperature profiles [2–4]. In addition, a uniform magnetic field was previously shown to affect equilibrium compositions [5,6] and theoretical rocket performance [7].

Magnetic susceptibility is used to quantify paramagnetic and diamagnetic behavior and is defined as the degree to which a substance will be magnetized when placed in a given magnetic field. The magnetic susceptibility of paramagnetic species can be specified by the Curie law, given as [8]

$$\chi_i = \frac{N_A g_L^2 \mu_B^2 S_i(S_i + 1)\mu_0}{3kTm_i} \tag{1}$$

As can be deduced from the preceding equation, an increase in temperature decreases the magnetic susceptibility. The magnetic susceptibility for paramagnetic species decreases rapidly for temperatures less than 1500 K and then reaches an asymptotic value when the temperature increases beyond this point. On the other hand, diamagnetic susceptibility is independent of the temperature. The magnitude of the magnetic susceptibility of paramagnetic substances varies in the range of 10^{-3} to 10^{-6} cgs units and is positive. Among the product species for the model reaction considered in this study (i.e., methane in air), NO (nitric oxide), O_2 (oxygen), and OH (hydroxyl) are the only paramagnetic species.

The present study is a continuation of the work done by Gupta and Baker [6], who examined the effect that uniform magnetic fields have on constant volume equilibrium combustion compositions. It was found that under isothermal conditions, an applied magnetic field could significantly change the equilibrium composition and decrease the equilibrium pressure. The impact on equilibrium pressure was more pronounced at higher temperatures and higher values of the applied magnetic-field strength. For the investigation detailed here, the equilibrium flame temperature and the equilibrium composition are taken as variable. The motivation for the work presented in this paper is the fact that changes in temperature can have a dramatic effect on the production of several species that are considered to be pollutants. There is little, if any, information on the impact that magnetic fields have on chemical kinetics. A thermodynamic equilibrium model, such as the one used in this study, provides an ideal first step for developing a fundamental understanding of how

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magnetic fields can be used to affect changes in the behavior of combustion processes. This is especially true given that computational models use a combination of chemical kinetics and chemical equilibrium models to model combustion processes.

The knowledge and understanding gained from examining the impact that uniform magnetic fields have on equilibrium chemical compositions and equilibrium flame temperature will be used to guide future emission reduction strategies. The specific objectives of this work are to 1) develop a model that can be used to examine the impact that uniform magnetic fields have on equilibrium flame temperature and 2) quantitatively study the effect of a uniform magnetic field on equilibrium flame temperature and equilibrium combustion composition under constant volume conditions.

Mathematical Formulation

A model reaction of methane in air was used to investigate the impact of a uniform magnetic field on equilibrium flame temperature under constant volume conditions. The specific reactants and products for this reaction are

$$\begin{aligned} CH_4 + n_{\mathrm{air}}(O_2 + 3.76N_2) \rightarrow\ & n_{CO_2}CO_2 + n_{CO}CO + n_{H_2O}H_2O \\ & + n_H H + n_{H_2}H_2 + n_{O_2}O_2 + n_{OH}OH + n_O O + n_{N_2}N_2 \\ & + n_{NO}NO + n_{CH_4}CH_4 \end{aligned} \tag{2}$$

The system is assumed to be a closed, constant volume, homogeneous, isotropic, stationary system (and, when specified, is assumed to be in the presence of a uniform applied magnetic field). The equilibrium composition is found using a minimization of the Helmholtz function at a specified temperature. The equilibrium flame temperature and composition are found using the following algorithm, along with the user-specified input data.

1) Determine the equilibrium flame temperature by dividing the enthalpy of the reactants by the total number of moles of nitrogen and assume this value to be the value of enthalpy for nitrogen at the equilibrium flame temperature.

2) Initialize the number of moles for each of the product species to 0.1, calculate various constants, populate the mass conservation matrix, read in the thermochemical data, and evaluate the normalized reference Helmholtz free energy for each of the product species.

3) Calculate the enthalpy of the reactants.

4) Calculate magnetic susceptibility for paramagnetic species at the current temperature and populate magnetic susceptibility for diamagnetic species. Note that in previous studies [1,5–7], the temperature dependence of the paramagnetic susceptibility was not considered.

5) Calculate the magnetic-field contribution for all of the species using the preceding magnetic susceptibilities.

6) Calculate the equilibrium composition at the current temperature and the product mole fractions as outlined in Gupta and Baker [6].

7) Calculate the enthalpy of the products.

8) Calculate the internal energy residual using the first law of thermodynamics:

$$\begin{aligned} \varepsilon_u = & \sum n_{r,i}\left[\bar{h}^o_{f,i} + \left(\bar{h} - \bar{h}^o_i\right)\right]_r - \sum n_{p,i}\left[\bar{h}^o_{f,i} + \left(\bar{h} - \bar{h}^o_i\right)\right]_p \\ & - R_u(n_r T_r - n_p T_{\mathrm{equil},p}) \end{aligned} \tag{3}$$

where the bar over the enthalpies implies values per unit mole.

9) If $|\varepsilon_u| \le 10^{-3}$, then the solution is taken to be converged, the data are written to a file, and the program terminates.

10) If $|\varepsilon_u| > 10^{-3}$, then a new equilibrium flame temperature estimate is calculated using linear interpolation/extrapolation using the equilibrium flame temperature estimates and the internal energy residuals from current and previous iterations, and control is returned to step 4. After the first iteration, the new equilibrium flame temperature estimate is determined by examining the sign and magnitude of the internal energy residual.

Table 1 Magnetic susceptibility of diamagnetic species [9]

Species	Magnetic susceptibility (cgs units)
N_2	-12.00×10^{-6}
H_2O	-12.63×10^{-6}
CO	-9.80×10^{-6}
CO_2	-21.00×10^{-6}
H	-2.93×10^{-6}
O	-4.61×10^{-6}
H_2	-3.99×10^{-6}
CH_4	-17.4×10^{-6}

Note that the equilibrium flame temperature is a function of the equilibrium composition and is calculated during every iteration cycle. Note also that during any given set of calculations, the externally applied magnetic field is a user-defined constant.

Results and Discussion

The magnetic susceptibility [9] values for diamagnetic species are listed in Table 1. As mentioned earlier, the magnetic susceptibilities for paramagnetic species were calculated using the Curie law. To calculate magnetic susceptibility, the value of Lande's g factor was assumed to be constant at 2.0 for all paramagnetic species considered (i.e., O_2, NO, and OH). The value of total electron spin was taken as 1.0, 0.5, and 0.5 for O_2, NO, and OH, respectively. An equivalence ratio of unity was used for all of the test cases (i.e., $n_{\mathrm{air}} = 2$ kmol). Three different volumes (5.0, 27.2, and 50.0 m^3) were used to examine the effect of magnetic fields on equilibrium flame temperature and equilibrium combustion compositions for different species. A constant volume of 27.2 m^3 is used, corresponding to a 1-atm reactant pressure. The other two volumes were selected on an ad hoc basis. The magnetic induction considered ranged from 0.00 to 0.04 T. The decision to examine this range was based solely on the fact that the impact of a magnetic field on equilibrium characteristics was easily observable in this range.

The validation of the equilibrium composition model developed was done by comparing the results with those obtained using GASEQ,[‡] and is the validation process that is detailed in Gupta and Baker [6]. GASEQ uses almost the same algorithm for calculating equilibrium flame temperature as that used in this study. A comparison was made between the results from GASEQ and the results obtained during this study for the three different volumes (5, 27.2, and 50 m^3). With the magnetic induction set to zero, the code used in this study produced results that almost exactly (a maximum of 0.01% difference with a 1-atm reactant pressure) match the results from GASEQ for the same conditions.

Figure 1 is a plot of equilibrium flame temperature and equilibrium mole fraction for carbon dioxide as a function of magnetic-field strength at constant volume conditions. The equilibrium flame temperature is plotted along the left y axis and equilibrium mole fraction is plotted along the right y axis on the same plot. From the figure, one can see that the equilibrium flame temperature and equilibrium mole fraction of CO_2 increase nonlinearly with the increase in magnetic-field strength for all volumes considered. At zero magnetic-field strength, it was observed that with the increase in volume, the equilibrium flame temperature decreases. A similar trend was observed for the equilibrium mole fraction of CO_2 at zero magnetic-field strength. The equilibrium flame temperature at a volume of 27.2 m^3 crosses the equilibrium flame temperature curve for a volume of 5.0 m^3 at around 0.015 T, and for a volume of 50.0 m^3, it crosses at around 0.012 T.

However, the equilibrium flame temperature plot for a volume of 50.0 m^3 crosses the equilibrium flame temperature for a volume of 27.2 m^3, at a value of even less than 0.01 T. This trend indicates that with the increase in volume, the increase in equilibrium flame temperature becomes steeper, as a function of magnetic-field strength. The increase in equilibrium flame temperature with an

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[‡] Data available online at http:// www.gaseq.co.uk [retrieved 24 July 2006].

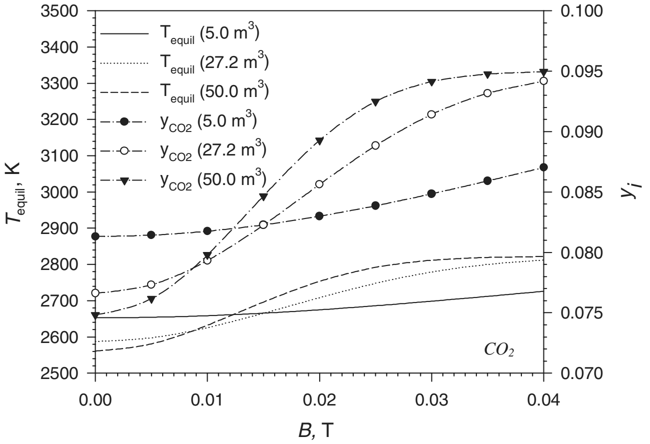

Fig. 1 Equilibrium flame temperature and mole fraction of CO_2 as a function of the applied magnetic field.

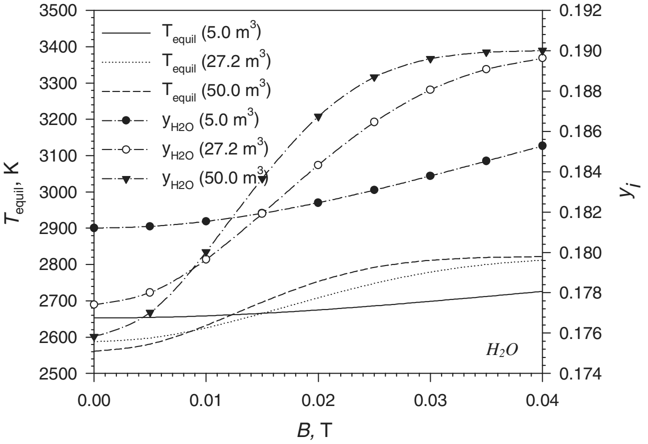

Fig. 3 Equilibrium flame temperature and mole fraction of H_2O as a function of the applied magnetic field.

increase in magnetic-field strength can be explained by using Le Châtelier's principle. According to Le Châtelier's principle, the effect of an increase in magnetic-field strength, with a constant volume and temperature, is to decrease the equilibrium pressure. It was shown earlier that an applied magnetic field will decrease equilibrium pressure [6]. A decrease in equilibrium pressure corresponds to a decrease in the total number of moles of products. A close examination of Eq. (3) indicates that with the decrease in the total number of moles of products, the enthalpy values of product species should increase to balance the equation. Higher enthalpy values of the products correspond to higher equilibrium flame temperature. The equilibrium combustion composition of carbon dioxide increases with an increase in magnetic-field strength, showing a trend similar to that of equilibrium flame temperature. As explained earlier, according to Le Châtelier's principle, the effect of an applied magnetic field is to disturb the equilibrium state, which results in the change of equilibrium combustion composition of all of the product species.

Figure 2 is a plot of equilibrium flame temperature and equilibrium mole fraction for nitrogen as a function of magnetic-field strength at constant volume conditions. As with CO_2, the mole fraction of N_2 also increases nonlinearly with increases in the applied magnetic field for all volumes considered. This trend is similar to the trend observed for the equilibrium flame temperature as a function of magnetic-field strength. For constant volumes of 5.0 m^3, the mole fraction of N_2 increases from a value of around 0.705 at 0.00 T magnetic-field strength to a value of around 0.709 at 0.04 T magnetic-field strength, whereas for constant volume of 50.0 m^3, the mole fraction of N_2 increases from a value of around 0.701 at 0.00 T magnetic-field strength to a value of around 0.715 at 0.04 T magnetic-field strength. This indicates that as the volume increases, the increase in mole fraction becomes steeper. It should be noted that as the value of the volume increases, the reactant pressure decreases, keeping the reactant temperature constant. Therefore, it can be inferred that at low reactant pressures, the equilibrium state becomes more sensitive to any change; hence, changes in the magnetic-field change the equilibrium combustion composition to a greater extent.

Figure 3 is a plot of equilibrium flame temperature and equilibrium mole fraction for water vapor as a function of magnetic-field strength at constant volume conditions. Similar to the preceding two plots discussed, there is a trend of increasing water mole fraction with increases in magnetic-field strength. This trend is again similar to the trend observed for equilibrium flame temperature as a function of magnetic-field strength for all volumes considered. The mole fraction curve for a constant volume of 50.0 m^3 crosses the mole fraction curve for constant volumes of 27.2 and 5.0 m^3 at a magnetic-field strength of around 0.009 T and 0.012 T, respectively. The equilibrium mole fraction for water at a volume of 5.0 m^3 increases from a value of approximately 0.182 at 0.00 T to a value of around 0.185 at 0.04 T, whereas for a constant volume of 50.0 m^3, the mole fraction increases from a value of around 0.176 at 0.00 T to a value of around 0.190 at 0.04 T. For a constant volume of 50.0 m^3, asymptotic behavior of the equilibrium mole fraction was observed at higher values of the magnetic-field strength of approximately 0.03 T and above.

Figure 4 is a plot of equilibrium flame temperature and equilibrium mole fraction for diatomic oxygen as a function of magnetic-field strength at constant volume conditions. It is evident from the figure that as the magnetic-field strength increases the mole fraction of O_2 decreases nonlinearly for all volumes. This trend is opposite to the trend observed for the equilibrium flame temperature at which there is a steady increase for all volumes considered. The equilibrium mole

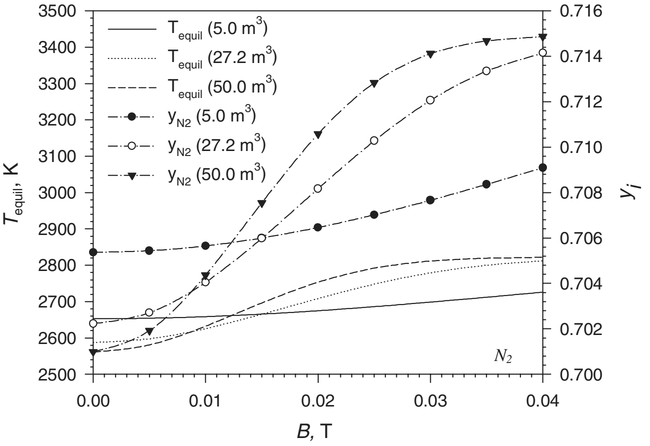

Fig. 2 Equilibrium flame temperature and mole fraction of N_2 as a function of the applied magnetic field.

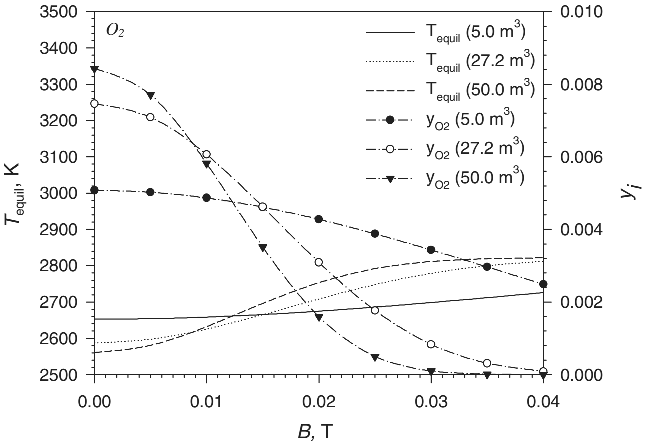

Fig. 4 Equilibrium flame temperature and mole fraction of O_2 as a function of the applied magnetic field.

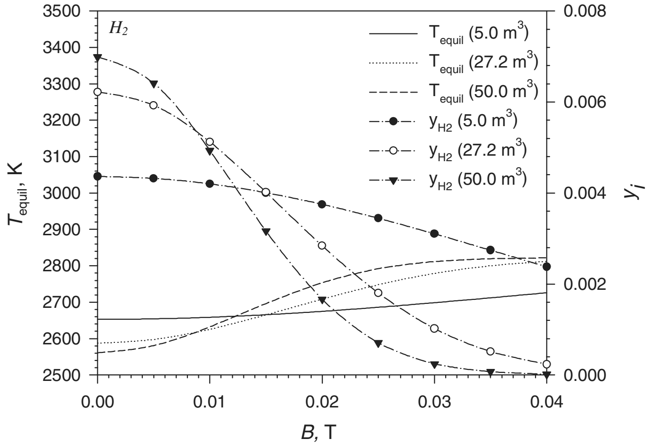

Fig. 5 Equilibrium flame temperature and mole fraction of H_2 as a function of the applied magnetic field.

fraction for a volume of 5.0 m^3 decreases from a value of around 0.005 at 0.00 T to a value of around 0.003 at 0.04 T magnetic-field strength, whereas for a volume of 50.0 m^3 the equilibrium mole fraction value decreases from a higher value of around 0.008 at 0.00 T to a value of 0.000 at 0.04 T magnetic-field strength. Clearly, with an increase in volume, the equilibrium composition of oxygen decreases sharply. For a volume of 50.0 m^3, an asymptotic equilibrium mole fraction of around 1.0×10^{-6} was observed at higher magnetic-field strengths of around 0.03 T and above.

Figure 5 is a plot of equilibrium flame temperature and equilibrium mole fraction for diatomic hydrogen as a function of magnetic-field strength at constant volume conditions. It was observed that diatomic hydrogen exhibited behavior similar to diatomic oxygen. The trend observed for the equilibrium flame temperature was opposite to that of equilibrium mole fraction of hydrogen as a function of magnetic-field strength. The maximum value of the equilibrium mole fraction for hydrogen was observed for a volume of 50.0 m^3 at a magnetic-field strength of 0.00 T, and the minimum was also observed for the same volume condition at a magnetic-field strength of 0.04 T. Asymptotic behavior of equilibrium mole fraction was observed at higher magnetic-field strengths of around 0.035 T and above for a volume of 50.0 m^3. Below a magnetic-field strength of 0.005 T, negligible change in equilibrium mole fraction of hydrogen was observed for a volume of 5.0 m^3.

Figure 6 is a plot of equilibrium flame temperature and equilibrium mole fraction for monatomic oxygen as a function of magnetic-field strength at constant volume conditions. From the figure, one can see that the equilibrium mole fraction of monatomic oxygen decreases with increases in the magnetic-field strength for all volume conditions. This trend is opposite to the trend observed for equilibrium flame temperature, which increases with increases in magnetic-field strength for all volumes considered. As explained earlier, according to Le Châtelier's principle, the effect of the magnetic field increases with increases in the difference of the total number of moles of products and reactants, which increases with increasing volume. For constant volume of 50.0 m^3, an asymptotic value of equilibrium mole fraction was observed close to a 0.025 T magnetic-field strength. For a volume of 27.2 m^3, an asymptotic value of equilibrium mole fraction was observed for values of magnetic-field strength greater than approximately 0.035 T.

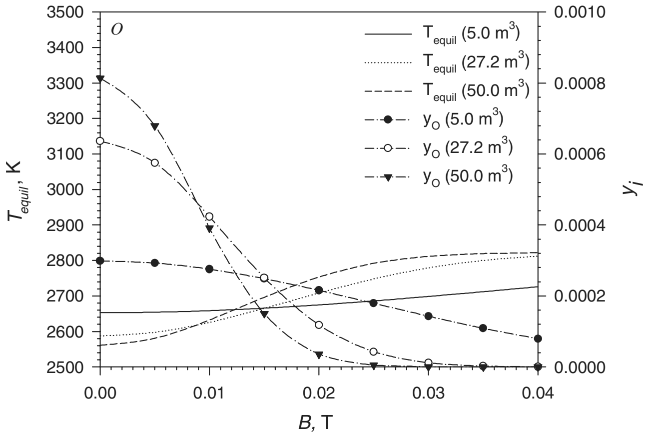

Fig. 6 Equilibrium flame temperature and mole fraction of O as a function of the applied magnetic field.

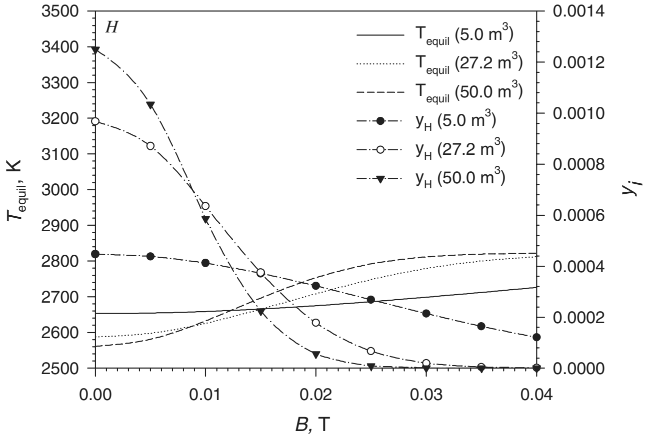

Fig. 7 Equilibrium flame temperature and mole fraction of H as a function of the applied magnetic field.

Figure 7 is a plot of equilibrium flame temperature and equilibrium mole fraction for monatomic hydrogen as a function of magnetic-field strength at constant volume conditions. As for monatomic oxygen, the equilibrium mole fraction of monatomic hydrogen decreases with increases in magnetic-field strength for all volumes considered. At a specified volume, the effect of the increase in the magnetic-field strength decreases the equilibrium mole fraction of monatomic hydrogen. For a constant volume of 5.0 m^3, the equilibrium mole fraction decreases from a value of around 4.0×10^{-4} at 0.00 T magnetic-field strength to a value of around 1.2×10^{-4} at 0.04 T magnetic-field strength, whereas for a constant volume of 50.0 m^3, the equilibrium combustion composition decreases from a higher value of around 1.2×10^{-3} at 0.00 T to a lower value of around 1.0×10^{-9} at 0.04 T magnetic-field strength.

Figure 8 is a plot of equilibrium flame temperature and equilibrium mole fraction for nitric oxide as a function of magnetic-field strength at constant volume conditions. As can be seen from the plot, at a particular magnetic-field strength, the NO mole fraction decreases with increases in volume. The trend observed for an equilibrium mole fraction of NO is opposite to that of the equilibrium flame temperature as a function of the magnetic-field strength for all volumes considered. For volumes of 5.0, 27.2, and 50.0 m^3, the equilibrium mole fraction decreases by around 24, 80, and 95%, respectively, as the magnetic-field strength is increased from 0.00 to

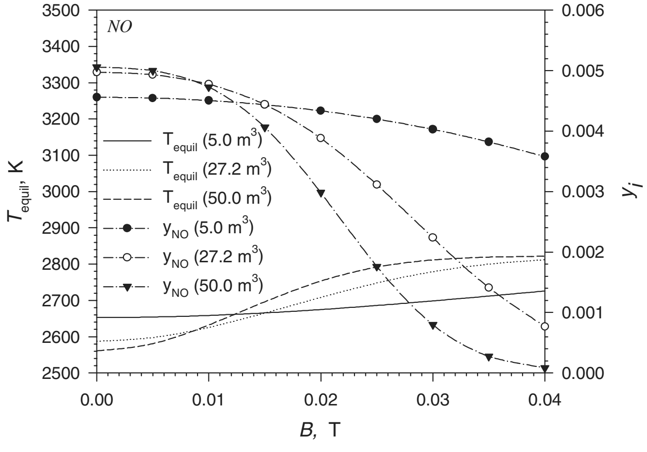

Fig. 8 Equilibrium flame temperature and mole fraction of NO as a function of the applied magnetic field.

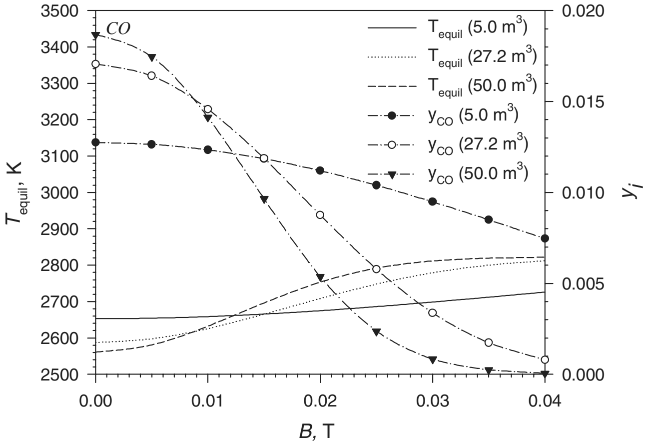

Fig. 9 Equilibrium flame temperature and mole fraction of CO as a function of the applied magnetic field.

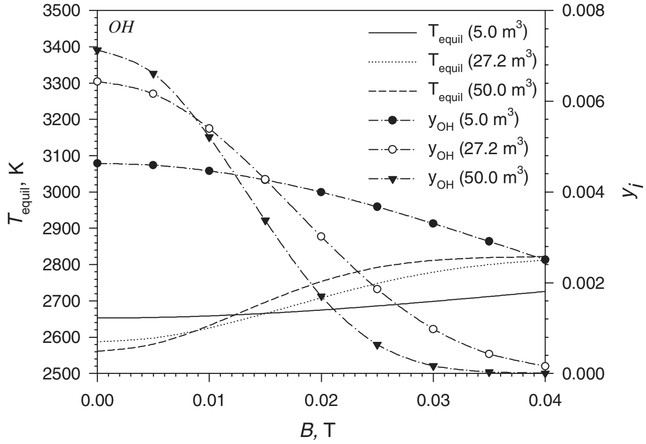

Fig. 10 Equilibrium flame temperature and mole fraction of OH as a function of the applied magnetic field.

0.04 T. At a particular magnetic-field strength, the decrease in mole fraction of NO with increasing volume increases with increases in magnetic induction. Because the analysis is a thermodynamic analysis, the equilibrium compositions shown here do not take into account the time duration to achieve these mole fractions. With the present study, a fundamental understanding of the trends of only equilibrium combustion compositions under the influence of uniform magnetic field can be achieved.

Figure 9 is a plot of equilibrium flame temperature and equilibrium mole fraction for carbon monoxide as a function of magnetic-field strength at constant volume conditions. For all volumes considered, the equilibrium mole fraction of CO decreases with increases in magnetic induction. This trend is opposite to the trend observed for equilibrium flame temperature as a function of magnetic-field strength. For a constant volume of 5.0 m^3, the equilibrium mole fraction of CO reduces from a value of around 0.012 at 0.00 T magnetic induction to a value of around 0.007 at 0.04 T magnetic induction, whereas for a constant volume of 50.0 m^3, the equilibrium mole fraction reduces from a value of around 0.018 at 0.00 T to a value of around 5.0×10^{-5} at 0.04 T magnetic-field strength. The decrease in equilibrium mole fraction of CO was again found to be highest for a constant volume of 50.0 m^3 with the application of 0.04 T magnetic-field strength.

Figure 10 is a plot of equilibrium flame temperature and equilibrium mole fraction for the hydroxyl radical as a function of magnetic-field strength at constant volume conditions. The mole fraction of hydroxyl reduces with the increase in magnetic-field strength for all volumes considered. This trend is opposite to the trend observed for equilibrium flame temperature as a function of magnetic-field strength. The equilibrium mole fraction of OH for a volume of 50.0 m^3 crosses the equilibrium mole fraction curves of OH for constant volumes of 27.2 and 5.0 m^3 at magnetic inductions of 0.009 and 0.012 T, respectively. Note that the decrease in the mole fractions may not be the same as those in practical engineering applications, because as the time duration of the reaction is not considered.

It should be noted that the influence of a constant uniform magnetic field on equilibrium composition and flame temperature even under constant volume conditions can be explained by considering the fact that the addition of the magnetic-field term in the formulation is analogous to applying a selective change in pressure to the product species. The magnitude of this pressure change is proportional to not only the magnitude of the magnetic-field strength but also to the magnitude of the magnetic susceptibility. From the results presented here, it is clear that there is a nonlinear interaction between this selective magnetic pressure and the equilibrium behavior, and that this interaction always produces an increase in the equilibrium flame temperature.

Conclusions

The impact of an applied uniform magnetic field on equilibrium flame temperature under constant volume conditions was investigated. A model reaction of methane in air was considered that included 11 product species. Thermodynamic equilibrium conditions were identified by minimizing the change in the Helmholtz free energy, modified to account for an applied magnetic field, using the method of Lagrange multipliers. The equilibrium flame temperature was calculated using an iterative procedure that minimized the residual of the reactant and product internal energies. The equilibrium flame temperature calculation was directly coupled to the equilibrium composition calculation. Results were presented in the form of plots of constant volume equilibrium flame temperature and equilibrium mole fractions for the different species as a function of magnetic induction. Based on these results, it may be concluded that the equilibrium flame temperature increases with increasing magnetic-field strength for all of the volumes considered. The degree of this increase in equilibrium flame temperature was generally more dramatic at larger volumes. In addition, the application of a magnetic field shifts the equilibrium composition toward higher mole fractions of water vapor and carbon dioxide and toward lower mole fractions of the reactant and other product species.

References

[1] Baker, J., and Calvert, M. E., "A Study of the Characteristics of Slotted Laminar Jet Diffusion Flames in the Presence of Non-Uniform Magnetic Fields," *Combustion and Flame*, Vol. 133, No. 3, 2003, pp. 345–357.

[2] Aoki, T., "Radical Emissions and Butane Diffusion Flames Exposed to Uniform Magnetic Fields Encircled by Magnetic Gradient Fields," *Japanese Journal of Applied Physics, Part 2: Letters*, Vol. 29, No. 5, 1990, pp. 952–957.

[3] Ueno, S., "Quenching of flames by magnetic fields," *Journal of Applied Physics*, Vol. 65, No. 3, 1988, pp. 1243–1245.

[4] Wakayama, N. I., "Effect of a Gradient Magnetic Field on the Combustion Reaction of Methane in Air," *Chemical Physics Letters*, Vol. 188, No. 3, 1992, pp. 279–281.

[5] Baker, J., and Saito, K., "Magnetocombustion: A Thermodynamic Analysis," *Journal of Propulsion and Power*, Vol. 16, No. 2, 2000, pp. 263–268.

[6] Gupta, A., and Baker, J., "Effect of Uniform Magnetic Field on Equilibrium Combustion Composition: Constant Volume," *AIAA Journal*, Vol. 43, No. 11, 2005, pp. 2438–2444.

[7] Baker, J., and Morgan, O. T., "Effect of Paramagnetism and Diamagnetism on Theoretical Rocket Performance," *Journal of Propulsion and Power*, Vol. 20, No. 6, 2004, pp. 1012–1017.

[8] Yamada, E., Shinoda, M., Yamashita, H., and Kitagawa, K., "Numerical Analysis of a Hydrogen-Oxygen Diffusion Flame in Vertical or Horizontal Gradient of Magnetic Field," *Combustion Science and Technology*, Vol. 174, No. 9, 2002, pp. 131–146.

[9] Weast, R. C. (ed.), *CRC Handbook of Chemistry and Physics*, 67th ed., CRC Press, Boca Raton, FL, 1986, pp. E119–E132.