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GENERATING EMISSIVITY CHARTS FOR FUEL GASES FROM HIGH-RESOLUTION SPECTRAL ABSORPTION DATA

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Abstract. *Although, the contribution of fuel vapors in overall radiation from the fire flame is conventionally ignored, in some cases such as fuel rich region just above the fuel surface in pool fires, it might be significant and should be considered. The aim of this study is to generate emissivity charts, which provide a prominent insight into the importance of radiation contribution of gases at various temperatures and optical thicknesses. Moreover, they can also be used as a starting point of model development and validation for radiative properties of gases as another purpose of this study. In the present work, experimentally measured spectral absorption coefficients were used to generate the emissivity charts of Methanol (CH_3OH), Propane (C_3H_8), Propylene (C_3H_6), MMA ($C_5H_8O_2$), Toluene (C_7H_8) and Heptane (C_7H_{16}). Here, the emissivity charts are presented for T=300K to 1400K and PL=0.01 atm.m to 10.0 atm.m. The results showed that Heptane had the lowest and MMA had the highest total emissivities. Additionally, the total emissivity of the studied fuel gases was independent of PL when PL>5.0 atm.m.*

Keywords: *Spectral thermal radiation, Emissivity charts, Fuel gas, Combustion, Fires*

1. INTRODUCTION

Radiative heat transfer has always been an attractive but challenging topic in heat transfer science. This mechanism may dominate other two mechanisms of conduction and convection in high temperature media, like in fires. The thermal radiation of the hot combustion products is summation of the contribution of the gaseous media and soot. Rapid developments in spectroscopy and the need to achieve accurate thermal heat transfer calculations motivated Hottel and co-workers to present the total emissivity charts for carbon dioxide and water vapor (Hottel (1954), Hottel and Sarofim (1965), Leckner (1972)) presented a comprehensive evaluation of Hottel's charts and corrected the inaccuracy of Hottel's measurements at small PLs. Later on, a new version of emissivity charts reported by Farag (1976). Hottel's (Hottel (1954), Hottel and Sarofim (1965)), Leckner (1972)) and Farag's (Farag (1976)) emissivity charts have been the most traditional and widely used resources for providing emissivity charts of CO_2 and H_2O. Using analytical methods, Felske and Tien (1973) reported total emissivity of luminous flames considering water vapor, carbon dioxide and soot. Coppalle and Vervisch (1983) calculated total emissivities of high temperature CO_2 and H_2O mixtures using Edward's exponential wide-band model (Edwards (1976)). The reviewed works focused on the primary applications of the emissivity charts. More recent studies about generating emissivity charts were conducted by Alberti et al. (Alberti *et al.* (2015a), Alberti *et al.* (2015b), Alberti *et al.* (2016), Alberti *et al.* (2017)). In Alberti *et al.* (2015b), they produced more accurate emissivity charts than those of Hottel's, applicable to 1 to 40 bar. Alberti *et al.* (2015a) evaluated the accuracy of H_2O and CO_2 emissivity charts calculated from HITEMP-2010 by comparing with experimental measurements. In another research, Alberti *et al.* (2016) extended the Hottel's emissivity charts to 40 bar pressure using HITEMP-2010 database. To this end, they employed linear interpolation for temperature scaling and logarithmic interpolation for pressure and pressure path length scaling.

Emission and absorption of fuel vapors in fire scenarios are conventionally ignored because most of the fuel vapors undergo a quick reaction converting. Therefore, their effect on radiation reaching outside of the flame zone is negligible. However, there are cases in which the contribution of fuel vapors in thermal radiation is important and cannot be ignored. For instance, the radiation reaching a liquid pool in a pool fire is affected by a layer of rich fuel vapor with a relatively lower temperature just above the surface of the pool (Consalvi and Liu (2014a), Consalvi and Liu (2014b)). Hence, the spectral absorption and emission of the fuel gases can affect the radiative heat flux reaching the pool. This heat flux provides the heat for evaporation and then evolution of the fire (Bordbar and Hostikka (2019), Bordbar *et al.* (2020b)). In practice, total emissivity is usually sufficient to evaluate the emission from a hot gas that reaches a point in environment. Total emissivity is defined as the emission of the gas at atmospherics pressure over a gas column when the collisions between the molecules of the gas are neglected, i.e. self-absorption is ignored.

Solving thermal radiation in combustion gases is a challenging task due to the strong spectral dependency of absorption coefficients Bordbar *et al.* (2019). Several simplified models were developed to include the drastic change of the absorption coefficient with wavenumbers in overall thermal radiation calculations, such as Modest (1991), Modest and Zhang (2002), Denison and Webb (1993), Solovjov and Webb (2001). These models provide an accurate approximation of radiative heat transfer with affordable computational costs (Bordbar *et al.* (2020a)) where emissivity charts have some attractive applications. Total emissivity is also used for validation of numerical thermal radiation models and radiation exchange. Its application can be found in Dorigon *et al.* (2013); Bordbar *et al.* (2014, 2020a); Bordbar and Hyppänen (2013).

The aim of this study is to generate emissivity charts, which provide a prominent insight into the importance of radiation contribution of fuel gases at various temperatures and optical thicknesses. Moreover, they can also be used as a starting point of model development, namely WSGG model, and validation for radiative properties of gases as another purpose of this study. While most of the previous relevant works of total emissivity, as the literature review indicates, focused on obtaining emissivity charts for CO_2, H_2O and CO, the present research aims at generating the emissivity charts of Methanol (CH_3OH), Propane (C_3H_8), Propylene (C_3H_6), MMA ($C_5H_8O_2$), Toluene (C_7H_8) and Heptane (C_7H_{16}). Here, the emissivity charts are presented for T=300K to 1400K and PL=0.01 atm.m to 10.0 atm.m. These fuels are some of the most common fuels in combustion and fires.

2. SPECTRAL DATABASES

In this work, the high resolution spectral absorption coefficients needed for generation of the emissivity charts are taken from two different sources of experimental measurements and line-by-line calculations. Wakatsuki (2005) measured the spectral absorption coefficients of Heptane, Methanol, MMA, Propane, Propylene and Toluene using high-resolution FTIR at seven tempratures. The wavenumber range was 700 cm^{-1} to 4000 cm^{-1} with 0.5 cm^{-1} resolution. Here, the experimental data were interpolated and extrapolated whenever needed for 300K to 1400K (Wakatsuki *et al.* (2005)). Wakatsuki (2005) showed that for the abovementioned six fuel gases, the contribution of the weak absorption lines outside the main absorption bands can be safely ignored. We obtained the needed high-resolution absorption spectra of Methane by line-by-line calculations. In the LBL calculations, HITRAN2008 (Rothman *et al.* (2009)) spectral database was used. The spectral absorption data were obtained for the temperatures from 300K to 2450K. A uniform spectral resolution of 0.02 cm^{-1} was chosen for the spectrum from 150 cm^{-1} to 15000 cm^{-1}. Chu *et al.* (2011) reported that this resolution is optimum for the LBL calculations in combustion applications. Figures 1 and 2 show the pressure-based absorption spectra at T=300K obtained from LBL calculations for Methane and the experimental measurements for Heptane, Methanol, Propane, Propylene, MMA and Toluene. As Figures 1 and 2 illustrate, all the gases have absorption coefficients less than 10^2 $atm^{-1}cm^{-1}$. These bands identify each gas and lead to different spectral characteristics and total emissivities.

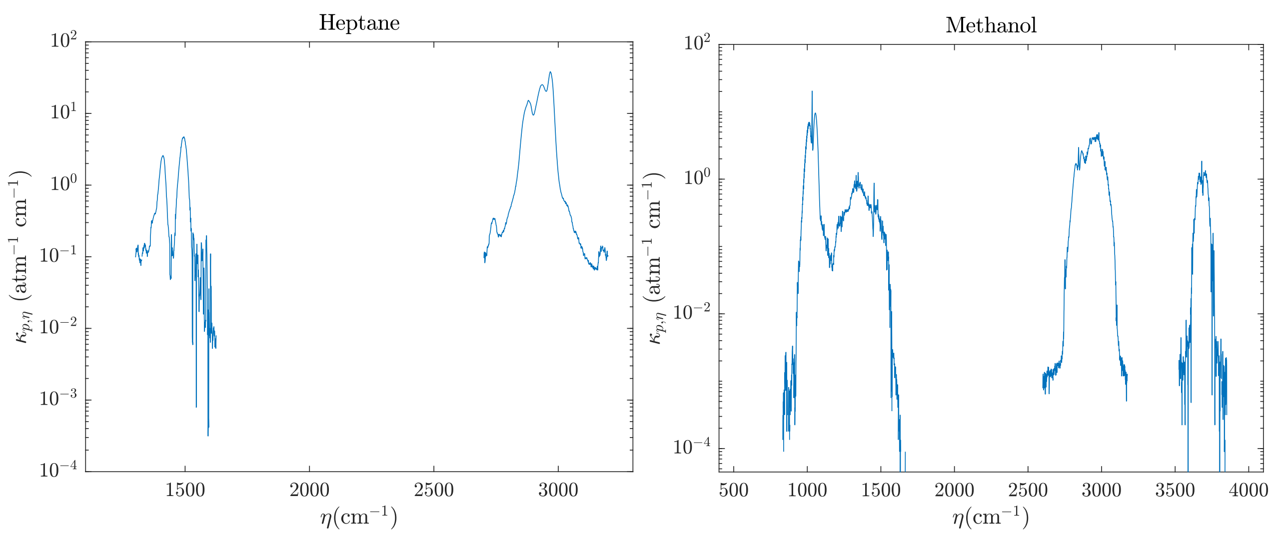

Figure 1: Absorption spectra of the fuel gases

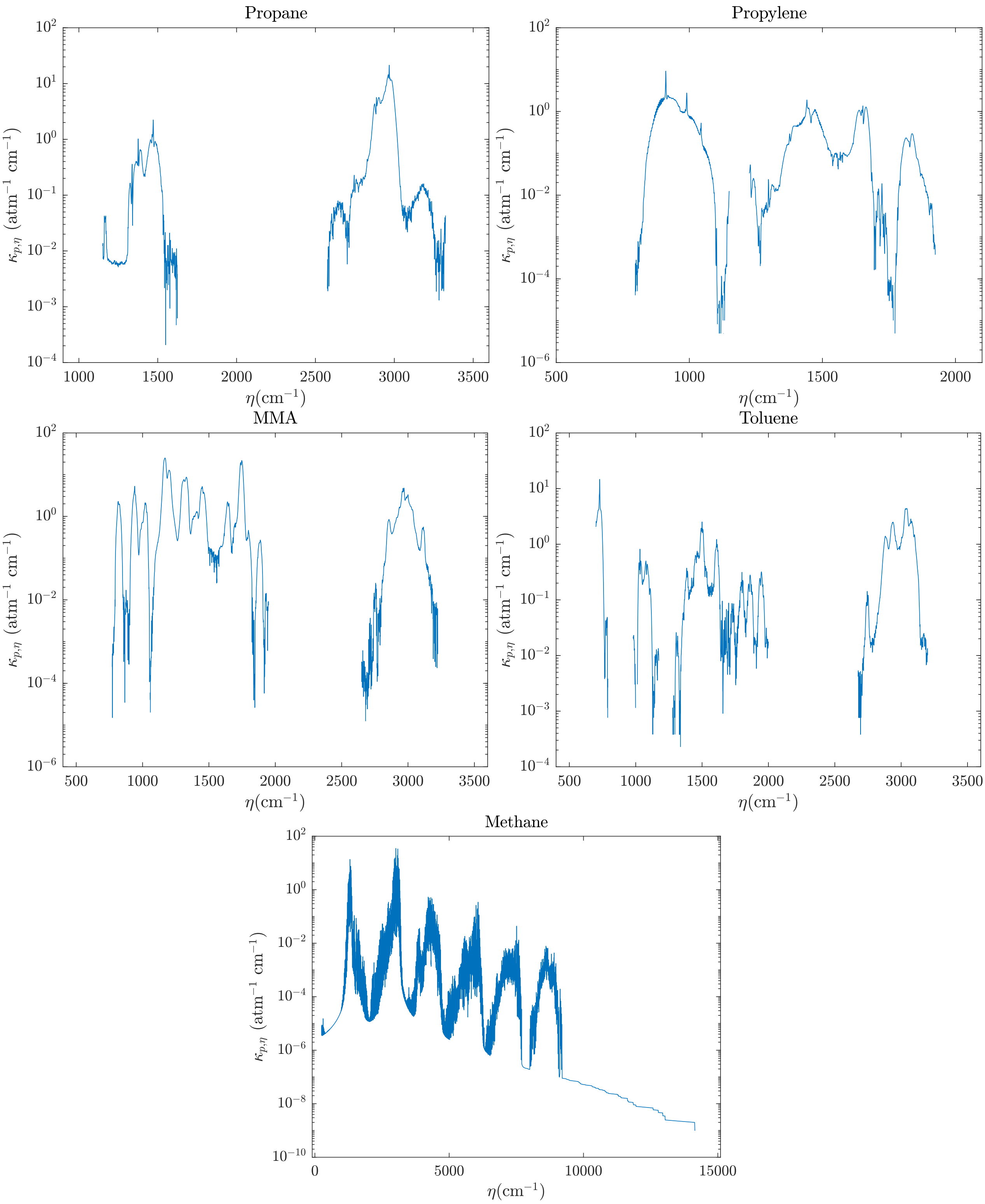

Figure 2: Absorption spectra of the fuel gases

3. PROBLEM STATEMENT

Emissivity is defined as the share of energy emitted over a certain path that escapes into a given direction without being absorbed between the point of emission and the point of exit. The total emissivity represents the portion of total emitted radiation over a path Y that is not attenuated by self-absorption divided by the maximum possible emission. The spectral emissivity can be calculated as:

$$\epsilon_\eta = 1 - e^{\kappa_\eta PYL} \tag{1}$$

where κ_η is spectral absorption coefficient at wavenumber η, P is total pressure of the medium, Y is molar fraction of the gas and L is the pathlength. To calculate total emissivity over all the spectrum at a given temperature,

$$\epsilon_t = \frac{\int_0^\infty I_{b\eta}(1 - e^{-\kappa_\eta PYL})d\eta}{\int_0^\infty I_{b\eta}d\eta} \tag{2}$$

where $I_{b\eta}$ is Planck function defined as

$$I_{b\eta} = \frac{2hc^2\eta^3}{n^2\left[e^{\frac{hc\eta}{nk_BT}} - 1\right]} \tag{3}$$

In Eq.3, h and k$_B$ are Planck and Boltzmann constants, respectively. c is the speed of light in vacuum media and n is refractive index which is considered n = 1 for gases. Spectral absorption coefficients are needed to solve Eq.2. Wakatsuki (2005) performed experiments for high resolution transmission measurements using a Mattason Galaxy 7020 FTIR for seven temperatures between 295K to 1000K over the wavenumber of 700 cm^{-1} to 4000 cm^{-1}. Here, absorption coefficients with 0.5 cm^{-1} resolution were interpolated and extrapolated based on Wakatsuki (2005) for 300K to 1400K. Wakatsuki (2005) showed that for the abovementioned six fuel gases, the contributions of the weak absorption lines outside the main absorption bands can be safely ignored.

4. RESULTS AND DISCUSSION

The calculated total emissivities of two fuel gases are presented in Figure 3. Emissivities are calculated using Eq. (2) for the temperatures of 300-1400 K for Heptane, Methanol, MMA, Propane, Propylene and Toluene and for 300-2450 K for Methane, with a temperature step of 10K. Here, the partial pressure of the species is defined as $p = PY$ where P is the total pressure and Y is the molar ratio. As seen in Figures 3 and 4, all the emissivity charts have increasing and then decreasing trends versus temperature. In comparison with other fuels, MMA has higher values of total emissivities, up to 0.63 for the studied pLs and among all the studied gases, Heptane has the lowest total emissivities with a maximum of 0.23 at T=800 K at the highest pL. Figure 4 indicates that Propane has a specific behaviour at $0.01 < pL < 1$, showing a significant decrease of the total emissivities around T =450 K.

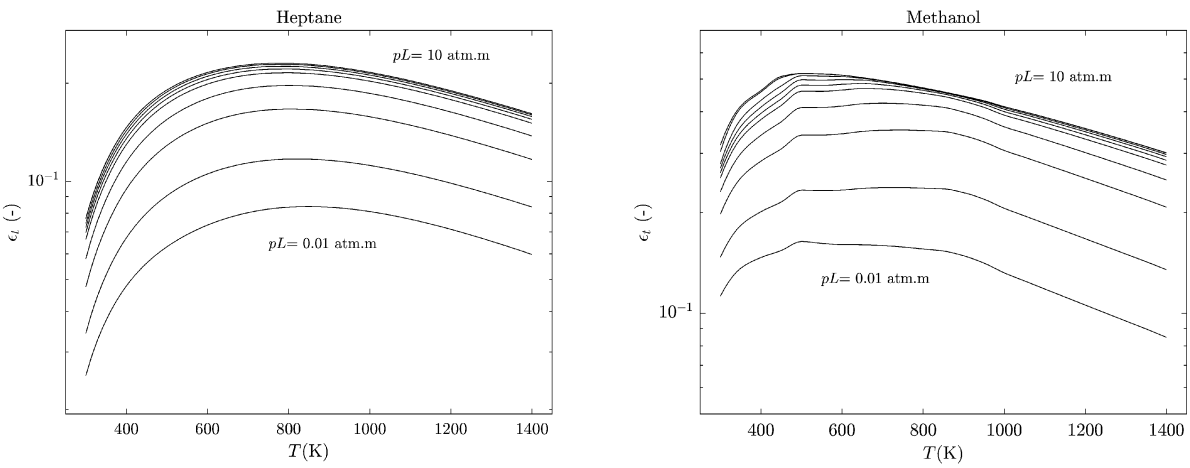

Figure 3: Total emissivity of the fuel gases

As seen in Figure 4, except for Methane, the emissivity charts sensibly vary up to $pL = 0.2$ atm.m and at higher pLs, the emissivity charts have very close values. Additionally, the total emissivity of Heptane, Methanol, MMA, Propane, Propylene and Toluene was independent of pL when $pL > 5.0$ atm.m. To understand the cause of this behaviour, we investigated the variation of the integrand of Eq. (2), normalized by total emitted power, i.e. $I_{b\eta}\epsilon_\eta/\sigma T^4$. Figure 5 shows the variation of this parameter with wavenumber for Propane and $pL = 0.02$ atm.m at three temperatures. In the chosen region of spectrum, η=1150-1330 cm^{-1}, the value of $I_{b\eta}\epsilon_\eta/\sigma T^4$ at T= 450K is generally lower than at T=400 K and T=500 K, leading to the lower value of total emissivity.

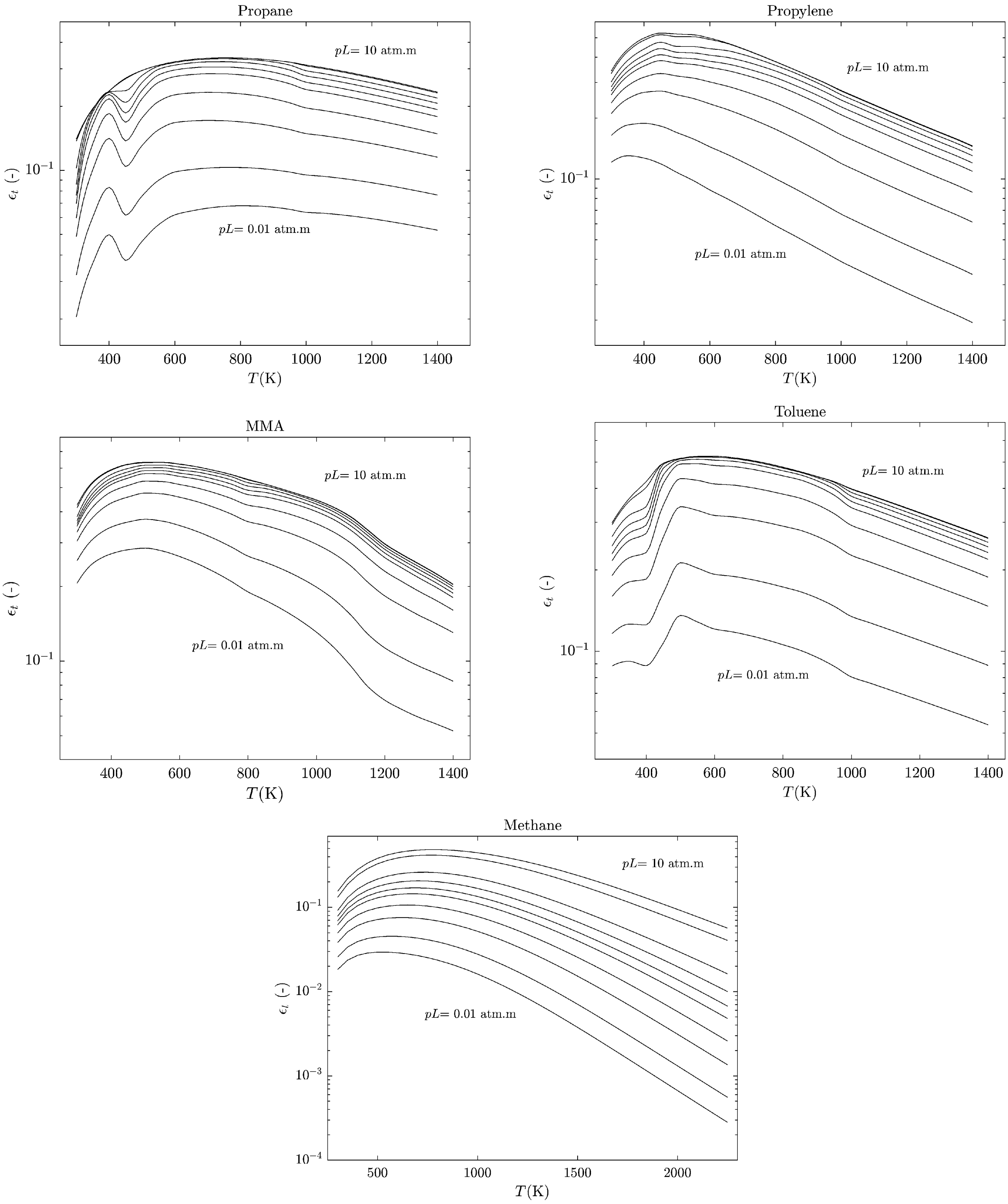

Figure 4: Absorption spectra of the fuel gases

5. CONCLUSION

In this work, emissivity charts of seven fuel gases were presented. Fuel gases had similar behaviour in general, meaning that the total emissivity of each increased until a certain temperature and then it decreased. For the studied gases, the maximum emissivities were observed between T=500 K and 800 K. In addition, total emissivities increased by increasing pL values due to the higher concentration of the fuel gas molecules. However, the total emissivities were independent of pL at $pL > 5$ atm.m

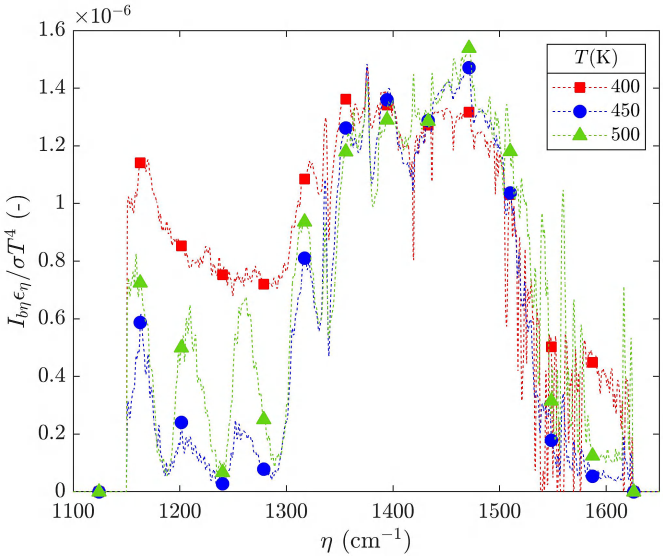

Figure 5: Absorption spectra of the fuel gases

6. ACKNOWLEDGEMENT

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