A VERTICAL DIFFUSION MODEL TO PREDICT PROFILES OF TEMPERATURE WITHIN THE LOWER ATMOSPHERIC SURFACE LAYER: SIMPLE OR COMPLICATED?

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Abstract—Knowledge of urban and rural climates is of crucial importance in urban climate control and wind farm development. A vertical diffusion model that predicts vertical profiles of temperature in a rural area was developed. This model has the capability to predict the thermally stable and unstable conditions as they vary diurnally. A different parameterization, which is independent of the well-known Obukhov length, was introduced to calculate the turbulent diffusion coefficient. The source/sink term in the diffusion equation was also parameterized based on heat fluxes at surface level. The net heat flux was composed of shortwave/longwave radiation fluxes and release of sensible/latent heat fluxes from vegetation/ground. As a result, the model can transition between thermally stable and unstable conditions over the diurnal cycle. The assumption of a constant specific humidity profile in this model was assessed by comparing vapour and saturation vapour pressures up to low altitudes, well within the lower portion of the atmospheric surface layer. In addition, a Doppler miniSoDAR system was operated to sample the vertical wind speed profiles in a typical rural area. The diurnal wind speed profile was compared to the logarithmic law. From an urban climate point of view, this model can be employed on its own or it can be coupled to existing urban canopy models to predict the urban microclimate.

Keywords-component; length scale, temperature profile, vapour pressure, vertical diffusion, wind profile

I. INTRODUCTION

Modeling the vertical profile of meteorological quantities in the lowest range of altitudes within the atmospheric surface layer is becoming important since this layer drives the microclimate environments. For example, accurate wind speed profiles are required to perform wind energy feasibility studies and to predict shear loads on the wind turbine blades. In the context of urban planning, vertical profiles of wind speed and temperature in both urban and rural areas are of great importance to predict and control the urban environment to meet human comfort.

It has been suggested that turbulent transport in rural areas, which is characterized by horizontally uniform distribution of temperature and wind, is only significant in the vertical direction. The well-known $K - theory$, which is based on the down-gradient transport hypothesis, is generally accepted to approximate turbulent transport in the vertical direction, where K_t is turbulent diffusivity governing the strength of transport [1]. This hypothesis indicates that, for example, heat flows down from warm regions to cold regions at a rate proportional to K_t multiplied by gradients of mean temperature. In this theory, vertical motion is accounted for small scales of turbulent mixing based on mixing length scales [2].

During the last few decades, numerous studies have focused on modeling vertical profiles of wind speed and temperature based on turbulent mixing length models [2-4]. The very first version of the length scale parameterization suggested a linear relationship between mixing length and height for near neutral conditions but $(-1/2)$ and $(-1/4)$ power laws for unstable conditions [3]. It has been suggested that wind speed and temperature profiles, specifically turbulent diffusion coefficient within the surface layer, is largely controlled by friction velocity, surface roughness, and stability condition [2]. The majority of existing models parameterize the mixing length scale using the Obukhov length, which is defined as

$$L = \frac{-u_{*0}^3}{\kappa(g/T)\overline{w'T'}}, \tag{1}$$

where u_{*0} is friction velocity near the ground, κ is the von Kármán constant, (g/T) is buoyancy parameter, and $\overline{w'T'}$ is the kinematic turbulent vertical heat flux at the surface. It has been suggested that the sign of (z/L), where z is the height above the surface, implies the stability condition: negative represents the thermally unstable atmosphere and positive represents the thermally stable atmosphere [5]. Despite extensive use of L to relate momentum and heat fluxes to bulk meteorological parameters, serious limitations have been found with the use of L particularly for near neutral and stable atmospheric conditions [6]. During neutral condition, vertical heat flux approaches close to zero leading to large values (positive or negative) for

Obukhov length. Hogstrom [7] also showed substantial scatter between experiments for wind and temperature gradient as a function of L for neutral conditions. Efforts have been made to parameterize the turbulent mixing length scales in the lowest few hundred meters of the atmospheric boundary layer using alternative methods [8]. For example, it has been suggested that turbulent mixing length scales can be divided into three regions. In the first region mixing length increases linearly with height within the surface layer considering stability correction; in the next region just above the surface mixing length depends only on stability condition; and in the last region at the top of the surface layer the mixing length is negligible compared to the other two regions [8].

II. OBJECTIVE

Many studies in the literature parameterize turbulent diffusivity based on mixing length scales, which are still suffering from Obukhov length limitations. To cope with these problems, a different parameterization for turbulent diffusivity is introduced, which is mainly inspired by explicit formulation of the turbulent length scale [9] and systematic scaling analysis of turbulent flow [10]. The model will distinguish between stable and unstable conditions based on direct solar radiation in a rural area. The study also investigates how well the rural wind speed profile can be formulated using field measurements in a typical area in Guelph, Canada.

III. OBSERVATION SITE

In this study, data was collected from a rural field campaign held in the Guelph Turfgrass Institute from July 14, 2018 to September 4, 2018. The rural area is far away from the nearby urban areas by 1-2 km (Fig. 1).
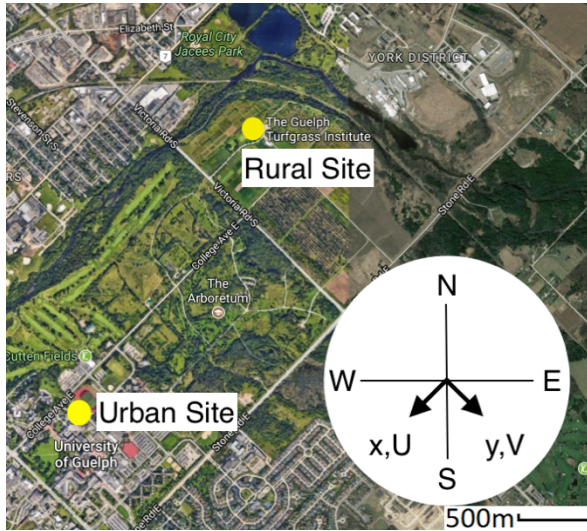

Figure 1.   Top view of rural area which is located at the Guelph Turfgrass Institute at $43.5473°$N and $80.2149°$W.

In the rural site, a Doppler miniSoDAR was operated to measure wind speed and wind direction from 30 m to 200 m at 10 m vertical resolution (Fig. 2). It outputs average data every 30 minutes. In the same location, Environment and Climate Change Canada is operating a meteorological station by measuring temperature and humidity at 2 m elevation and wind speed and direction at 10 m elevation.

Figure 2.   The Doppler miniSoDAR instrument operated in the rural area to measure the wind speed and direction profiles

IV. METHODOLOGY

In this study, wind speed profile is calculated using the logarithmic equation

$$\bar{S} = \frac{u_*}{\kappa} \ln\left(\frac{z-d}{z_0}\right), \tag{2}$$

where d is rural displacement height and z_0 is rural aerodynamic roughness length scale. Raupach et al. [11] suggested that z_0 is 0.2 for trees. u_* is friction velocity. Aliabadi et al. [10] performed a systematic scaling analysis of turbulence parameters using data collected from a microclimate field campaign in Guelph, Canada, to parameterize u_*. They found a high linear correlation coefficient between u_* and mean horizontal velocity and suggested the following equation for the rural cite

$$u_* = 0.07\bar{S} + 0.12. \tag{3}$$

Fig. 3 shows measurements from the miniSoDAR from 30 meters up to five times of average building height (around 80 m) in the surrounding areas compared to logarithmic wind speed profile. The logarithmic model with a new equation for friction velocity predicts wind speed profile in the rural area reasonably well. However, it very often overestimates wind speed up to the height of 50 m under thermally stable conditions.
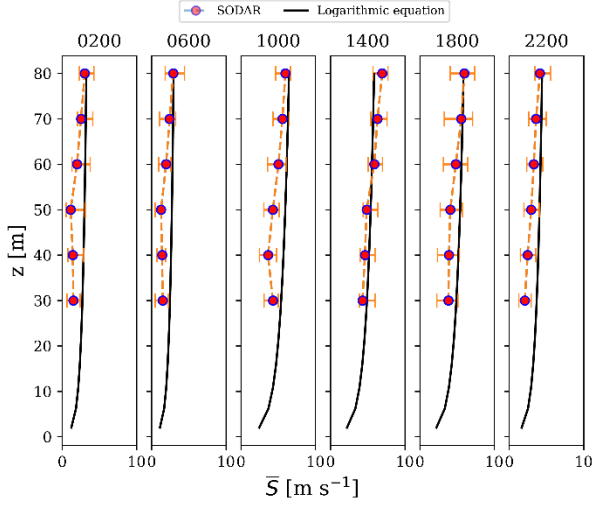
Figure 3. Comparison between logarighmic wind speed profile and miniSoDAR measurerments; times in Local Standard Time (LST)

In atmospheric modeling, it is a common practice to characterize turbulence using vertical diffusion of an atmospheric quantity of interest, such as momentum, heat, and humidity [12]. This approach follows the Reynolds averaging procedure in which the variable of interest (here temperature) is decomposed into mean and fluctuating parts. The heat equation in the horizontally-homogeneous region is reduced to

$$\frac{\partial \bar{\theta}}{\partial t} + \overline{W} \frac{\partial \bar{\theta}}{\partial z} = \frac{\partial \overline{w'\theta'}}{\partial z} + \gamma, \tag{4}$$

where $\bar{\theta}$ is the potential temperature, $\overline{W}$ is the mean velocity component in the z or vertical direction, $\overline{w'\theta'}$ is the kinematic turbulent vertical heat flux, and γ is the heat sink/source term also known as cooling or heating rate. Assuming steady state conditions and zero mean vertical velocity the left-hand side of equation (4) is forced to zero. From $K - theory$, turbulent heat flux is proportional to the gradient of mean potential temperature. Thus, equation (4) can be simplified to

$$0 = \frac{\partial}{\partial z}\left(-\frac{K_t}{Pr_t}\frac{\partial \bar{\theta}}{\partial z}\right) + \gamma, \tag{5}$$

where K_t is turbulent diffusivity and Pr_t is the turbulent Prandtl number (assumed to be one here [13] but can be changed). It has been suggested that K_t is a function of mixing length scale, which needs to be parameterized given the stability condition [8].

A. Parameterization of Mixing-Length

Prandtl [14] proposed that turbulent diffusivity is proportional to wind shear and it can be formulated by length scale (ℓ), which inherently depends on atmospheric stability condition

$$K_t = \ell^2 \frac{\partial \bar{S}}{\partial z}, \tag{6}$$

where $\bar{S}$ is the mean horizontal wind speed. The approach to parameterize length scale, as opposed to previous models, is not a function of Obukhov length. As mentioned before, the diurnal variation of Obukhov length exhibits very large values in neutral

or weakly stable conditions, where the vertical heat flux is negligible (see Fig. 4 in local standard time (LST) as obtained from a climate model). According to previous formulations for mixing length [8], it can cause unexpected values for mixing length and consequently turbulent diffusivity.
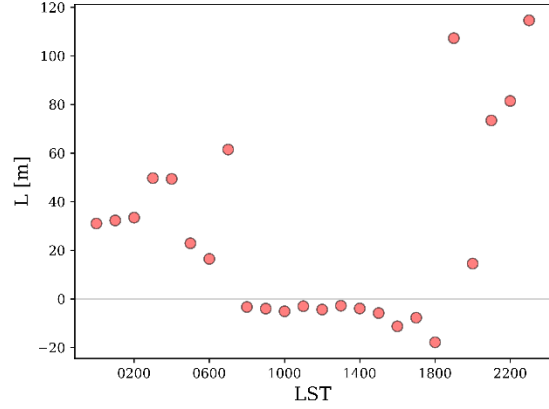

Figure 4. Diurnal variation of Obukhov length; times in Local Standard Time (LST)

Inspired by Gryning et al. [8], the mixing length scale can be parameterized as

$$\frac{1}{\ell} = \frac{1}{C_{cr}}\left(\frac{1}{\kappa z} + \frac{1}{C_* u_*}\right), \tag{7}$$

where the first term on the right-hand side indicates a linear relationship with height near the surface, while the second term restricts the value of length scale in the upper part of the atmospheric surface layer, and C_* is a correction factor for the second term. C_{cr} is a scaling correction factor which can be optimized to 2 during unstable conditions and 1.5 during stable conditions. The most appropriate and practical indicator for thermally unstable conditions is presence of incoming solar radiation on the surface while the absence of incoming solar radiation on the surface indicates stable conditions. This approach is mostly applicable for not-so-much humid air at short vertical scales.

B. Parameterization of Heat Sink/Source Term

We still need to parameterize heat sink/source term (γ) to close equation (5). Cooling or heating of the atmospheric surface layer is tightly coupled to heat transfer with the earth surface. When a positive upward heat flux from the surface is injected into the atmosphere, unstable conditions are created with the consequence that the column of air warms above the surface. On the other hand, a negative upward heat flux from the surface, i.e. heat sink into the earth surface, will create stable conditions while cooling the column of air above the surface. Such heat fluxes can be estimated using sensible and latent heat components.

Parameterization of γ, which is composed of sensible and latent heat fluxes from the rural site, requires meteorological information measured at the rural area. For example, a weather file typically contains information about direct and diffusive

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solar radiations, temperature at the height of 2 m and wind speed at the height of 10 m on an hourly basis. In this study, we assumed the following equations to formulate γ

$$\gamma = C_\gamma \left(\frac{Q_{net}}{\rho C_p}\right)\frac{1}{H_{bl}}, \tag{8}$$

$$Q_{net} = \underbrace{\left(Q_{Hveg} + h_{conv}(T_0 - T_{air})\right)}_{sensible\ heat\ flux} + Q_{rad} + \underbrace{(Q_{Lveg} + Q_{Lsoil})}_{latent\ heat\ flux}, \tag{9}$$

where Q_{net} is the net heat flux (positive upward from the surface into the atmosphere at the rural site), ρ is air density near the rural surface, C_p is air specific heat capacity, C_γ is a scaling factor for heat sink/source term (optimized to be 10) and H_{bl} is the diurnally-averaged boundary layer height taken to be 2000 m. In equation (9), Q_{Hveg} is the sensible heat flux from vegetation, h_{conv} is the convection heat transfer coefficient at the rural surface, T_0 is the rural surface temperature, T_{air} is the air temperature at the height of 2 m, Q_{rad} is the long wave and shortwave radiation absorbed by the rural surface, Q_{Lveg} is the latent heat flux from vegetation, and Q_{Lsoil} is the latent heat flux from soil. Bueno et al. [15] provided more details about calculation of these heat fluxes. Palyvos [14] suggested that the convection heat transfer coefficient is a linear function of wind speed

$$h_{conv} = 3.7\bar{S}_0 + 5.8, \tag{10}$$

where $\bar{S}_0$ is mean wind speed obtained from the rural weather station.

V. RESULTS AND DISCUSSION

From the above parameterization of mixing length and heat source/sink term we can now determine the diurnal variation of temperature and wind speed profiles in the rural area. Note that the model is only applied to rural climate up to the height of 5 times of average building height in the surrounding urban area, which is 80 m for the top of the domain for the vertical diffusion model. The boundary conditions for potential temperature are fixed value at the bottom of the domain, set to temperature at 2m elevation, and zero gradient on the top of the domain. Wind shear gradient is estimated from the logarithmic law at any elevation. However, this assumption is more accurate during thermally-neutral conditions.

As shown in Fig. 5, vertical profile of turbulent diffusivity exhibits negligible value very near the surface under all stability conditions. It is also known that the turbulent diffusivity very far from the surface close to the top of the planetary boundary layer is also negligible (not shown here). K_t increases with height at different rates depending on the stability condition. Under unstable conditions, atmospheric turbulence is mostly driven by thermal convection and shear production, as opposed to stable condition. Thus, as shown in Fig. 5, turbulent mixing at 1000 LST, 1400 LST and 1800 LST increases at higher rates.
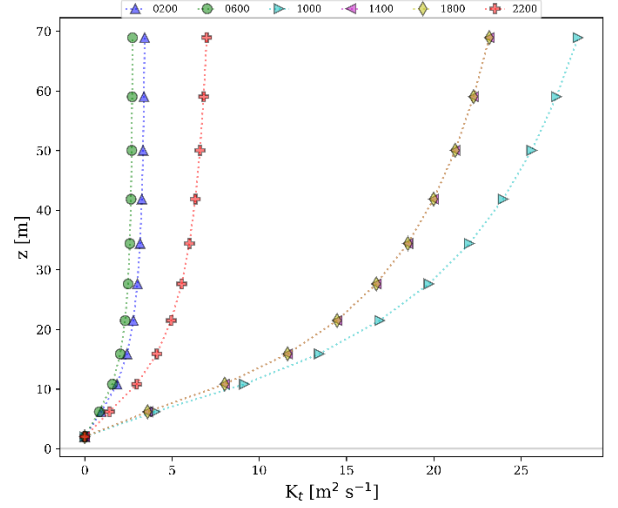

Figure 5. Diurnal variation of turbulent heat diffusivity profiles in the rural area; times in Local Solar Time (LST)

Fig. 6 shows the potential temperature profiles in the rural area over the course of a day. The atmosphere goes through a cycle starting from strongly stable conditions in the early morning (0200 LST) to unstable condition in the midafternoon (1400 LST). Under stable conditions, potential temperature increases with height and the atmospheric surface layer is weakly turbulent. As potential temperature profiles evolve with time and the sun rises, the rural surface begins warming up and the atmosphere becomes more turbulent. At 0200 LST the rural surface layer retains the heat from the previous day, explaining higher potential temperatures aloft, but the atmosphere is calm and stable near the surface where cooling occurs. As time evolves into the night and close to the morning, the surface layer potential temperature further drops at all altitudes. During the day, higher surface temperatures cause upward heat flux and the atmosphere becomes more turbulent. A clear transition between unstable to stable condition is evident at 1800 LST, where the potential temperature profile does not exhibit any significant change with height near the surface, representing the neutral condition.
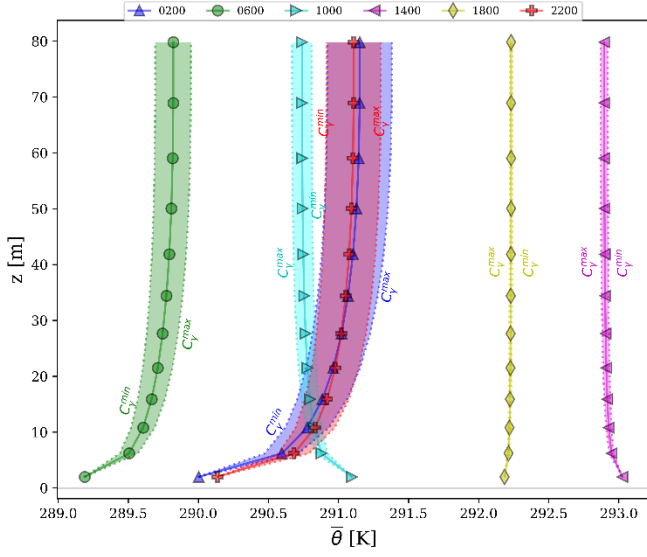
Figure 6. Diurnal variation of temperature profile in the rural area; times in Local Solar Time (LST)

An important parameter which can significantly affect parameterization of cooling/heating rate is C_γ. The effect of this coefficient on γ and the potential temperature profile is investigated by performing a sensitivity analysis. C_γ is varied in the range 8, 10, 12. As shown in Fig. 6, temperature profiles during stable atmospheric condition shift more under the influence of C_γ. In addition, diurnal variation of the heat sink/source term is provided in Fig. 7. This figure clearly shows that the rural heat flux varies between negative to positive values under a cycle of stable-neutral-unstable-neutral conditions. Sensitivity of the sink/source term to C_γ is also shown in Fig. 7.

Another sensitivity analysis is conducted to understand the effect of scaling correction factor C_{cr} for the mixing length scale on the temperature profile. For this purpose, C_{cr} is set to vary in the range 1.2, 1.5, 1.8 under stable condition and 1, 2, 3 under unstable condition. As shown in Fig. 8, this scaling factor has a large effect on the potential temperature profiles particularly during the stable condition.
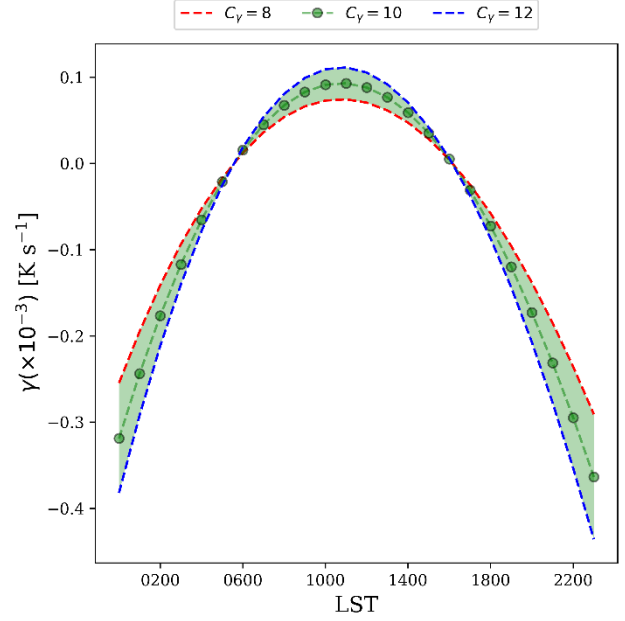

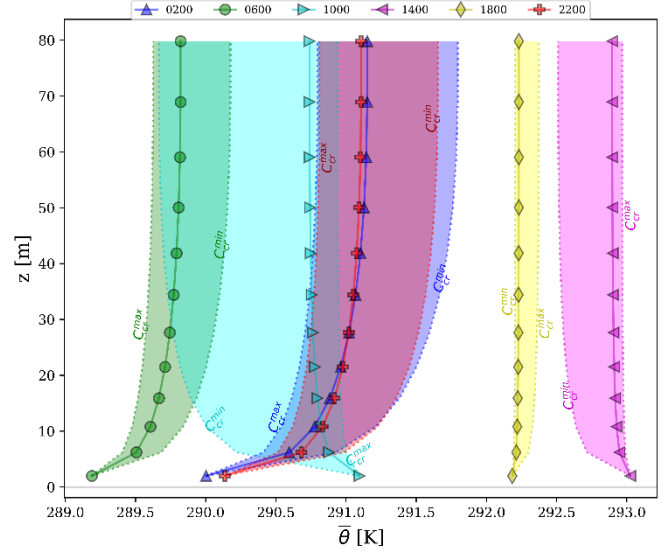Figure 7. Diurnal variation of cooling or heating rate for different C_γ; times in Local Solar Time (LST)

Figure 8. Effect of scaling factor on diurnal variaion of temperature profile; times in Local Solar Time (LST)

Another assumption made in this rural model is to consider that the specific humidity is constant, i.e. invariant with height. This assumption is valid until vapour pressure is less than the saturation vapour pressure for a given altitude. This condition must be checked to validate the adequacy of this assumption. From the specific humidity equation, we have

$$q = \frac{\rho_v}{\rho_a} = \frac{\rho_v}{\rho_v + \rho_d}, \tag{11}$$

where ρ_v is the water vapour density, ρ_a is the air density and ρ_d is dry air density. This can be simplified more using the ideal gas law

$$q = 0.622 \frac{P_v(z,T)}{P_a(z,T)}, \qquad (12)$$

where P_v and P_a are the water vapour pressure and the air pressure, respectively, as a function of height and real temperature (T) (not potential temperature). Using the Clausius-Clapeyron equation, we can determine the saturation pressure (P_{sat}) for water using

$$P_{sat}(T) = 0.61094 \, exp\left(\frac{17.625T}{T+243.04}\right), \qquad (13)$$

where P_{sat} is in kPa and T is in $^\circ$C. Note that the temperature in the diffusion equation is the potential temperature, so, a density profile is required to convert potential temperature to real temperature. Using density (ρ_0), real temperature (T_0) and pressure (P_0) at the surface level from the weather station at 2 m elevation, and considering a lapse rate of -0.000133 kg m^{-3} m^{-1} for density within the surface layer, the density profile can be simplistically parameterized by

$$\rho = \rho_0 - 0.00133(z - z_0). \qquad (14)$$

Now, we can calculate the vapour pressure and saturation vapour pressure at the top of the domain using equations (12) and (13), respectively. Fig. 7 shows the time series of P_{sat} and P_v on the domain top over the course of a day. Vapour pressure is almost always less than saturation pressure, particularly during the day. However, vapour pressure tends to saturation pressure under strongly stable condition from 0000 LST to 0600 LST. Assuming constant specific humidity up to the height of five times of average building height in the surroundings, i.e. 80 m, does not significantly violate the requirement for vapour pressure to remain below saturation vapour pressure on the top of the domain. So the assumption for constancy of specific humidity within the lowest range of altitudes in the surface layer is a practical assumption. Note, however, that this assumption does not apply to high altitudes where condensation may occur due to vapour pressure exceeding saturation vapour pressure.
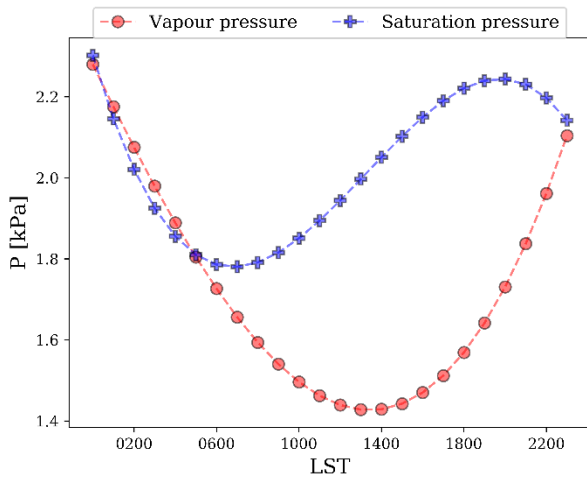

Figure 9. Diurnal variaion of vapour pressure and saturation vapour pressure on the top of the vertical diffusion model domain; times in Local Solar Time (LST)

VI. Conclusion

A different approach was used to parameterize meteorological quantities, specifically vertical profiles of the potential temperature, in the lowest range of altitudes for the atmospheric surface layer of a typical rural area. As opposed to previous models suffering from limitations on Obukhov length, the model was developed independent of Obukhov length to formulate turbulent heat diffusivity. A vertical diffusion equation was used for temperature using $K - theory$ with a new parameterization for the heat sink/source term, and subsequently the turbulent heat diffusivity. A relation between turbulent diffusivity and mixing length was established based on the availability of direct incoming solar radiation reaching the rural surface. In other words, a solar-basis correction factor for mixing length was introduced to consider effect of atmospheric stability, which is optimized as 2 under unstable condition (incoming solar radiation) and 1.5 under stable condition (lack of incoming solar radiation). Diurnal variation of turbulent heat diffusivity profile showed higher values during the day than over night, when the surface layer is less turbulent. Longwave and shortwave radiation, sensible and latent heat fluxes from soil and vegetation, and convection heat flux from the ground were considered as contributing factors in parameterization of heat sink/source term in the energy equation. As a result, vertical profile of the potential temperature clearly showed a cycle through stable, neutral, unstable, and neutral conditions. A logarithmic equation was used to determine the wind speed profile, which was more accurate during neutral and unstable conditions. The diurnal variation of the logarithmic wind profile was compared to measurements from a miniSoDAR in the rural area. An important assumption in this rural climate model was to consider specific humidity to be constant, i.e. invariant with height. This was assessed by comparing the vapour pressure and the saturation vapour pressure at the top of the vertical diffusion model domain (five times of building height in the nearby urban areas), and it was shown that almost always the vapour pressure is less than the saturation vapour pressure. However, vapour pressure approached saturation pressure over night. Future work shall involve integration of this rural climate model into an urban climate model to predict the vertically-resolved microclimate of urban areas. The vertical diffusion model, however, may have many other potentials for use such as wind farm assessment as well.

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