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A SIMPLE METEOROLOGICAL PREPROCESSOR (SIMETPRO) FOR OPTIMIZING HANDS-ON APPLICATION OF AIR POLLUTION DISPERSION MODELS IN LIMITED DATA SCENARIOS

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ABSTRACT

This study presents preliminary test case of a Simple Meteorological Preprocessor (SIMETPRO) that is coupled from boundary layer scaling relationships for estimating deterministic surface layer parameters. The SIMETPRO is intended for teaching hands-on basics of meteorological preprocessing in limited data scenarios of West African sub-region and its subsequent application in air pollution dispersion models. A two-year dataset of routine meteorological parameters obtained from near-surface gradient measurement around a characteristic scrap-iron smelting industry in Ile-Ife, southern West Africa was used to test run the preprocessor. An independent field experiment of Eddy Covariance (EC) system complimented with profile measurement of air temperature, relative humidity and wind speed was used to validate sensible heat flux and friction velocity estimates from the SIMETPRO. Diurnal trend of the SIMETPRO outputs were realistic in representing diurnal changes of atmospheric dynamics. Time variation analyses of daytime (07:00-18:00 GMT+1) minimum-maximum values were; friction velocity (FRV) 0.05 – 0.65 ms^{-1}, mixing height (MH), 200 – 3100 m, sensible heat flux (SHF) 25 – 135 Wm^{-2}, potential temperature gradient (PTG) – 0.4 – (-0.01) $^{o}C/m$, convective velocity (COV) 0.2 – 1.5 ms^{-1}. Nighttime (19:00 - 06:00 GMT+1) values were less variant with MH mostly below 500m, VPG between 0 – 0.6 $^{o}C/m$ and SHF below 5 Wm^{-2}. Inter-annual trend level shows varied degree of values between seasons and years, mostly with peak values occurring in dry seasons. Preliminary limitations of the SIMETPRO validation were highlighted and future refinement direction pointed out. In summary, a handy meteorological tool for stepwise understanding of basic parameters required for running dispersion models was proposed and tested. Though further refinement is required, the SIMETPRO is nonetheless efficient in delivering the targeted objective.

Keywords: meteorology; preprocessor; air pollution; dispersion models; surface layer parameters

INTRODUCTION

Estimating air pollutants' emissions and their atmospheric dispersion from natural and anthropogenic sources has become a global demand to compliment limited in-situ measurement required for regulatory, compliance and environmental protection purposes especially in developing countries. Reliable ambient air pollutants estimates are therefore derived from well-formulated and tested regulatory air pollution models. To execute such models, deterministic surface layer parameters which describe the dynamical state of the atmospheric boundary layer are required as input. These parameters include the mean wind speed, ambient air temperature, boundary layer height, Bowen ratio, sensible heat flux, friction and convective velocity, atmospheric stability parameters, Monin-obukhov's length, mechanical and convective mixing heights among others (Perry *et al*., 2003). However, not all of these parameters are routinely measured at meteorological stations due to spatio-temporal constraints in deploying equipment, technical capability and manpower. The need therefore arises to estimate the surface layer parameters in terms of routinely measured meteorological variables using well tested and validated parametric relationship through meteorological preprocessing (Jegede, 1994a). A number of meteorological preprocessors have been developed and well tested (Perry. 1992; Hanna and Chang, 1993, Karppinen *et al*., 1997; Cimorelli *et al*., 2004), but none was experimented in Africa. As a result, they do not fully represent the conditions in tropical locations (Jegede, 1994a). This is mainly because many of the empirical parameters used in developing the preprocessors were obtained using boundary layer measurements from the mid-latitudes which is quite different from the conditions at low-latitudes (Jegede, 1994b). In addition, the available preprocessors require input of upper air data which is not readily available for tropical locations and when available, they are often not on a sufficient timescale and the accessibility might be limited. As a result, the output parameters from these preprocessors do not accurately describe the atmospheric dynamics at the site of application. It is of great need therefore to provide alternative route to obtaining fairly reliable estimates of important atmospheric parameters for executing regulatory dispersion models at a tropical locations of Africa for instance. Hence, this study presents the architecture for a simple meteorological preprocessor for optimizing the use of air quality dispersion models for teaching atmospheric Physics/Science students and the appreciation of hands-on application in Nigeria. The aim of this study is not to discuss the dynamics of the parameters but rather to show the feasibility of the SIMETPRO output as an input for dispersion models. Depending on the dispersion model of choice, users who intend to apply SIMETPRO may have to convert the outputs into readable formats.

MATERIALS AND METHODS

Meteorological Measurement

Quality-assured and high time resolution meteorological dataset (ambient air temperature, relative humidity, wind speed and direction, sensible and soil heat flux, net and global radiation) acquired in March – December, 2013 and January – June 2014 was utilized in this study. The dataset were products of a site specific measurement conducted in the vicinity of a scrap-iron smelting factory in Fashina, Ile-Ife to model the dispersion of pollutants emission from the factory. Detailed description of the metrological mast installation, height configuration, meteorological parameters and corresponding sensors used, data archiving and post quality-assurance procedure has been given by Abiye *et al.*, (2017).

Parametric Models

The following sub-sections describe the parametric models employed in estimating the surface layer characteristics at the study site.

Lapse Rate (Γ_a) and Potential Temperature Gradient (Γ_d)

From the logarithmic finite difference approximation method (Arya, 2001), the gradients of ambient air temperature and potential temperature were estimated as follows

$$\Gamma_a = \frac{\partial T}{\partial z} \cong \frac{1}{z_m}\frac{\Delta T}{\ln(z_2/z_1)} \qquad (1)$$

$$\Gamma_d = \frac{\partial \Theta}{\partial z} \cong \frac{\partial T}{\partial z} + \Gamma \qquad (2)$$

z_1 and z_2 are the heights for the two levels of wind speed measured from the ground surface. z_m is the geometric mean height of the two levels. Γ is the dry adiabatic lapse rate, approximately - 10 ^{0}C/km or 0.01 ^{0}C/m (Beychok, 2005).

Richardson Number (R_i) and Monin-Obukhov's (M-O) Stability Parameter (ζ)

The dimensionless dynamic stability parameter (Richardson number, (R_i), was used as a measure of the intensity of turbulent mixing and also as criterion for the existence or non-existence of turbulence in the stably stratified environment (Arya, 1999). The Richardson number which is a ratio of buoyancy force to shear stress and the M-O stability parameter ζ (ratio of height z, to buoyancy length scale L) were estimated from the formulations of Arya (1999). The buoyancy length scale L also known as Monin-Obukhov's length is a measure of the depth of the near-surface layer in which shear effects are likely to be more significant under any stability condition. The empirical relationships used in this study are given as follows

$$R_i = \frac{g}{T}\frac{\frac{\partial \Theta}{\partial z}}{\left(\frac{\partial u}{\partial z}\right)^2} \qquad (3)$$

$$\zeta = \begin{cases} R_i, & R_i < 0 \\ \dfrac{R_i}{1-5R_i}, & 0 \le R_i < 0.2 \end{cases} \qquad (4)$$

$$\zeta = {}^{z}/_{L} \tag{5}$$

Surface Friction Velocity (u_*)

The magnitude of the surface friction velocity u_* which serves as a measure of the vertical transport of horizontal momentum and hence the atmosphere's ability to drift and lift pollutants from the earth's surface was determined from gradient measurement of wind speed. This method was preferred to the usual iterative scheme proposed by Businger *et al* (1971) because the iterative method was found to always fail under stable conditions especially in a low wind condition (Berkowicz and Prahm, 1982; Stull and Bruce, 2006) typical of the of the present study site. Hence, an alternative method to avoid this disadvantage (Arya, 2001) was adopted as follows

$$u_* = \frac{k \triangle u}{\phi_m \ln(z_2/z_1)} \tag{6}$$

The M-O dimensionless similarity heat and momentum stability terms ϕ_h and ϕ_m as a function of geometric mean height of the measurement levels (z_m) and Obukhov's length L were determined as follows:

$$\phi_m = \begin{cases} (1 - 15\zeta)^{-\frac{1}{4}}, & \zeta(z_m/L) < 0 \\ 1 + 15\zeta, & \zeta(z_m/L) > 0 \end{cases} \tag{7}$$

$$\phi_h = \begin{cases} (1 - 15\zeta)^{-\frac{1}{2}}, & \zeta(z_m/L) < 0 \\ 1 + 15\zeta, & \zeta(z_m/L) > 0 \end{cases} \tag{8}$$

Bowen Ratio (β)

The Bowen ratio, β (Kakosimos *et al.*, 2011); the ratio of sensible heat flux (H) to latent heat flux (λE), was estimated from the gradient of air temperature (T) and specific humidity (q) as follows:

$$\beta = \frac{H}{\lambda E} \cong \gamma \frac{\Delta T}{\Delta q} \tag{9}$$

where γ is the psychometric constant (0.4 g/kg·K^{-1}). ΔT and Δq are gradients of air temperature and specific humidity, respectively. In order to obtain the specific humidity, an estimate of the saturated vapor pressure (*SatVP*) and vapor pressure (*VP*) is required. A polynomial approximation method by Lowe (1977) was adopted.

$$SatVP = 0.1(A_0 + A_1T + A_2T^2 + A_3T^3 + A_4T^4 + A_5T^5 + A_6T^6) \tag{10}$$

where

$A_0 = 6.107799961, A_1 = (4.436518521)^{-01}$, $A_2 = (1.428945805)^{-02}, A_3 = (2.650648471)^{-04}$, $A_4 = (3.031240396)^{-06}, A_5 = (2.034080948)^{-08}$, $A_6 = (6.136820929)^{-11}$

The vapor pressure (KPa) was estimated from

$$VP = \frac{SatVP * RH}{100} \tag{11}$$

RH is the relative humidity (%)

Sensible Heat Flux (H)

Simple parameterizations were made from the surface energy balance equation in (12) (Oke, 1978) with λE = H/β from (9)

$$R_N = H + \lambda E + G \tag{12}$$

In cases when direct measurements of R_N (net radiation) and G (ground heat flux) are available, the above expression for sensible heat flux was represented as

$$H = \frac{(R_N - G)}{1 + 1/\beta} \tag{13}$$

In order to ensure that the estimated sensible heat flux obtained from the method above was bounded within the limits of reasonable values [it is known that the Bowen ratio breaks down in the region -1.25 < β < - 0.75 (Ohmura, 1982; Jegede *et al.*, 2001)], an approximation for the sensible heat flux was introduced using tested empirical relationship obtained from measured dataset at the study site. Whenever there is a breakdown, $H_{est} = aR_N$ was used where α is a constant that is location dependent.

Convective Velocity Scale (ω_*)

The convective velocity scale ω_* of turbulence in the surface layer was estimated following the formulation of Deardorff (1970)

$$\omega_* = \left(\frac{g}{T}\frac{H}{\rho C_p} z_{md}\right)^{1/3} \tag{14}$$

However, for the periods when estimates of the mixed layer depth $z_{ic,im}$ are unrealistic, Wyngaard and Brost (1984) formulation was adopted to calculate the convective velocity scale as in (15).

$$\omega_* = 4.74\left(\frac{H}{\rho C_p}\right)^{1/2} \tag{15}$$

Monin-Obuhkov's Length (*L*)

With a known estimate of the surface friction velocity u_* and sensible heat flux H_s in equation (6) and (13) respectively, the Monin-Obukhuv's length for the stable (Venkatram, 1980) and convective (Cimorelli *et al.*, 2004) boundary layer was estimated from equation (16) and (17) respectively.

$$L = \frac{Tu_*^2}{kg\theta_*} \tag{16}$$

$$L = -\frac{\rho c_p T u_*^3}{kgH} \tag{17}$$

Where, ρ is the density of dry air (kgm^{-3}), c_p is the specific heat capacity of air (Jkg^{-1}K^{-1}), T is the ambient temperature (K), and g is the acceleration due to gravity (ms^{-1})

Mixed Layer Height, z_i

For unstable conditions (stability classes A, B and C), equation (18) from Giovannoni (1993) was adopted for estimating the convective mixing height z_{ic}. For stable and neutral conditions, equation (19) from Cimorelli *et al* (2004) was used to estimate the mechanical mixing height z_{im}. Schematics of the SIMETPRO is presented in Figures 1 and 2.

$$z_{ic} = -kL\left(\frac{\omega_*}{u_*}\right)^3 \tag{18}$$

$$z_{im} = 2300u_*^{3/2} \tag{19}$$

Test validation for H_s and u_*

To validate the estimates of sensible heat flux (H_s) and friction velocity (u_*) obtained from SIMETPRO, direct measurements were obtained from an independent field experiment carried out at Obafemi Awolowo University Teaching and Research Farm, Ile-Ife between 20 and 21 July, 2014. The measurement site (Figure 3) was a grass covered 20 x 20 m^2 with well-levelled surface. The instrumentation at the site comprised a 6 m mast and an Eddy-Covariance (EC) measurement system. The EC sytem is the most accurate and straight forward (direct) technique available for

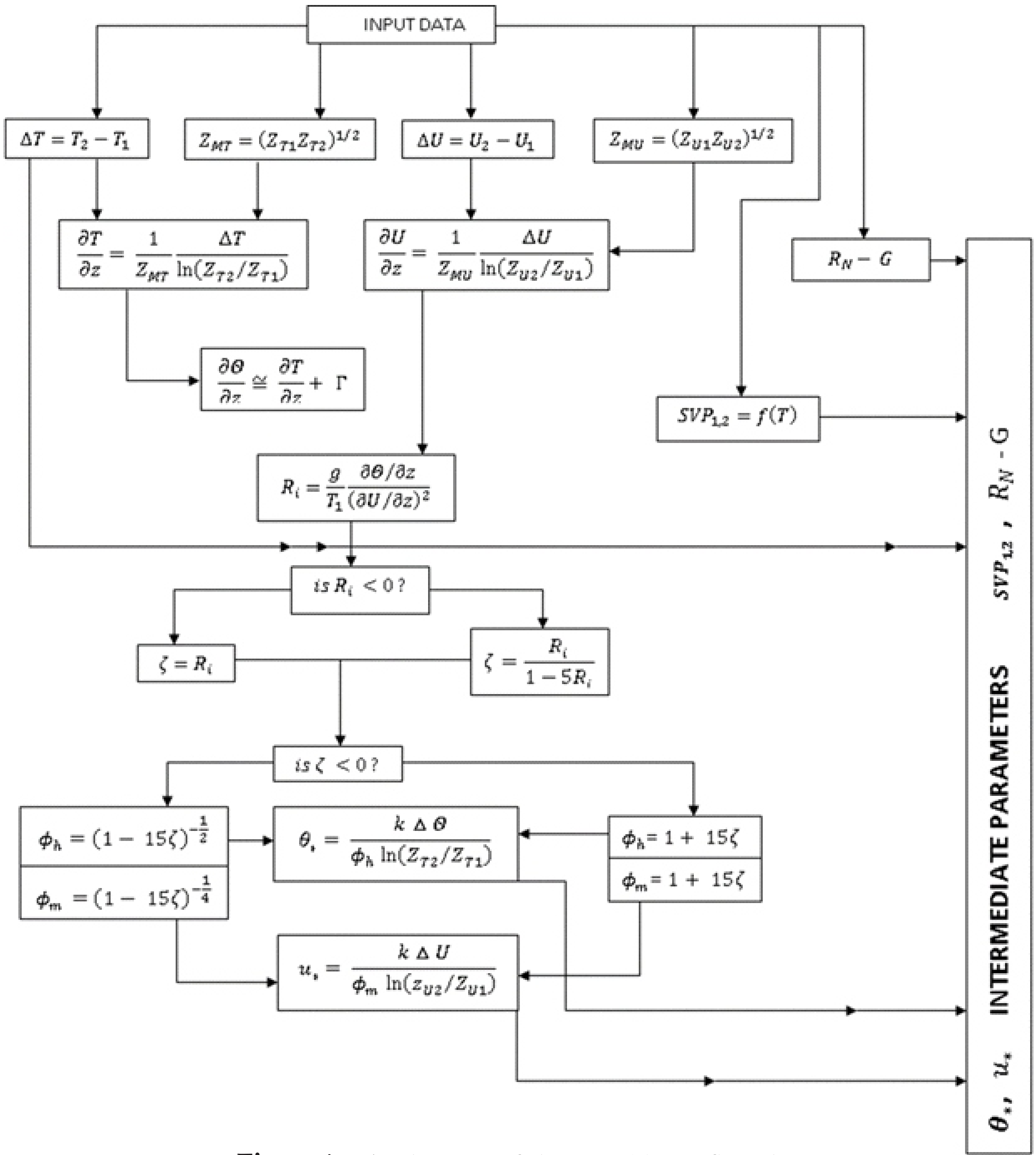

Figure 1: A schematic of the SIMETPRO flow chart

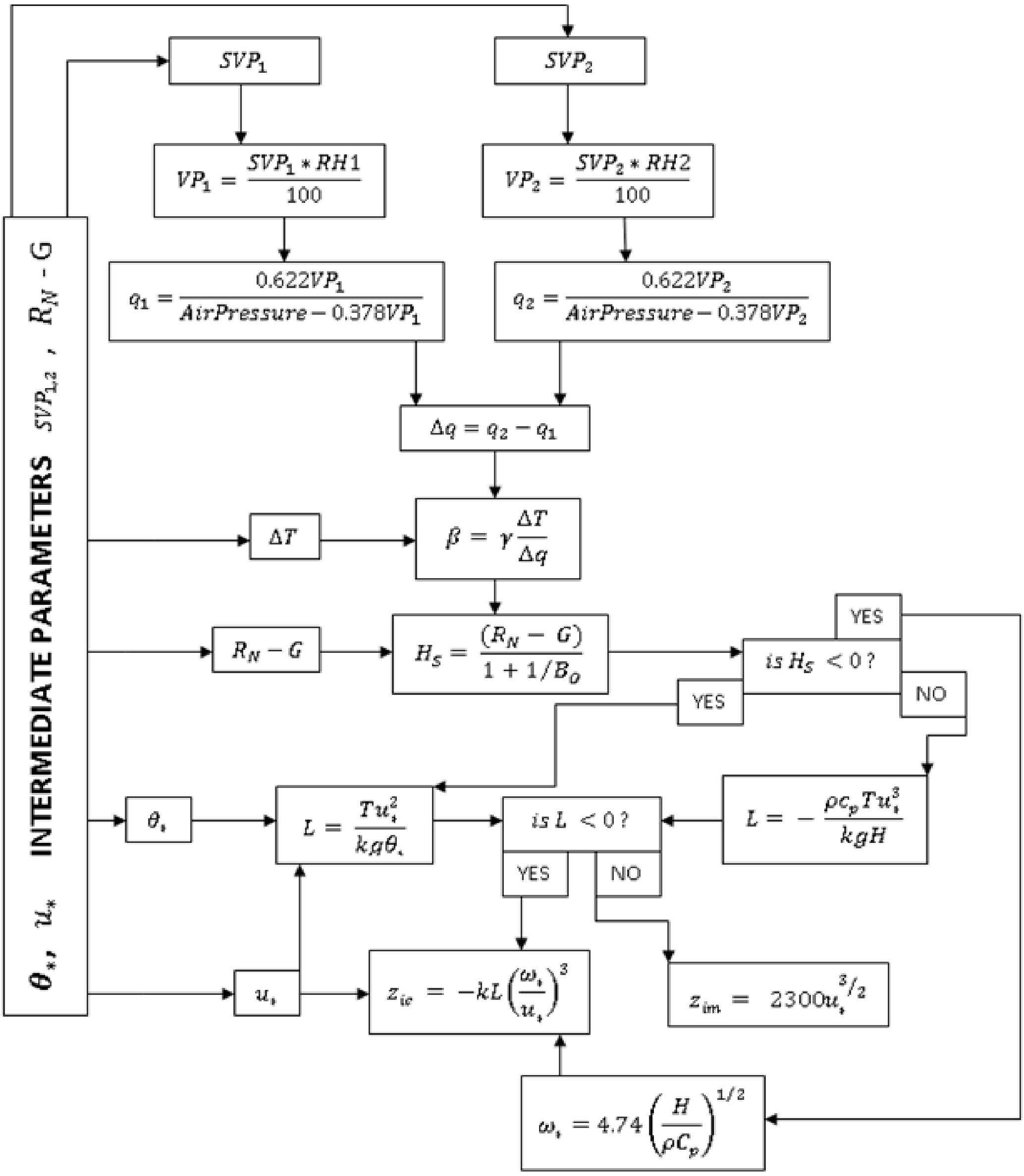

Figure 2: SIMETPRO flow chart (cont'd)

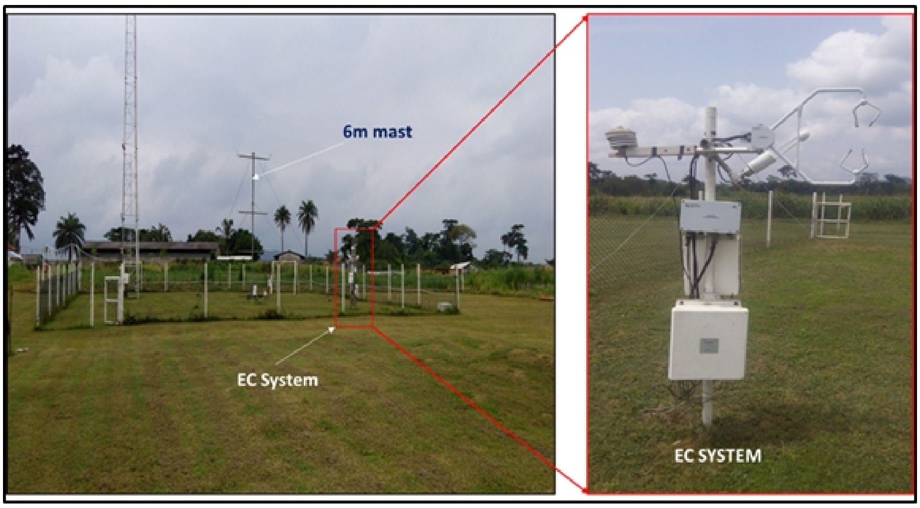

Figure 3: The independent Eddy covariance measurement site at Obafemi Awolowo University Teaching and Research Farm. (station is maintained by the Atmospheric Physics Research Group)

measuring energy fluxes at the surface (Jegede, 2001). The meteorological mast was designed purposely for profile measurements of wind speed, air temperature and relative humidity at three heights (0.5m, 2.0m, 5m) each, net radiaton flux (1.5m) and ground heat flux (5cm below surface). The height configurations were so chosen in such a way that the Bowen ratio energy balance (BREB) method adopted in the SIMETPRO can be tested. Thirty minutes averages of measured meteorological variables at the experimental site were used to compute the sensible heat flux from the preprocessor and its values were compared with those measured by the EC system. It was observed that the BREB method mostly breaks down during the early morning period, this is particularly so when the β is in the range $-1.25 < \beta < -0.75$ and thus the sensible heatflux estimate becomes unrealistic. The criterion to discard all values of β in the range $-1.25 < \beta < -0.2$ (Ohmura, 1982) were jettisoned in this study. Instead of rejecting data points in this range, a boundary condition was imposed on the BREB method in the interval of the breakdown. The boundary condition employs an empirical constant (an average value of 0.23) obtained from probing the ratio of sensible heat flux to the net radiation flux as a rough estimate for H_s to minimise the number of data gap in the final analysis. The estimated H_s was capped at a maximum value of 250 Wm^{-2} which is typical for a tropical location such as Nigeria, following the results of Jegede (2001).

SIMETPRO Outputs

Diurnal trend of the test validation for H_s and u_* are presented in Figure 4. Although the temporal changes in the fluxes were well reproduced by the SIMETPRO, it tends to overestimate the values in both cases. H_s was overestimated by a factor of 0.8 – 1.6 and 1.2 – 4.5 for u_* during the more convective period of 20 July. The day was characterized by intense solar with the net all-wave radiation reaching up to 900 Wm^{-2}. Ground heat flux for the same period reached 250 Wm^{-2}. With less intense heating of the surface i.e. less convective period, the estimates were much improved. Clearly, this indicates that the stability characterization scheme of the preporocessor needed to be reviewed. Figure 5 presents the diurnal trend (at mean, 25/75 and 5/95th quantiles) for some parameters processed from the SIMETPRO which are required in dispersion models. Mean friction velocity drops below 0.2 ms^{-1} with instantaneous value up to 0.6 ms^{-1}. 95^{th} quantile of boundary layer mixing height was 2000 meters driven by an equivalent sensible heat flux of 180 Wm^{-2}. Generated potential temperature gradient fully represents the physical dynamics of day-night transition with extreme stability conditions at morning hours, 95^{th} quantile between 0.3 and 0.6. Inter-year comparion of the output is presented in Figure 6. The fluctuations in the estimates could be linked to changes in the underlying atmospheric variables within seasons and also the influence of the pollution plume in the measurement environment.

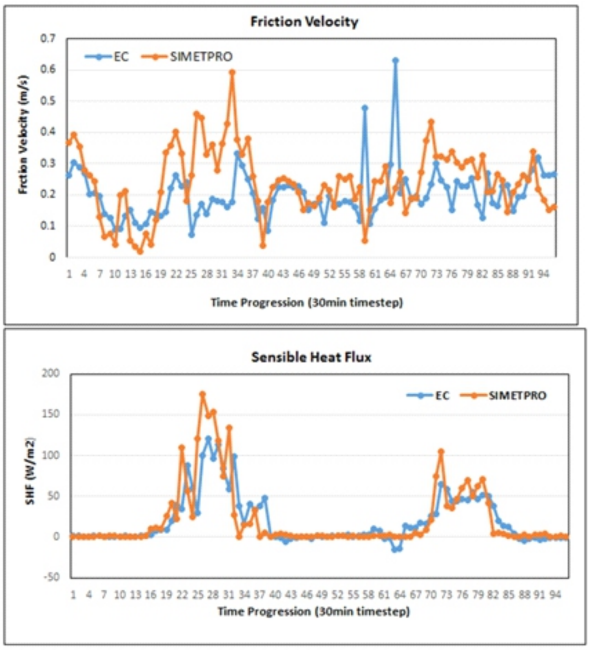

Figure 4: Test validation for H_s and u_* from EC and SIMETPRO.

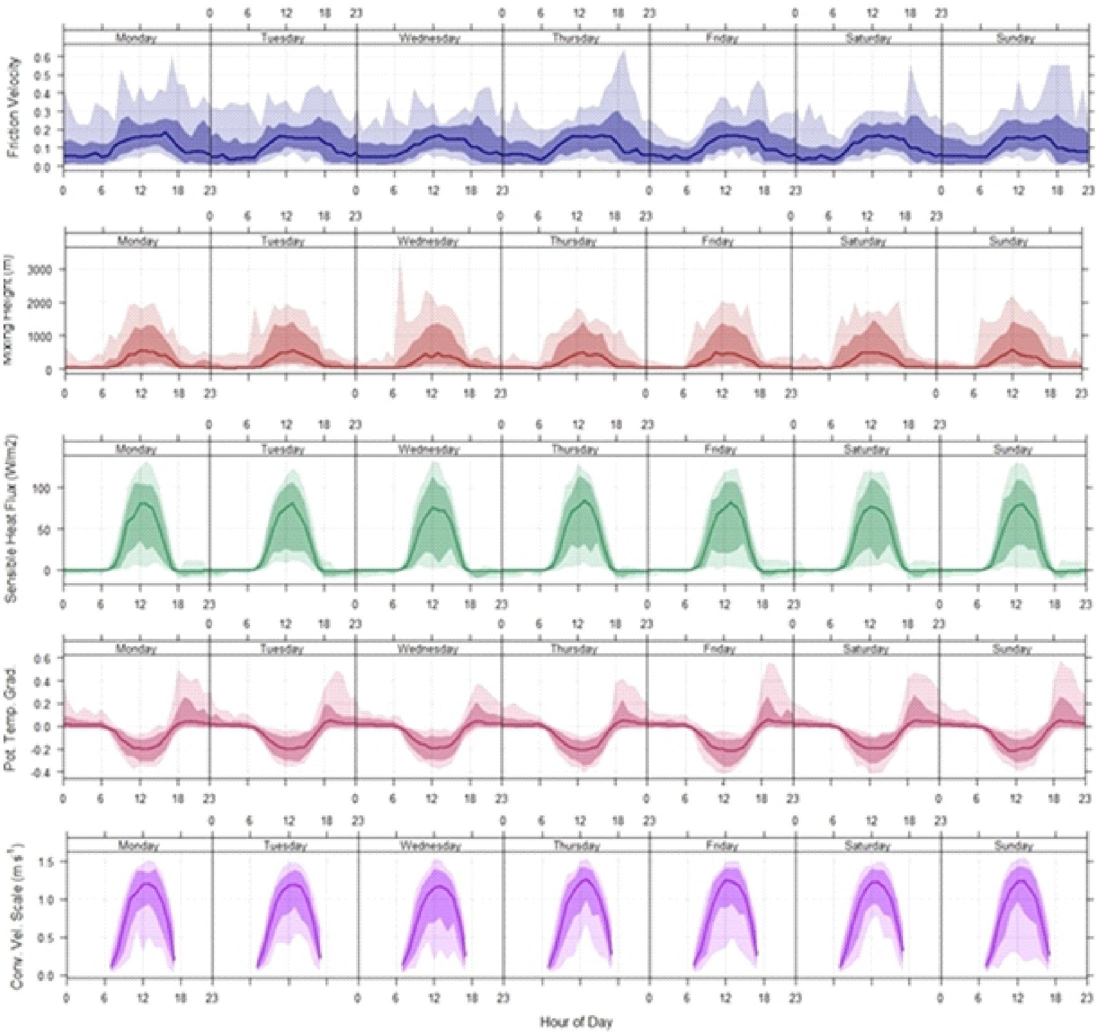

Figure 5: Diurnal trends of SIMETPRO outputs

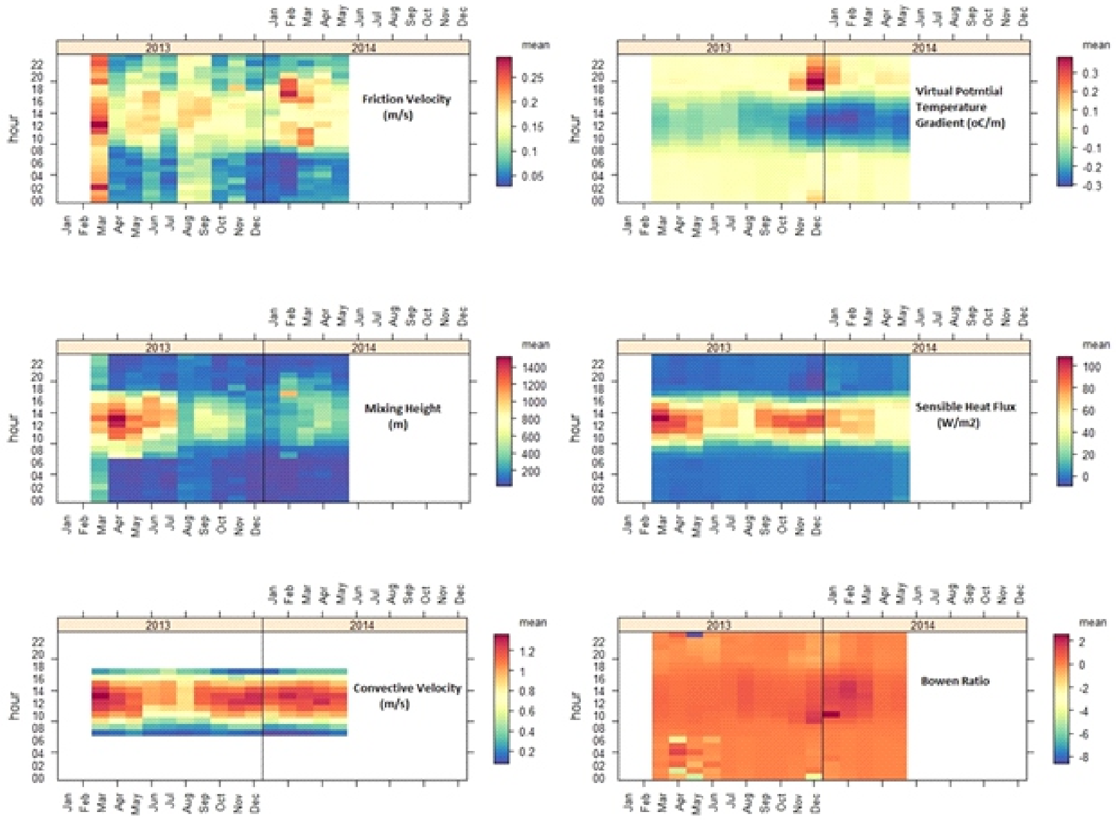

Figure 6: Inter-year comparison of SIMETPRO outputs.

Limitations and Future Improvement

Of all the deterministic parameters generated from SIMETPRO, this study was only able to validate the estimates of sensible heat flux and friction velocity with direct measurement from Eddy covariance (EC) system. It is important to note that the EC system was setup independently at a location different from the primary study site. Given this condition, certain limitations are obvious and herein enumerated; (1) the difference in terrain and fetch requirement/availability between the location of the EC system and the study site constitute a source of error which may arise due to inhomogeneity in the measured surface parameters used in running the preprocessor (2) albeit the substantial effort, validating only two parameters (sensible heat flux and friction velocity) among many others is rather insufficient and considering also that a scanty two-day dataset was used. Regardless of the fact that procuring, setting-up and maintaining an EC system together with an operational meteorological station is capital and human resource intensive, longer measurement period would be more appropriate (3) the gradients of air temperature and wind speed measurement were taken from a meteorological mast that is less than 10 m (a minimum requirement stipulated by World Meteorological Organization). As such, the surface wind shear may not have been adequately represented.

In the future when funding and research equipment are available, the SIMETPRO needs to be refined and well-tested. This would require an intensive observation period at an integrated experimental site comprising a tetheredsonde/radiosonde for mixing height profiling, setup of an EC system for measuring surface energy fluxes, radiation sensors, and profile measurement of air temperature, relative humidity and wind speed up to 10 m and above. While the SIMETPRO is not intended as a replacement for standard preprocessors such as AERMET, it is however important to compare its performance for assessment of uncertainties when used to run dispersion simulation; a core goal for future study.

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