Accepted Manuscript

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PII: S0169-8095(14)00147-1
DOI: doi: 10.1016/j.atmosres.2014.03.023
Reference: ATMOS 3128

To appear in: Atmospheric Research

Received date: 11 October 2013
Revised date: 24 March 2014
Accepted date: 28 March 2014

Please cite this article as: Hariprasad, K.B.R.R., Srinivas, C.V., Singh, A. Bagavath, Vijaya Bhaskara Rao, S., Baskaran, R., Venkatraman, B., Numerical Simulation and Intercomparison of Boundary Layer Structure with different PBL schemes in WRF using experimental observations at a Tropical site, Atmospheric Research (2014), doi: 10.1016/j.atmosres.2014.03.023

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Numerical Simulation and Intercomparison of Boundary Layer Structure with different PBL schemes in WRF using experimental observations at a Tropical site

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Abstract

In this study the performance of seven PBL parameterizations in the Weather Research and Forecast (WRF-ARW) mesoscale model was tested at the tropical site Kalpakkam. Meteorological observations collected during an intense observation campaign for wind field modelling called Round Robin Exercise (RRE) were used for comparison. High resolution simulations were conducted for a warm summer condition in 22-24 September 2010. The observations included GPS Sonde vertical profiles, surface level data from meteorological towers and turbulent fluxes from sonic anemometers. Sensitivity experiments with seven PBL schemes [Mellor-Yamada-Janjic (MYJ), Mellor-Yamada-Nakanishi-Niino (MYNN), Quasi Normal Scale Elimination (QNSE), Yonsei University (YSU), Asymmetric Convective Model (ACM2), Bougeault- Lacarrére (BL), Bretherton-Park (UW)] indicated that while all the schemes similarly produced the stable boundary layer characteristics there were large differences in the convective daytime PBL. It has been found that while ACM2, QNSE produced highly unstable and deep convective layers, the UW produced relatively shallow mixed layer and all other schemes (YSU, MYNN, MYJ, BL) produced intermediately deep convective layers. All the schemes well produced the vertical wind directional shear within the PBL. A wide variation in the eddy diffusivities were simulated by different PBL schemes in convective daytime condition. ACM2, UW produced excessive diffusivities which led to relatively weaker winds, warmer and dryer mixed layers with these schemes. Overall the schemes MYNN, YSU simulated the various PBL quantities in better agreement with observations. The differences in the simulated PBL structures could be partly due to various surface layer formulations that produced variation in friction velocity and heat fluxes in each case.

[Keywords: Mesoscale, WRF, Boundary Layer, PBL parameterization, RRE experiment]
1. Introduction

Mesoscale atmospheric models have been widely used in short-range weather prediction, atmospheric dispersion and air quality assessment (e.g., Hu et al., 2010; Jimenez et al. 2006; Zhang et al. 2006). Among a number of factors physics parameterizations in numerical models are very important to simulate the atmosphere realistically. The Planetary Boundary Layer (PBL) turbulence is especially influential in the simulation of low level atmospheric winds and clouds and diffusion of dynamical and thermodynamical quantities. The turbulent mixing in PBL determines the vertical transport of heat, moisture, momentum and other physical properties (Garrat, 1994; Stull, 1988). Excessive turbulent mixing leads to too warm, dry and thick PBLs, which influences the simulation of important meteorological systems such as convective storms through alteration of convective available energy and hurricanes by influencing the friction and winds (Braun and Tao, 2000). The vertical mixing due to turbulent motions in the PBL is not explicitly resolved in atmospheric models even at the highest possible resolution. The net effect of all the scales of eddies is parameterized using closure techniques based on gradients of resolved quantities. The key parameters that determine the to-and-fro transfer and diffusion of fluxes between the surface and atmosphere are surface drag coefficients for momentum ($C_d$), moisture and heat ($C_k$), eddy diffusivity for momentum ($K_m$), and moisture and heat ($K_h$).

The PBL schemes influence the simulation of various atmospheric phenomena by producing substantial differences in the simulated temperature and moisture profiles and subsequent interaction with other model physics (Fast et al., 1995; Bright and Mullen 2002; Fast et al. 1995; Misenis and Zhang 2010). The uncertainty in the estimates of the PBL parameters with various PBL schemes is due to different assumptions regarding the transport of mass, moisture, and energy leading to variation in the structure of simulated atmospheric phenomena.
Hong and Pan (1996) showed precipitation simulations given by numerical weather forecast models were sensitive to the vertical mixing formulation. In the case of Hurricanes a number of studies (Bhaskar Rao et al. 2006; Braun and Tao 2000; Gopalakrishnan et al. 2013; Montgomery et al. 2010; Nolan et al. 2009 a, b; Smith and Thomsen 2010; Srinivas et al. 2007a; Srinivas et al. 2012) have shown that the structure, intensity, track and precipitation simulations were influenced by the PBL physics through alteration of primary and secondary circulation. With the continuous developments in models and improvements in PBL physics several intercomparison studies have been made to study the suitability and application of specific schemes over various regions. Berg et al. (2005) have shown that the MM5 simulated PBL characteristics at an extra-tropical observation station were sensitive to the turbulence closure schemes and that simple first order schemes like Blackadar (1979) well represented the observed convective boundary layer structure. Steeneveld et al. (2008) compared simulations of PBL diurnal patterns from three regional models with observations from Cooperative Atmosphere-Surface Exchange Study (CASES-99: Poulos et al. 2002) experimental campaign. Their study reported that the simulated diurnal structures in both daytime and night time were sensitive to the selected PBL parameterization schemes. In the case of air quality studies Yerramilli et al. (2010; 2012) showed that the surface ozone simulations produced by WRF/Chem model were influenced by the PBL parameterization schemes and that the k-theory based first-order YSU scheme produced better results than the ACM2, MYJ schemes for simulating the diurnal cycle and Ozone mixing ratios in the Mississippi Gulf coastal region. Hu et al. (2010) studied three PBL parameterizations within WRF-ARW model for air quality application in Texas, and it was shown that the YSU, ACM2 produced better simulations for both stable and unstable conditions and that the MYJ produces coldest and moistest biases in the PBL. Madala et al (2013) have shown that the
thunderstorm simulations at a tropical station Gadanki were influenced by the PBL parameterization and cores of strong convective updrafts were obtained with Mellor-Yamada-Janjic scheme. The PBL parameterizations in numerical models have been mostly tested in subtropical and higher latitudes and very few studies (Srinivas et al. 2007b; Sanjay et al 2008) exist over tropical regions. Recently Shin and Hong (2011) compared five PBL schemes within WRF model using CASES-99 field data. Interestingly their study revealed that the PBL structure was better represented by non-local schemes under unstable / convective conditions and TKE closure local schemes in stable conditions. Such studies are generally rare in the tropical regions mainly due to lack of experimental observations. However, the tropical regions are interesting cases where convection is a dominant turbulent process and assessing the PBL parameterizations becomes important under convective conditions. The objective of the present work is to study the performance of the turbulence parameterization schemes in the WRF mesoscale model for the simulation of boundary layer flow structure at a tropical site. Towards this objective the observations collected at the Kalpakkam station, India during the Round Robin Exercise (RRE) field meteorological experiment (Srinivas et al. 2011) were used for validation of the simulated PBL structure. The paper is organized as follows: In section 2 model and design of numerical simulations are described. In section 3, the conceptual differences in PBL physics are presented. Section 4 provides the details of observations used for model comparison. Results of the simulations for winds, surface level variables, PBL height are presented in section 5. In section 6 conclusions and summary of main findings along with a discussion for future research are given.

### 2. Numerical model and simulations

The Advanced Research WRF (WRF-ARW v3.2) mesoscale model developed by National Center for Atmospheric Research (NCAR), USA was used for the simulations in this study. It is
a mass conservative finite difference model and uses non-hydrostatic compressible Euler equations, terrain-following hydrostatic pressure vertical coordinate and Arakawa-C type horizontal grid (Skamarock et al., 2008). The prognostic variables include the three-dimensional wind, perturbation quantities of potential temperature, geopotential, surface pressure, turbulent kinetic energy and moisture. The model is flexible with a number of options for spatial discretization, diffusion, nesting, lateral boundary conditions and physics parameterizations as well as the terrain & topographic datasets compatible to different regions.

In this study the WRF model was configured with 4-domains of horizontal resolutions 27 km, 9 km, 3 km, 1 km (Figure. 1a). The inner fine nest covers the experimental site Kalpakkam and adjoining areas. The model physics included Kain-Fritsch scheme (Kain and Fritsch, 1993) for convection, WRF single moment (WSM3) scheme for cloud microphysics, NOAH scheme (Chen et al. 2001) for land surface processes, RRTM scheme (Mlawer et al. 1997) for longwave radiation and Dudhia scheme for shortwave radiation. No convection scheme was employed for the fine domains 3 and 4. The domain and physics are given in Table 1. Simulations were conducted for 22-24 September 2010 in a summer warm period characterized with southwesterly synoptic flow condition. The model was initialized at 00 UTC on 22 September 2010 and integrated for 48 hours. The 3-dimensional National Centers for Environmental Prediction (NCEP) Global Forecasting System (GFS) meteorological analysis data available at 0.5 degree resolution (~50 km) was used for the initial conditions. The boundary conditions to the outer domain were updated from 3 hourly GFS forecasts. The USGS elevation data, FAO soil data and MODIS land use data available at 10 min, 5 min, 30 sec resolution were used to define the surface fields in the model.
As mentioned earlier, the PBL physics influences the simulation of winds, mixed layer height and other state variables in the lower atmosphere. To study the above features seven different PBL schemes were used. The selected PBL schemes were Yonsei University (YSU) non-local diffusion (Hong et al. 2006), Mellor-Yamada-Janjic (MYJ) TKE closure (Janjic, 1994), Mellor-Yamada-Nakanishi-Niino level 2.5 (MYNN) local closure (Nakanishi and Niino 2004), Asymmetric Convective Model (ACM2) (Pleim, 2007), Bougeault and Lacarrère (1989) (BL), Quasi Normal Scale Elimination (QNSE) (Sukoriansky et al. 2005), University of Washington Moist Turbulence scheme (UW) (Bretherton and Park, 2009) respectively. Surface layer schemes compute friction velocities and surface exchange coefficients that facilitate the estimation of surface heat, moisture fluxes by the land-surface models and momentum fluxes consistent with the flux-profile relationships. The surface fluxes provide the lower boundary condition for the computation of vertical transport in the PBL. The surface layer schemes used in experiments were: Eta similarity theory (Janjic, 1990) with MYJ, Pleim-Xue (PX) similarity (Pleim 2006) with ACM2, QNSE similarity (Galperin and Sukoriansky 2010) with QNSE, UW similarity scheme with UW, and MM5 similarity (Zhang and Anthes 1982) with YSU, MYNN, BL as per their compatibility. The YSU, ACM are first-order and the rest are one-and-half order closures. The conceptual differences in different PBL schemes are discussed below.

3. Description of PBL closures

Two approaches of PBL turbulence closure called ‘local’ or ‘non-local’ are generally followed in numerical models to obtain closed solution for the turbulence terms (Stensrud, 2007). In local closure the turbulent fluxes are derived from known quantities or their vertical derivatives at the same grid point. In non-local closure the turbulence fluxes are related to known quantities at any number of grid points elsewhere in the vertical (Stull, 1988; Shin et al 2011). The first order
closure is formulated following the gradient transport or K-theory where the second moments are parameterized. Here, any variable \( c(u,v,ө,q) \) is written as

\[
\frac{\partial c}{\partial t} = ... - \frac{\partial}{\partial x_j} \left( \overline{c'u'_j} \right)
\]  

(1)

where the turbulent flux of \( \overline{c'u'_j} \) is given by

\[
\overline{c'u'_j} = -K \frac{\partial}{\partial x_j} (\overline{c})
\]

(2)

where ‘K’ is the eddy diffusivity coefficient. To overcome the deficiencies of unrealistic near surface adiabatic layers under strong heating condition and to obtain flux transports under strongly unstable environments higher order closures are proposed. They solve additional prognostic equation for turbulent kinetic energy (TKE) for the higher moments (Mellor and Yamada, 1982; Janjic, 994). Here, the eddy diffusivity coefficients for momentum and heat are parameterized through the use of TKE following the mixing length theory as

\[
K = Sl e^{1/2}
\]

(3)

where ‘S’ is the dimensionless stability function \( (S_m \text{ for momentum, } S_h \text{ for heat or moisture}) \), ‘l’ is the turbulent macroscale or master length scale and ‘e’ is the TKE. \( S_m \) and \( S_h \) are coefficients modifying ‘l’ as a function of Richardson number (Ri) quantifying wind shear and buoyancy. The diagnostic equations used to obtain parameters ‘S’ and ‘l’ differ in different TKE closures MYJ, MYNN, QNSE, BouLac and UW. The TKE is predicted using the relation

\[
\frac{\partial \overline{e}}{\partial t} = -\overline{u'w'} \frac{\partial u}{\partial z} - \overline{v'w'} \frac{\partial v}{\partial z} + \frac{g}{\rho} \overline{w' \theta'} - \frac{\partial}{\partial z} \left( \frac{\overline{w' p'}}{\rho} + \overline{e w'} \right) - \varepsilon
\]

(4)
The first and second terms on the right hand side of equation (4) represent production due to shear, the third term represents the buoyancy, the fourth term represents the vertical TKE flux and pressure fluctuation, and the last term \( 'c' \) represents dissipation of TKE by molecular processes. The PBL height is diagnosed using a TKE threshold. The equations for heat and moisture include a term that allows mixing against local-gradient to represent large-eddy effects.

In the YSU ‘non-local’ scheme (Hong et al 2006) the diffusion equations for prognostic variables \((u,v,o,q)\) are expressed as

\[
\frac{\partial c}{\partial t} = \frac{\partial}{\partial z} \left[ K_c \left( \frac{\partial c}{\partial z} - \gamma_c \right) - \overline{(w'c')} h \left( \frac{z}{h} \right)^3 \right] \tag{5}
\]

where \( \gamma_c \) is a correction to the local gradient to represent effects of large-scale eddies under \.

Here, the eddy diffusivity for momentum is defined as

\[
K_m = kzw_s \left( 1 - \frac{z}{h} \right)^p \tag{6}
\]

where ‘\( k \)’ is the von Karman constant (=0.4), ‘\( z \)’ is the height above the ground, ‘\( h \)’ is the height of the boundary layer, ‘\( w_s \)’ is the mixed layer velocity scale defined form surface friction velocity and wind profile function at the surface layer top and the exponent ‘\( p \)’ (\( p \sim 2 \)) is the profile shape constant (Holtslag and Boville, 1993; Troen and Mahrt, 1986). The counter gradient flux is expressed as

\[
\gamma_c = b \overline{(w'c')} \tag{7}
\]

where \( \overline{(w'c')} \) is the surface flux for \( u,v,q \) and \( \theta \) and \( b \) is a constant of proportionality. The term on the right side in Eq.(5) is the entrainment flux which is taken proportional to the surface buoyancy flux. The eddy diffusivity for temperature and moisture \((K_h)\) is computed from \( K_m \) in
Eq. (7) by using the Prandtl number relationship. The stability functions are derived from PBL height and Obukhov length. The boundary layer height is determined by

\[ h = \frac{\beta_{\nu} |U(h)|^2}{g[\theta_v(h)-\theta_s]} \]  

(8)

where \( \beta_{\nu} \) is the critical bulk Richardson number, \( U(h) \) is the horizontal wind speed at \( h \), \( \theta_v \) is the virtual potential temperature at the lowest level (30 to 50 m), \( \theta_v(h) \) is the virtual potential temperature at \( h \), and \( \theta_s \) is the potential temperature near the surface. The Asymmetric Convective Model (ACM2: Pleim, 2007) uses local-closure for stable conditions and non-local closure for unstable conditions.

4. Observational Data

The observations used in the present work were gathered in special field experiments under Round Robin Exercise (RRE) study program to validate the atmospheric flow field models for airborne effluent dispersion at the tropical coastal site Kalpakkam (Srinivas et al. 2011). Under this programme meteorological observations were collected during an Intensive Observation Period (IOP) 14-24 September 2010 in a domain of 100 km range from Kalpakkam (12.565° N and 80.160° E) (Figure.1b) station situated between Chennai and Pondicherry cities on the southeast coast of India. The observations were collected in three spatial domains (meso, local, microscale) around Kalpakkam from August 2010 to February 2011 by deploying multi-level meteorological towers, portable masts, Ultrasonic Anemometers, Automated Weather Stations, UHF Doppler Wind Profiler, GPS Radiosonde, Pyrhelio/Pyrgeometers, soil moisture and temperature probes. Measurements during the IOP included micrometeorological observations, turbulent components (\( u' , v' , w' , \theta' \)) at 5 locations (Kalpakkam, Anupuram, Vittalapuram, Chennai, Kattankulathur, Gadanki), vertical profiles of winds, temperature, humidity at 2
locations (Kalpakkam, Chennai), short-wave/ long-wave, soil temperature, soil moisture at 1 location (Kalpakkam) respectively. The mesoscale domain has plain topography with a few hillocks located at about 45 km on the western and northwestern sides. The land cover primarily comprises agriculture fields, scrubland and wastelands. The soil textural type is red loamy at the site and changes to silt loam at the coast.

5. Results
The synoptic weather condition during the IOP in September 2010 was analysed from NCEP GFS global model meteorological analysis (Figure 2). A south north pressure gradient existed over the Indian Peninsula with high pressure distributed to the south and low pressures along the axis of the monsoon trough extending from northwest India to the head of Bay of Bengal near Calcutta during the observation period. The surface winds in September 2010 were mostly westerly / south-westerly with wind speed of order of 4 to 7 ms$^{-1}$ in the southern Peninsular India. In the upper air at 200hPa (~14km, top of troposphere) the winds were easterly. Results of qualitative and quantitative comparison of simulated PBL variables winds, temperature, humidity, surface fluxes, vertical profiles of the above parameters and their time-height variations from the fine nest domain are presented.

a) Diurnal evolution of Surface variables: The time variation of the surface level meteorological variables simulated by ARW at Anupuram and Kalpakkam stations along with observations are presented in Figures 3-6. The diurnal wavy pattern in surface level temperature, humidity and winds could be simulated as in observations at both the stations. However, the magnitudes of simulated variables differed among various schemes. Most PBL schemes produced a warm bias in the daytime air temperature and a slight cold bias in the night time air temperature. Among the
non-local schemes the ACM2 scheme simulated considerable overestimation of daytime temperature and a small underestimation in the night time temperature. The YSU produced a slight warm bias in both day and night temperatures. Among the higher order schemes MYNN produced a slight warm bias and simulated the night time temperature in better agreement with observations than other TKE schemes. The local closures MYJ, QNSE, UW, BL produced considerable warm and cold biases in the day and night time temperatures. The MYJ and QNSE simulated the largest cold and warm bias in the air temperatures. At the inland station Anupuram most PBL schemes produced a slight cold bias and the ACM2 scheme produced a warm bias in day temperature. Shin and Hong (2011) also reported warmer bias with ACM2 scheme and a cold bias with QNSE while comparing with observations during the convective time. Surface level relative humidity comparisons (Figure 4) shows that humidity was underestimated with all the PBL schemes at both the stations. Underestimation of humidity by MYJ and YSU schemes was also reported by Misenis and Zhang (2010) in air quality simulations over the coastal Mississippi. YSU, MYNN, MYJ, QNSE and BL schemes exhibited lower dry bias in both day and night time humidity relative to other schemes. The non-local scheme ACM2 produced a large dry bias in both day and night time humidity. Among the TKE schemes MYJ and QNSE simulated humidity in better agreement with the observations followed by BL, MYNN and UW. Overall MYJ and QNSE simulated the surface relative humidity reasonably well. The above results are similar to those found in Hu et al. (2010) in Texas (USA) and in Garcia-Díez et al (2013) over Europe. The above studies also reported significantly less bias with YSU than MYJ, ACM2 for temperature, humidity. The comparisons indicate that the differences among surface thermodynamic variables from different schemes were maximum at daytime and minimum at nighttime as also found in Shin and Hong (2011).
The time variation of winds at 10-m level from different experiments (Figure 5) indicated considerable overestimation of winds with MYJ, QNSE in both day and nighttime. The other schemes YSU, MYNN, BL, UW and ACM2 produced moderately stronger winds in both day and night time relative to observed winds at both stations. Overestimation of winds with WRF was also reported by Steeneveld et al (2008). Overall the ACM2 produced lesser deviations in both day and night time wind speed simulations. Wind speed predictions with YSU, MYNN, BL were better at Kalpakkam than at Anupuram. MYJ and QNSE simulated the highest wind speed errors at both the stations. Unlike in Shin and Hong (2011) where the wind components were more divergent at nighttime, present study shows the winds from different schemes were divergent at the tropical site in both daytime and nighttime with large deviations from observations. There were large directional shears in the simulations MYJ, QNSE in the initial time period (Figure 6). Unlike at Anupuram the directional deviations of about 25-50 deg were found with all the PBL schemes for the coastal site Kalpakkam, which could be due to the abrupt contrast of land-water terrain at the Kalpakkam site. Barring these few deviations all the PBL schemes well simulated the windflow direction.

The differences in the simulated surface level winds and thermodynamical variables can be explained from the differences in the friction velocity (u*) and surface fluxes. Comparison of time variation of u* (Figure 7) indicated that the frictional velocity was generally underestimated indicating underprediction of the shear force in the surface boundary layer in all simulations. The u* values simulated by YSU, MYNN, BL were nearly similar which is due to the use of a common surface layer scheme in the above simulations. The ACM2 and UW schemes that use their respective surface layer schemes (Pleim-Xue, UW M-O theory) produced large underestimation of frictional velocity. The variation in exchange coefficients and friction
velocity can influence simulated sensible heat fluxes. The sensible heat and latent heat flux comparisons show that a large bias is simulated in the daytime flux by various schemes (Figure 8). All the PBL schemes overestimated the sensible heat flux on the first day of simulation and an improvement was noted in the simulated heat flux on the second day. This could be due to certain spinup time taken by the Noah land surface model for adjusting to the soil and vegetation processes to evolve the surface fluxes. While all the schemes similarly simulated the night time fluxes the MYJ, QNSE, ACM2 schemes produced higher daytime fluxes relative to observed fluxes. Further the latent heat flux was almost comparable in magnitude to sensible heat which could be due to high soil moisture and transfer of energy by evaporative process in the coastal environment. Overall, the MYNN and YSU show a better comparison of the surface heat flux simulation. The same time variations were found in the latent heat flux simulation and the schemes MYNN, YSU produced better latent heat flux simulations. The higher/lower sensible heat flux in QNSE/YSU in convective condition may be attributed to the simulated surface exchange coefficients in the respective schemes (Shin and Hong, 2011).

b) Boundary layer flow field: The simulated surface level (10 m) flow field from the fine nest is analysed during the unstable daytime at 12 IST (Figure 9). In the morning conditions calm westerly flow (~1 ms\(^{-1}\)) was simulated over the land in all the experiments and the winds were slightly stronger (1 to 1.5 ms\(^{-1}\)) over the ocean relative to the land (0.5 to 1.5 ms\(^{-1}\)) region. During the daytime large variations were found in the simulated surface temperature and flow field in different simulations. Large air temperature gradients (~5-7°C) across the land and sea interface at the coast were found in the simulations ACM2, MYJ, QNSE. Correspondingly stronger sea breeze with ACM2, MYJ, QNSE (4-5 ms\(^{-1}\)) and weaker winds with YSU, MYNN, BL, UW (2 to 3 ms\(^{-1}\)) were simulated. The relatively higher atmospheric temperatures simulated
with ACM2, MYJ, QNSE indicated relatively higher convective turbulence, higher diffusion and therefore a relatively deep boundary layer formation in these cases. Sea breeze flow was more organized with YSU, ACM2, MYNN, UW and was highly divergent in the cases MYJ, QNSE, and BL. The vertical extent of the sea breeze was found up to 700 m with MYJ, QNSE, and up to 400 m / 500 m in the other cases (not shown). Factors such as PBL height, wind shear, and entrainment of free atmospheric air into the PBL affect the wind distribution and mesoscale circulations (Arya, 2001). These factors are inturn related to the surface fluxes and PBL diffusivities which are analysed further in the following discussions.

c) **Vertical PBL structure:** Vertical profiles of simulated potential temperature, relative humidity, wind speed and wind direction at 06 IST, 12 IST, 16 IST corresponding to morning, daytime and sea breeze time in the afternoon for Anupuram station are shown in Figures 10, 11, 12 and 13 respectively. The potential temperature profiles indicate slight overestimation in the temperature during the morning time. Above 50 m, highly stable conditions were simulated with all the PBL schemes giving similar vertical temperature variation in the morning as in observations. The local-closures QNSE, MYJ, UW, and BL produced highly stable conditions compared to other schemes. During the convective conditions at 12 IST the radiosonde data indicate development of a well mixed layer growing up to 900 m above ground level (AGL). A shallow unstable surface layer (extending to ~100 m AGL) was also found. The profiles with MYJ, BL, UW indicated a shallow 600 m deep mixed layer, YSU, MYNN indicated 800 m deep mixed layers whereas ACM2 and QNSE produced deeper (~1000 m) convective layers. During the sea breeze hours the potential temperature profiles show shallow convective mixed layer with a vertical extent of about 400 m AGL. This shallow mixed layer during sea breeze is well known as the thermal internal boundary layer (TIBL) in coastal regions. The development of sea breeze
in the afternoon at the coastal site can be recognized from a change in the wind direction from
southwesterly (~225) to southeasterly (~120), strengthening of the winds from 3 ms\(^{-1}\) to 5 ms\(^{-1}\)
and increase in the relative humidity from 50% to 80%. While ACM2 produced a deeper (~750
m deep) mixed layer during the sea breeze time, the experiments QNSE, MYJ, UW produced
relatively shallow mixed layers (<400 m deep) than that was found in the actual profile. Of all
the seven experiments YSU, MYNN, BL well simulated the mixed layer (350 m deep)
characteristics during the sea breeze time. Well developed deep convective mixed layers using
YSU, and shallow layers with MYJ were also reported by Misenis and Zhang (2010) in air
quality simulations using WRF-Chem.

With reference to the relative humidity, the profile comparisons show vertically decreasing
humidity in the morning, increasing humidity in the convective daytime up to 1000 m AGL at 12
IST and up to 400 m AGL during the sea breeze hours. The morning humidity profiles ingeneral
show a steep unstable surface layer with humidity drastically falling up to 100- 150 m AGL and
then increasing to a height of 400 m AGL. The MYNN, YSU, UW and to some extent the
ACM2 experiments produced these stable layer humidity characteristics well, while the rest of
the simulations (MYJ, QNSE, BL) produced a continuously falling humidity in the lower
atmosphere. Observations at this time, however, were erroneous which may be due to the failure
of the humidity sensor of the Radiosonde. During the convective daytime conditions the
humidity profiles given by QNSE, ACM2 indicated an increasing moist bias with height as in the
case of temperature. The vertical variations of humidity simulated with MYJ, UW and BL were
indicative of a relatively shallow (~500 m deep at 12 IST; ~250 m deep at 16 IST) mixed layer
development in comparison to the observed layer with radiosonde. The humidity profiles
simulated with MYNN and YSU were more realistic both in convective noon time (12 IST) as
well as during sea breeze time (16 IST). The simulated thermodynamic properties show that QNSE, ACM2, YSU, UW generally produced dry and warm layers which could be due to excessive mixing (by larger eddy exchange coefficient for heat and moisture) computed in these schemes. The other schemes MYJ, MYNN, BL produced relatively cold and humid layers. The above results of YSU simulating slightly more warm and dry layers than MYJ are consistent with those obtained by Hu et al (2010) using WRF over Texas and Kim et al (2006) using WRF-Chem in airquality study. The deficiencies in reproducing the temperature and humidity by various schemes at the coastal site in the present study could be attributed to the deficiencies in capturing small-scale meteorological phenomena under complex weather patterns involving land/sea interactions as was also reported by Misneis and Zhang (2010).

Comparison of wind speed profiles (Figure 12) shows that during the stable morning conditions all the simulations overestimated wind speed in the first 600 m AGL. Here, the ACM2, MYNN and YSU indicate better comparisons than the other experiments. Above 600 m most of the simulations produced lower wind speeds than the observations except ACM2 and UW. Similarly, during the convective daytime conditions except ACM2 all the experiments especially QNSE and MYJ produced higher wind speed in the lower 400 m region of the atmosphere. In the layer above 400 m AGL the QNSE shows a better comparison than the other schemes. During the sea breeze (16 IST) the same pattern of vertical variation of wind speeds as at noon time were found in the simulations. Overall, the YSU, MYNN, BL, ACM2 schemes produced better wind speed comparisons than the rest. The large differences between simulated and observed wind profiles in the layer above 600 m could be due to the horizontal drift of the radiosonde from its release location.
Comparison of the vertical variation of wind direction (Figure 13) indicated that all the simulations well produced the vertical wind directional shear in the boundary layer. All the schemes indicate westerly / southwesterly boundary layer flow in the late night/ morning time and the occurrence of sea breeze in the 0-500 m layer in the daytime. The simulated direction profiles with YSU, QNSE, BL and MYNN were in better agreement with observations than the others in both stable and unstable conditions. The direction comparisons clearly show southeasterly sea breeze flow simulation in the lower levels up to 500 m AGL in agreement with observations. ACM2 produced slightly higher shear than other schemes at about 1 km region. Santos-Alamillos et al (2013) in a study of wind flow with WRF over southern Spain showed the wind direction estimates were more sensitive to the terrain characteristics rather than the model physics. Our present results also show less direction deviations with different PBL physics for the coastal site.

c) Time Evolution of PBL: Intercomparison of the time-height variations from 00 UTC 22 to 00 UTC 24 September 2010 in potential temperature (θ) (Figure. 14) and specific humidity (q) (Figure 15) for the model grid at Kalpakkam indicates the model simulated the evolution of the boundary layer generally well in all the PBL schemes, but with some differences. During the period from local night (00 IST / 18 UTC) to local morning (08 IST/ 02 UTC) the simulated mean potential temperature increased with height indicating stable stratification in all the cases. Both the local as well as the non-local diffusion schemes similarly produced the nocturnal boundary characteristics at the observation site. At around 06 IST/ 00 UTC all the simulations showed highly stable temperature stratification and the local closures (MYJ, QNSE, BL, UW) more clearly depicted the stable boundary layer formation in agreement with the corresponding Radiosonde observations (Figure 10a). In the daytime from 09 IST/03 UTC onwards the
potential temperature remained uniform up to a certain height and then increased from 0.6 km upwards indicating development of well mixed conditions from 09 IST onwards. The layer within which the temperature remained uniform had reduced from 0.6 km to 0.4 km at 12 IST/06 UTC and further to 0.2 km at 15 IST/09 UTC. This alteration in the mixed layer depth to a minimum value in the afternoon is a unique feature of coastal locations and is due to the well known phenomena of TIBL formation at the coast. The vertical extent of the daytime convective (or unstable) boundary layer was variously simulated in different experiments. The well mixed layer height was simulated as 0.6 km with YSU, MYJ, MYNN; 0.7 km with ACM2, 0.9 km with QNSE, 0.55 with UW, BL schemes. The QNSE, produced the deepest boundary layer followed by ACM2, YSU, MYNN, MYJ, BL, UW schemes. The PBL schemes QNSE, ACM2 and UW produced extremities (deep/shallow) in mixed layer simulations. The above results of formation of deeper convective boundary layers with QNSE, ACM2; shallow layers with UW and moderately deep convective layers with YSU, MYNN, BL, MYJ schemes were supported by Radiosonde observations in the earlier discussion. Simulation of deep boundary layers with ACM2 and moderately deep layers with YSU and MYJ were also reported by García-Díez et al (2013) over Europe.

The diurnal evolution of the PBL could also be analysed from the time-height variations in specific humidity (Figure 15). The stable boundary layers during the night and morning were marked with decreasing specific humidity whereas the unstable layers in the daytime were marked with near uniform vertical humidity distribution. The deepest boundary layers during the daytime were found with QNSE followed by ACM2, MYJ, YSU, MYNN, BL and UW. The local closure TKE schemes (MYJ, MYNN, QNSE, BL and UW) produced steep vertical gradients in the humidity distribution during the night stable atmospheric conditions (at 03 IST/
21 UTC) as compared to the non-local schemes. However, the non-local schemes produced distinctly uniform humidity distributions during the convective day time conditions (12 IST/06 UTC) as compared to the local-closure schemes thus showing the expected well mixed conditions. The local schemes produced relatively higher humidity (0.019 kg/kg) in the lower layers as compared to the non-local schemes (~0.017 kg/kg) under convective conditions indicating lesser mixing as compared to the non-local schemes.

d) PBL Height: Various methods are used in model PBL formulations for the estimation of boundary layer height involving thermodynamics, dynamics, using parameters like the critical Richardson number, threshold TKE, potential temperature etc (e.g., Noh et al. 2003; Troen and Mahrt, 1986; Vogezezang and Holtslag, 1996; Shin and Hong, 2011). The PBL height is diagnosed from bulk Richardson number by comparing with critical Richardson number in YSU and ACM2 schemes. In YSU scheme bulk Richardson number is calculated from the surface. For convective conditions its value is set to zero, whereas in stable conditions \( R_i \) is taken > 0 (0 to 0.25). In the case of ACM2, PBL is considered to comprise a free convective layer and an entrainment layer. The height of free convective layer is diagnosed from the temperature of the rising plume. The height at which the temperature of the rising plume is equal to the temperature of the surrounding environment is considered as the top of the free convective layer. The depth of the entrainment layer estimated from the critical Richardson number is added to the height of the free convection layer to obtain the height of the PBL. In the case of local PBL schemes (i.e., MYJ, QNSE, MYNN, BL, UW), PBL height is diagnosed as the height where prognostic TKE reaches a sufficiently small value (of the order of 0.005 m\(^2\)/s\(^2\)) (Shin and Hong, 2011). In the present study the PBL height was analysed from daytime Radiosonde observations using potential temperature profile specifically for the morning (06 IST) and noon (12 IST) conditions.
The comparison shows that during daytime the QNSE, ACM2 simulated very deep boundary layers, UW simulated shallow PBL while MYJ, MYNN, YSU, BL simulated intermediately deep layers (Figure. 16). During the night time while ACM2, BL, YSU, UW produced very shallow layers MYNN, QNSE, MYJ simulated unrealistic deep layers. The time variations show that while ACM2, QNSE, MYJ, UW produced a sudden decay of PBL around the day/night transition (15IST), the MYNN, YSU, BL schemes simulated extended mixed layers through night indicating a gradual decay of PBL and higher nocturnal PBL height (439 m to 575 m) (Table 2). During the stable morning conditions the local closures (QNSE,MYJ, MYNN, BL) except UW produced deeper layers in contrast to the non-local schemes YSU and ACM2 (Table 2). However, during the daytime, except QNSE and MYJ, the local closures produced relatively shallow convective layers in comparison to the non-local closures. Among nonlocal PBL schemes ACM2 produced deeper boundary layers (PBL height: 1262.8m/59m) relative to the YSU (PBL height: 871.9m/29.97m) during both convective and stable conditions. Among the local PBL schemes QNSE produced very deep boundary layers (PBL height: 1308m/259m) and UW produced shallow (PBL height: 402m/29m) boundary layers during the convective and stable conditions respectively indicating extremities. From the diurnal cycle the YSU, MYNN, BL schemes produced more realistic time variation in the PBL heights in better agreement with profile observations. Shin and Hong (2011) while evaluating WRF PBL formulations with CASES observations also reported simulation of deep mixed layers with QNSE, ACM2, MYJ; moderate layers with YSU and shallow layers with BL. Our present results from the tropical site corroborate findings of the above study.

e) Eddy diffusivities: The differences in the simulation of dynamic and thermodynamic variables in the lower atmosphere could be related to the variation in the simulation of the eddy exchange
coefficients for momentum ($K_m$) and heat / moisture ($K_h$) by various schemes. We analysed the $K_h$, $K_m$ parameters from various schemes and presented in Figure 17 and Table 3. Among the seven PBL schemes used ACM2 and BL assume the eddy diffusivity for momentum as identical to that for enthalpy (Prandtl number $K_m/K_h \sim 1$) whereas in MYJ, MYNN, QNSE, YSU and UW schemes $K_h$ is larger than $K_m$. Under unstable conditions or strong shear the assumption of $K_m=K_h$ may not be valid. The time averaged $K_m$, $K_h$ for the period (01 UTC-19 UTC) representing unstable conditions and for the period (19 UTC 22 September 2010 - 01UTC 23 September 2010) representing stable conditions are presented in the above figure. Each TKE scheme used a different approach to calculate $S$ and $I$ parameters used in the expression for $K$. As expected though all the schemes indicated higher eddy diffusivities during unstable regime relative to the stable regime the ACM2, MYNN and UW produced higher $K_m$ and $K_h$ values relative to other PBL schemes. While the ACM2, UW produced the largest diffusivities, the BL and QNSE simulated least diffusivities indicating extremities in turbulent mixing in the above schemes. The $K_m$ values with ACM2, UW were about 5 times higher relative to most PBL schemes. This had lead to stronger simulated winds with QNSE, MYJ schemes relative to the ACM2, UW as discussed earlier. Similarly the $K_h$ was comparatively higher in ACM2, UW which tend to produce higher mixing of heat or moisture and hence warmer and dry boundary layer. During the stable atmospheric conditions the simulated $K_m$, $K_h$ were nearly of the same order of magnitude and ACM2, UW produced slight higher values of $K_m$, $K_h$. Hence in stable atmospheric conditions the simulated quantities from all the schemes nearly converged. Thus in general ACM2, UW simulated higher diffusivities for momentum and heat/ moisture in comparison to MYJ, YSU, MYNN, QNSE, BL which resulted in variations in the simulated PBL parameters. Overall the $K_m$, $K_h$ values simulated with YSU, MYNN schemes are in the
intermediate range of the seven PBL schemes in both stable and convective conditions and hence produced lesser errors in the simulated mean variables.

The mean model error statistics from various PBL simulations for different variables are presented in Table 4. As discussed earlier YSU/MYNN has shown better results in 2m-temperature prediction (RMSE=1.03/1.123, Bias=-0.004/-0.28) and MYJ/QNSE has shown largest cold bias (-0.68/-0.84; RMSE =1.33/1.43) relative to other schemes. For humidity, MYJ/QNSE showed less dry bias (-9.59/-9.76) and less RMSE (11.88/12.08) relative to other schemes. In the case of 10m-wind speed, ACM2 produced least bias 0.35 and RMSE (1.19) and MYJ/QNSE generated largest biases (1.44/1.37) and RMSE (1.87/1.79) of various PBL schemes.

6. Conclusions

In this study numerical simulations were conducted with WRF-ARW mesoscale model to study the Planetary Boundary Layer characteristics at the tropical site Kalpakkam on the southeast coast of India. The ability of the model to reproduce the observed features was studied by conducting simulations with seven PBL schemes and by intercomparison. The observations collected during an intensive field measurement campaign RRE were used to verify the results from different numerical experiments. Diagnosis of the surface level meteorological variables (winds, temperature, humidity, surface fluxes) and their vertical variation indicated that for temperature the non-local PBL scheme YSU and the higher order local-closure TKE scheme MYNN produced better results. For humidity MYJ, MYNN, QNSE simulated reasonably well while ACM2, YSU produced large dry bias in the night time. For wind speed the combined local/ non-local scheme ACM2 produced better simulations, and local closures MYJ, QNSE considerably overestimated the winds while the other schemes (YSU, MYNN, BL, UW)
simulated moderately stronger winds relative to observations. However, all the PBL schemes reproduced the wind direction reasonably well. Though large underestimation of friction velocity was found in the case of ACM2, the higher eddy diffusivities found with ACM2 seem to provide better wind simulations than the other cases.

While all the PBL schemes well simulated the stable morning profiles, there were large differences in the convective daytime profiles. The vertical extents of unstable surface layer, well mixed layer and inversion layer were differently simulated by different PBL parameterizations. A wide variation was found in the simulated PBL heights by different schemes. Relatively shallow convective boundary layers with UW (402 m), very deep mixed layers with ACM2, QNSE (1200m to 1308m) and moderately deep layers with YSU, BL, MYJ, MYNN (800m to 1070m) were simulated. This variation in mixing height simulation could be due to the use of different formulations for PBL height in different schemes. Considering the diurnal cycle the YSU, BL, MYNN schemes produced more realistic time variation in the PBL heights in better agreement with radiosonde profile data. Of all the seven experiments YSU and MYNN well simulated the mixed layer characteristics (lesser temperature, higher humidity, moderate winds) during the sea breeze time. A wide variation of diffusivities ($K_h, K_m$) was produced by different PBL schemes which had led to variations in the vertical extent of mixed layer, magnitudes of thermodynamic variables and momentum. The ACM2, UW, MYNN simulated higher diffusivities than MYJ, YSU, QNSE, BL for momentum and heat/ moisture in both stable and unstable atmospheric conditions. The higher exchange coefficients in the case of ACM2, UW, MYNN produced relatively lesser winds, warm and dry mixed layers in these cases in comparison to the other PBL schemes. The $K_m, K_h$ values from YSU, MYJ and BL were in the intermediate range of the seven PBL schemes and they
produced lesser errors in the simulated mean variables. The variations in the simulated quantities could be partly also due to the variation in the use of different surface layer formulations with different PBLs as evident from the variation in the simulated friction velocity and surface fluxes.

A comprehensive examination of all the schemes in the present study indicated that no scheme perfectly works for all the variables and for all the stability conditions. In general the observational comparison indicated the non-local scheme YSU produced more realistic atmospheric structures during the convective conditions and the TKE closures MYNN produced more realistic vertical structures during the stable conditions. These results corroborate the findings from earlier intercomparison studies by Hu et al. (2010), Shin et al. 2011 and Steeneveld, (2008) with WRF model. The simulations in the present study were focused on a warm convective period at the tropical coastal site. The boundary layer structure simulated by WRF needs to be assessed for a stable cold season as well as an inland station to further study the performance of the PBL schemes in tropical conditions. It is also required to use continuous observations like Wind profiler to assess the temporal evolution of the PBL simulated by the model.

**Acknowledgements:**

Authors thank S.A.V. Satya Murty, Director, EIRSG, for the encouragement in carrying out the study. The observations used in the study were obtained from the Round Robin Exercise project coordinated by IGCAR and funded by Board of Research in Nuclear Sciences, DAE, Mumbai. Authors acknowledge NCEP/NOAA for the public access of GFS analysis/forecasts used in the study. ARW model was obtained from NCAR, USA. Thanks are due to anonymous reviewers for their technical comments which helped to improve the manuscript.

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<td>Time-height section of specific humidity (kg/kg) in 22-24 September 2010 at Kalpakkam from different numerical experiments a)YSU, b)ACM2, c)MYJ, d)MYNN, e)QNSE, f)BL, g)UW. Times indicated on the x-axis are in UTC.</td>
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<th>WRF V3.4</th>
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<td>Dynamics</td>
<td>Primitive equation, non-hydrostatic, fully compressible, terrain following</td>
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<td>Vertical resolution</td>
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<td>Horizontal resolution</td>
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<td>Dudhia scheme for short wave radiation</td>
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<td>Surface-layer</td>
<td>Monin-Obukhov similarity scheme (MM5 scheme, Eta scheme, Pleim-Xue MO similarity)</td>
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<td>Land Surface scheme</td>
<td>NOAA Land Surface scheme</td>
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<td>PBL turbulence</td>
<td>YonSei University(YSU),Mellor-Yamada-Janjic(MYJ),Mellor-Yamada Nakanishi-Niino(MYNN2.5), BouLac, UW (Bretherton and Park), ACM2(Pleim),and Quasi-Normal Scale Elimination</td>
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<td>Cloud microphysics</td>
<td>WRF single moment 6-class scheme (WSM6)</td>
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Table 2. Comparison of simulated PBL height from different experiments

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<th>Expt No.</th>
<th>PBL Height (m)</th>
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<td>UW</td>
<td>29.94</td>
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<table>
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<th>Expt No.</th>
<th>Stable Condition</th>
<th>Unstable Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$K_m$(m$^2$s$^{-1}$)</td>
<td>$K_h$(m$^2$s$^{-1}$)</td>
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Table 4. Model Error Statistics

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<th>MAE (°C)</th>
<th>RMSE (°C)</th>
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Highlights

- The performance of PBL parameterizations in WRF model to simulate lower atmospheric fields was examined.
- The simulation of vertical profiles, surface fluxes, winds, temperature, humidity and mixed layer evolution were assessed.
- Wide differences in variables, fluxes, diffusivity and PBL height were found among the schemes.
- The non-local closure YSU and local closure MYNN produced better PBL structure in stable and unstable conditions.