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An Updated Parameterization of the Unstable Atmospheric Surface Layer in WRF Modeling System

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Abstract. Accurate parameterization of atmospheric surface layer processes is crucial for weather forecasts using numerical weather prediction models. Here, an attempt has been made to improve the surface layer parameterization in the Weather Research and Forecasting Model (WRFv4.2.2) by implementing similarity functions proposed by Kader and Yaglom (1990) to make it consistent in producing the transfer coefficient for momentum observed over tropical region (Srivastava and Sharan 2015). The surface layer module in WRFv4.2.2 is modified in such a way that it contains all commonly used φ_m and φ_h under convective conditions instead of the existing single functional form. The updated module has various alternatives of φ_m and φ_h, which can be controlled by a flag introduced in the input file. The impacts of utilizing different functional forms have been evaluated using the bulk flux algorithm as well as real-case simulations with the WRFv4.2.2 model. The model-simulated variables have been evaluated with observational data from a flux tower at Ranchi (23.412N, 85.440E; India) and the ERA5-Land reanalysis dataset. The transfer coefficient for momentum simulated using the implemented scheme is found to agree well with its observed non-monotonic behaviour in convective conditions (Srivastava and Sharan 2022). The study suggests that the updated surface layer scheme performs well in simulating the surface transfer coefficients and could be potentially utilized for parameterization of surface fluxes in the numerical weather prediction model.

1 Introduction

Inadequate representation of near-surface turbulent processes adds significant uncertainty in both climate projections and seasonal weather forecasts obtained from atmospheric models (Bourassa et al., 2013). Most of the numerical weather prediction and general circulation models utilize Monin-Obukhov similarity theory (MOST; Monin and Obukhov 1954) to parameterize surface turbulent fluxes. To estimate these fluxes and near-surface atmospheric variables, the theory utilizes similarity functions of momentum (φ_m) and heat (φ_h) often prescribed as functions of ζ (stability parameter). However, the exact functional forms for these functions have not been provided by MOST, rather it suggests some asymptotic predictions under near neutral to very stable and unstable conditions which are tuned with field data. Over the years, researchers have developed many functional forms for these functions based on the different experiments, conducted over different locations and have separate expressions for stable and unstable stratifications (Webb, 1970; Businger, 1971; Carl et al., 1973; Dyer, 1974; Hicks,

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1976; Holtslag and De Bruin, 1988; Brutsaert, 1992; Bruin, 1999; Wilson, 2001; Cheng & Brutsaert, 2005; Grachev et al., 2007; Gryanik et al. 2020; Srivastava et al. 2020).

In most of the atmospheric models, the commonly used similarity functions under convective conditions are those proposed by Businger (1966) and A. J. Dyer [1965, unpublished work; see Businger (1988)] and referred to as Businger-Dyer (BD) functions. However, these functional forms are unable to follow the classical free convection limit. The study by Rao et al. (1996) suggests that the MOST using Businger relations is unable to define transfer coefficient for momentum (C_D) consistent with its observed behaviour, specifically at low wind convective conditions, indicating that MOST needs to be modified in the (nearly) windless free convection limits. As a result, a revised scaling of heat flux for weakly forced convection in the atmosphere has been proposed by Rao et al. (2006). Later, the issues of using BD functions in the surface layer scheme based on the fifth-generation Pennsylvania State University-National Centre for Atmospheric Research Mesoscale Model (MM5) of a regional scale model (Weather Research and Forecasting; WRF) have been reported in a study by Jimenez et al. (2012). They implemented the new scheme (referred to as revised MM5 scheme; Jimenez et al., 2012) in WRF modeling system and replaced the BD functions by those proposed by Fairall et al. (1996) (F96) under convective conditions. F96 functions are the combination of BD functions and the functions suggested by Carl et al. (1973) and are valid for the entire range of atmospheric instability. Note that the most recent version of the WRF model still utilizes F96 functions under convective conditions.

Srivastava and Sharan (2015) analyzed the observed behaviour of C_D over an Indian land surface and suggested that the observed C_D shows non-monotonic behaviour with $-\zeta$, unlike the behaviour of predicted C_D from MOST based parameterization using commonly used φ_m and φ_h (Businger et al., 1971; Carl et al., 1973; Fairall et al., 1996). Later, a theoretical study by Srivastava and Sharan (2021) revealed that the three-sublayer model based on Kader and Yaglom (1990) is able to predict C_D consistent with its observed non-monotonic behaviour. Note that the three-sublayer model has not yet been incorporated and evaluated in WRF modeling framework. However, it is already being operational in the surface layer scheme (Community Land Model; CLM) of National Centre for Atmospheric Research Community Atmosphere Model version 5 (NCAR-CAM5) as well as Regional Climate Model (RegCM).

The study by Srivastava and Sharan (2021) also analyzed the possible uncertainties associated with the use of different functional forms of φ_m and φ_h under convective conditions. To quantify the impacts of different functional forms, they classified available φ_m and φ_h in four classes based on the exponents appearing in the expressions of φ_m and φ_h as (1) functional forms having the exponents of φ_m and φ_h as $-1/4$ and $-1/2$, respectively (Businger et al. 1971; Hogstrom 1996). (2) functional forms having the exponent of φ_m and φ_h as $-1/3$ (Carl et al. 1973). (3) functional forms having the exponent of φ_m and φ_h as $-1/4$ and $-1/2$, respectively in near neutral conditions while $-1/3$ in very unstable conditions (Fairall et al. 1996; Grachev et al. 2000; Fairall et al. 2003). (4) functional forms having the exponent of φ_m and φ_h as $-1/4$ and $-1/2$, respectively in near neutral conditions however, $1/3$ for φ_m and $-1/3$ for φ_h in strong unstable conditions (Kader and Yaglom 1990; Zeng et al. 1998). This study concluded that utilizing different functional forms of similarity functions in the bulk flux algorithm results in a large deviation in the values of estimated fluxes. The detailed description of different functional

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forms for φ_m and φ_h considered in different classes are given in Appendix B. We wish to highlight that the available functional forms for φ_m and φ_h under convective conditions fall in one of the classes stated above.

The revised MM5 surface layer scheme of WRF model version 4.2.2 (WRFv4.2.2) employed φ_m and φ_h based on Fairall et al. (1996), which, belong to class 3. As a result, this scheme is not appropriate in producing C_D consistent with its observed behaviour, specifically over the Indian land as stated above. Recently Namdev et al. (2023) argue that the performance of NWP models varies a lot over different seasons and surface types depending upon the functional behaviour of φ_m and φ_h. Thus, to enhance the potential applicability of WRF modeling framework, this study attempted to incorporate all the commonly used similarity functions under convective conditions along with KY90 as well as existing functional forms in the revised MM5 surface layer scheme of WRFv4.2.2. A namelist flag has been introduced in WRF model to choose between various φ_m and φ_h in the modified scheme. The modified surface layer scheme proposed in this study has been evaluated using offline simulations with bulk flux algorithm as well as the real-case simulations with WRFv4.2.2 during the pre-monsoon season (March-April-May) of 2009 over a domain centered around the location of the flux tower installed at Ranchi (23.412N, 85.440E), India.

2 Methodology and data

2.1 Surface flux computation in the WRF modeling system

The Monin-Obukhov similarity theory serves as the foundation for the surface layer parameterization (revised MM5 scheme) in the WRF model, and the surface turbulent fluxes are calculated based on the bulk approach using bulk transfer coefficients for momentum (C_D) and heat (C_H) (Namdev et al., 2024; Srivastava et al., 2021; Srivastava and Sharan, 2021). A brief description and different numerical expressions used in the computation of surface fluxes in WRF model are provided in Appendix A.

The default version of the revised MM5 scheme in WRF model utilizes similarity functions suggested by Cheng and Brutsaert (2005) under stable atmospheric conditions ($\zeta > 0$), which are developed using CASES-99 dataset. The integrated forms of functions proposed by Cheng and Brutsaert are

$$\psi_m(\zeta) = -a \ln\left(\zeta + \left[1 + \zeta^b\right]^{1/b}\right), \qquad \zeta > 0 \tag{1}$$

$$\psi_h(\zeta) = -c \ln\left(\zeta + \left[1 + \zeta^d\right]^{1/d}\right), \qquad \zeta > 0 \tag{2}$$

where $d = 1.1, c = 5.3, b = 2.5$ and $d = 6.1$.

On the other hand, the similarity functions for unstable atmospheric surface layer ($\zeta < 0$) are those proposed by Fairall et al. (1996). The corresponding integrated functional forms ψ_m and ψ_h are defined as:

$$\psi_\alpha(\zeta) = \frac{\psi_{\alpha_{BD}}(\zeta) + \zeta^2\, \psi_{\alpha_{conv}}(\zeta)}{1 + \zeta^2}, \qquad \alpha = m, h. \tag{3}$$

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where $\psi_{\alpha_{BD}}$ and $\psi_{\alpha_{conv}}$ denote the integrated functional forms based on Businger and Dyer, and Carl et al. (1973), respectively. The expressions for $\psi_{\alpha_{BD}}$ and $\psi_{\alpha_{conv}}$ are

$$\psi_{m_{BD}}(\zeta) = 2\ln\left(\frac{1+x}{2}\right) + \ln\left(\frac{1+x^2}{2}\right) - 2\tan^{-1}x + \frac{\pi}{2}, \tag{4}$$

$$\psi_{h_{BD}}(\zeta) = 2\ln\left(\frac{1+x^2}{2}\right), \tag{5}$$

in which $x = (1-16\zeta)^{1/4}$ and

$$\psi_{\alpha_{conv}} = \frac{3}{2}\ln(y^2 + y + 1/3) - \sqrt{3}\tan^{-1}\left(2y + 1/\sqrt{3}\right) + \frac{\pi}{\sqrt{3}} \tag{6}$$

with $y = \left[1 - \beta_{m,h}\zeta\right]^{1/3}$. The values of the constants β_m and β_h are taken as 10 and 34 based on Grachev et al. (2000).

2.2 Implementation of different similarity functions

In this section, we briefly describe the implementation of different similarity functions under unstable stratification of surface layer parameterization of WRFv4.2.2.

2.2.1 Functions by Businger et al. (1971) (BD71)

Similarity functions suggested by Businger et al. (1971) are based on the KANSAS dataset. These functions do not satisfy the classical free convection limit as predicted by the MOST. These functions are already implemented in the old version of the MM5 surface layer scheme (Grell et al., 1994) in WRF model. The integrated functional forms (ψ_m and ψ_h) for φ_m and φ_h stated in Appendix B (Eqs. B1 and B2) are given in Eqns. (4) and (5). BD71 functions have already been used in the old version of the MM5 scheme.

2.2.2 Functions by Carl et al. (1973) (CL73)

Carl et al. (1973) proposed an expression of similarity functions φ_m and φ_h valid for the stability range $-10 \leq \zeta \leq 0$. The expressions for φ_m and φ_h are given in Eqns. (B3, and B4: Appendix B). The similarity functions proposed by Carl et al.

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(1973) have not been analyzed in the surface layer scheme of WRF model. The integrated forms (ψ_m and ψ_h) of similarity functions φ_m and φ_h are given in Eqn. (6).

2.2.3 Functions by Kader and Yaglom (1990) (KY90)

Kader and Yaglom (1990) introduced a three-sublayer model for convective conditions. The three sublayers are categorized based on ζ values as (1) the dynamic sublayer which corresponds to near neutral conditions, (2) the dynamic convective sublayer which corresponds to moderately unstable conditions and (3) the free convective conditions. The present study utilized φ_m and φ_h expressions (given in Eqns. B9, and B10 in Appendix B) that are being used in the surface layer scheme (CLM4.0; Zeng et al. 1998) of NCAR-CAM5 model. The corresponding integrated forms for φ_m and φ_h are

$$\psi_m(\zeta) = \begin{cases} \psi_{m1}(\zeta_m) + \ln\frac{\zeta}{\zeta_m} - 1.14\left[(-\zeta)^{1/3} - \right], & \zeta \leq -1.574 (= \zeta_m) \\ \psi_{m1}(\zeta) = 2\ln\left(\frac{1+x}{2}\right) + \ln\left(\frac{1+x^2}{2}\right) - 2\tan^{-1}x + \frac{\pi}{2}, & -1.574 < \zeta < 0 \end{cases} \quad (7)$$

$$\psi_h(\zeta) = \begin{cases} \psi_{h1}(\zeta_h) + \ln\frac{\zeta}{\zeta_h} - 0.8\left[(-\zeta)^{-1/3} - (-\zeta_h)^{-}\right], & \zeta \leq -0.465 (= \zeta_h) \\ \psi_{h1}(\zeta) = 2\ln\left(\frac{1+x^2}{2}\right), & -0.465 < \zeta < 0 \end{cases} \quad (8)$$

where $x = (1 - 16\zeta)^{1/4}$.

Note that all the functions stated above have been incorporated in the revised MM5 surface layer scheme of WRFv4.2.2 and can be used in place of F96 functions already employed in the model. Here, we have introduced a new surface layer module where different options for φ_m and φ_h can be controlled using an appropriate value of namelist parameter (psimhu_opt). The parameter psimhu_opt is added under the physics section of the namelist file. The variable psimhu_opt can have values 0, 1, 2, and 3 for different options for functions F96 (default), BD71, CL73, and KY90 respectively. A brief structure and different choices for psimhu_opt based on different incorporated and default functional forms of φ_m and φ_h in the default and modified revised MM5 scheme are shown in Figure 1.

2.3 Characteristics of default and incorporated similarity functions

The expressions of φ_m and φ_h for different functional forms utilized in this study are stated in Appendix B. Figure S1 (supplementary material) shows the variation of different (a) φ_m and (b) φ_h under moderately to strongly unstable conditions. It is evident from Figure S1 that all the different functional forms provide similar values of φ_m and φ_h in near neutral to moderately unstable conditions (up to $\zeta = -0.1$ approximately). However, at higher instabilities one can expect noticeable differences between different functional forms of φ_m and φ_h. Note that the functional forms for φ_m corresponding to BD71 and CL73 decrease continuously on increasing instability; however, φ_m corresponding to KY90 functional forms show decreasing behaviour in near-neutral to moderately unstable conditions and attain a minimum at $\zeta = -1.574$, and, as the instability further increases, it starts increasing with $-\zeta$ (Figure S1a). This implies that φ_m based on class 4 functions shows non-monotonic behaviour which contradicts the classical MOST prediction. On the other hand, in case of φ_h, all the functional forms provide continuously decreasing behaviour of φ_h from near neutral to moderately unstable conditions (Figure S1b).

Figure 2 illustrates the variation of default (F96) and different incorporated integrated similarity functions ψ_m and ψ_h (BD71, CL73, and KY90) with respect to $-\zeta$. It is observed from Figure 2a that ψ_m corresponding to F96, BD71, and CL73 functional forms increases continuously with $-\zeta$ in moderately to strong unstable conditions. However, a non-monotonic behaviour has been observed for ψ_m corresponding to KY90 functions implying it first increases with $-\zeta$ and reaches a maximum at $\zeta = -1.574$ and then starts decreasing as instability further grows. On the other hand, ψ_h corresponding to all the considered functional forms increases continuously in near neutral to strong unstable conditions. However, the rate of increase is slightly higher for F96 in comparison to other three functions while ψ_h is found to be almost comparable obtained from other three functions BD71, CL73, and KY90 (Fig. 2b).

2.4 Observational data for model evaluation

For the evaluation of the real-case simulations, observational data derived from the micrometeorological tower installed at Ranchi (India) has been utilized (Srivastava and Sharan, 2019; Srivastava et al., 2020; 2021). The dataset (Ranchi data) is derived from an instrument mounted on a 32-m tall tower at the Birla Institute of Technology Mesra in Ranchi, India (Dwivedi et al., 2014). A fast response sensor (CSAT3 Sonic Anemometer) at a height of 10 m with an average elevation 609 m above sea level provides the temperature and the three components of wind at a 10 Hz frequency. The eddy covariance technique (Stull 1988) is used to estimate heat and momentum fluxes at one-hour time resolution, however the hourly temperature at 2 m is determined by averaging temperature observations available at a temporal scale of 1 minute from the slow response sensors located at logarithmic heights on the same tower. Sharan and Srivastava (2016); Srivastava and Sharan (2015; 2019) provided comprehensive descriptions of the dataset, quality control process and site. Apart from this we have also utilized the ERA5-Land reanalysis dataset available at $0.10^{o} \times 0.10^{o}$ spatial resolution to evaluate the spatial distribution of the model simulated near surface atmospheric variables. For consistency, we have regridded the model output to the same grid resolution of reanalysis/observed dataset.

3 Numerical simulations

Impacts of incorporated similarity functions together with the existing functional forms in surface layer scheme of WRFv4.2.2. For evaluation purpose, offline experiments as well as real case simulations have been conducted. The offline simulations are conducted using the transcendental relation given in Eqn. (A7 in Appendix A) to test the performance of incorporated functions without feedback to the atmosphere. In offline simulations, the value of ζ is estimated by calculating the root of least magnitude

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of Eqn. (A7 in Appendix A) for a given value of Ri_B. Once ζ is calculated then utilizing it in Eqns. (A8) and (A9), the values of C_D and C_H can be estimated. For the computation, z is taken as 10 m and Ri_B is in the range $-2 \leq Ri_B \leq 0$. The offline simulations are carried out over three different surface types by considering surface roughness (z_0) to be 0.01 m (smooth surface), 0.1 m (transition surface) and 1 m (rough surface) to analyze the impact of roughness of underlying surface on the simulation of ζ, C_D and C_H.

On the other hand, the real-case simulations with incorporated similarity functions have been done using WRFv4.2.2 model over an Indian land site during the pre-monsoon (March-April-May; MAM) season of the year 2009. The simulations have been conducted over a nested domain centred around the location of a micrometeorological tower installed at Ranchi (23.412ºN, 85.44ºE), India (Figure 3). Domain d01 ($\mathbf{6} \times \mathbf{6}$ km) consists of 233 east-west and 210 north-south grid points and domain d02 ($\mathbf{2} \times \mathbf{2}$ km) consists of 223 east-west and 196 north-south grid points which covers $\mathbf{1398} \times \mathbf{1260}$ km^2 and $\mathbf{446} \times \mathbf{392}$ km^2 spatial area around the centre point, respectively. Each domain was configured with 50 vertical eta levels from surface to top of the atmosphere. We kept five vertical levels below 100 m height. Initial and boundary conditions were taken from ERA5 global atmospheric reanalysis dataset at a resolution of $\mathbf{0.25^o} \times \mathbf{0.25^o}$ and boundary conditions were forced every 6 hours. For land use and land cover (LU/LC) information, we have used dataset from MODIS (Moderate Resolution Imaging Spectroradiometer; Friedl et al., 2002). Various physical parameterizations utilized in the simulations are listed in Appendix C. In this study, four sets of simulations were carried out, as given in Table 1.

The whole simulation period is divided into segments of 4 days with 24 h overlapping time between different segments to ensure continuity. The model is initialized at 0000 UTC of 1st day of each simulation and runs for 96 hours. In order to avoid the potential spin-up problems at the beginning of the simulation, we discard the first day of each simulation as spin up time and consider the last three days for the analysis (Jimenez et al., 2010; 2012).

For the evaluation of the real-case simulations, different statistical parameters such as mean absolute error (MAE), root mean square error (RMSE), mean bias (MB), index of agreement (IOA), different measures of correlation coefficient (CC), mean bias (%) (bias), and standard deviation of the model predicted output normalized by that of the observations are used. Brief description of the performance indicators for validation utilized in the present study is stated in Appendix C.

4 Results

4.1 Offline simulations

The offline simulations (Exp1, Exp2, and Exp3) have been conducted utilizing incorporated functions (BD71, CL73, and KY90) together with CTRL simulation using F96 functions for three different roughness lengths for momentum (z_0), which are representative of smooth ($z_0 = 0.01$ m), transition ($z_0 = 0.1$ m), and rough ($z_0 = 1.0$ m) surfaces. The simulated results for ζ (a1, a2, and a3) with Ri_B, C_D (b1, b2, and b3) and C_H (c1, c2, and c3) with ζ across various surface types and sublayers

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have been analyzed (Figure 4). The different sublayers associated with convective stratification include dynamic (DNS), dynamic-dynamic convective transition (DNS-DCS), dynamic convective (DCS), dynamic convective-free convective transition (DCS-FCS), and free convective (FCS) (Srivastava and Sharan, 2021). It is observed that the simulated values of ζ for smaller values of Ri_B (i.e., in DNS to DCS) from different experiments are found to be identical to the CTRL simulation (Figure 4a1-3). However, in FCS, large deviations have been observed in the simulated values of ζ for a given Ri_B from different experiments (Figure 4a1-3). Notably, Exp1, Exp2, and CTRL simulations predict relatively smaller absolute values of ζ for a given value of Ri_B. However, Exp3 is found to produce a relatively larger magnitude of ζ for a given value of Ri_B. This behaviour is observed to be consistent for all the values of ratio z/z_0 (Figures 4a1-3) representative of smooth, transitional, and rough surfaces. The substantially larger magnitude of ζ for a given value of Ri_B and the smaller values of ψ_m and ψ_h (Figure 2) in Exp3 implies that the momentum and heat fluxes predicted in Exp3 will be smaller than those anticipated in Exp1, Exp2, and CTRL simulation.

Figure 4b1-3 shows the variation of C_D with ζ predicted in CTRL simulation and Exp1-3 over different surfaces. Notice that the C_D values predicted in Exp1, Exp2, and CTRL simulations are substantially higher and continue to rise as instability progresses from DCS to FCS. On the other hand, Exp3 simulates significantly smaller values of C_D as compared to the other three experiments. It is important to highlight that C_D from Exp3 (KY90 functions) shows a non-monotonic behaviour, which is consistent with the observed behaviour of C_D over the Indian region reported in the literature (Srivastava and Sharan, 2019; 2021). Note that this non-monotonic behaviour is consistent for all three cases of different roughness lengths (Figure 4b1-3).

On the other hand, across all three surfaces, it is observed that the values of C_H predicted in all four experiments increases with increasing instability (Figure 4c1-3). While the rate of increase of C_H in Exp3 is noticeably slower. Moreover, Exp1, Exp2, and CTRL simulation predict almost similar values over all three types of surfaces. Noticeably, C_H also exhibits non-monotonic behaviour with ζ over rough surfaces, which contradicts the predictions of the other three experiments. In addition, it is important to note that C_D and C_H predicted by Exp3 are found to bound by twice their near-neutral values, while the other experiments predict continuously increasing values of C_D and C_H on increasing instability.

Hence, it is evident from the offline experiments that the functional forms adopted in Exp1 (BD71), Exp2 (CL73), and CTRL (F96) predict values of ζ, C_D, and C_H that are almost same. However, using KY90 functions compared to other commonly used φ_m and φ_h, one can expect a significant reduction in the estimated values of transfer coefficients in moderately to strongly unstable stratification.

4.2 Real-case simulations

In this section, observational and reanalysis datasets have been used to analyze the simulations performed with WRFv4.2.2 utilizing different incorporated and default φ_m and φ_h. The model simulated output has been extracted at the location of flux tower and compared against the observations derived from the flux tower installed at Ranchi (23.412N, 85.440E), India. The mean spatial patterns of certain variables averaged over daytime (04:00-12:00 UTC) have been compared against the ERA5-Land reanalysis dataset. Further, to access the effects of incorporated functions under free convective conditions, the mean spatial patterns of considered variables averaged across strong convective conditions (hours in which $\zeta < -10$ over most of the domain) have been analyzed against respective hours of ERA5-Land reanalysis data. Bilinear interpolation has been used to interpolate the model output to the same grid resolution as the ERA5-Land data in order to allow a consistent comparison.

4.2.1 Evaluation against observations derived from flux tower installed at Ranchi (India)

Figure 5 depicts the variation of (a) ζ with Ri_B, (b) C_D, and (c) C_H with ζ from different experiments (Exp1, Exp2, and Exp3) and CTRL simulation. The variation of simulated ζ with Ri_B, C_D, and C_H with ζ is found to be consistent with offline results. The values of simulated variables are found to be identical in DNS to DCS sublayers for all the experiments; however, in FCS, substantial differences between different experiments (Figures. 5a, b, and c) have been observed. Simulated ζ for a given Ri_B in Exp2 and CTRL simulation are similar and found to be smaller in magnitude than Exp1 and Exp3 in FCS. However, the absolute values of ζ in Exp3 (KY90 functions) are significantly larger in FCS than in all other experiments.

Figure 5b shows the variation of simulated C_D with ζ from different experiments. Yellow crosses denote the variation of observed C_D with ζ at the location of flux tower (Figure 5b). It is observed that the observed C_D increases as the instability increases from DNS to DCS and has the maximum value in the DCS (at $\zeta = -0.1$ approx.) and then starts to decrease as instability grows further from DCS to FCS. It is evident that C_D simulated using φ_m and φ_h based on class 4 functions (Exp3) exhibits non-monotonic behaviour (Figure 5b), which is consistent with the observed behaviour of C_D (Srivastava and Sharan, 2015; 2021). On the other hand, C_D simulated using φ_m and φ_h based on the first three classes (Exp1, Exp2, and CTRL simulation) increases continuously as instability grows from DNS to FCS (Figure 5b). However, it is found that the C_D predicted from the original forms of class 4 functions (EXP3) does not perfectly match with its observed behaviour, as the predicted C_D starts decreasing at ζ lying in FCS, which is different from that observed, i.e., ζ lying in DCS. In view of it, Srivastava and Sharan (2021) tuned the original forms of class 4 functions by enforcing the matching of the point at which both observed and model predicted C_D attain their maximum value. However, more studies in terms of predicting the observed variation of the non-dimensional vertical gradients of mean wind speed and temperature with ζ are essential to further tune the original KY90 functions for the Indian region using observed data from various locations under different seasons.

The magnitude of C_D predicted in Exp3 is significantly smaller than that simulated from other experiments as well as CTRL simulation, specifically in FCS. This may be due to the large differences between the KY90 functional forms of ψ_m and ψ_h and other forms of functions. We wish to highlight that utilizing KY90 (Exp3) functions in the revised MM5 scheme of WRF model makes it consistent in predicting C_D with its observed behaviour over the Indian region. The variation of simulated C_H with ζ from different experiments is shown in Figure 5c. C_H simulated from Exp1-3 as well as CTRL simulation shows continuously increasing behaviour with ζ. The magnitude of simulated C_H from CTRL simulation and Exp1-2 is

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relatively higher than that of Exp3 in FCS beyond $\zeta < -10$ (approximately). It is also evident that at higher instabilities, even C_H shows non-monotonic behaviour with ζ (Figure 5c).

The analysis presented here indicates that the KY90 functions in the revised MM5 surface layer scheme are found to be appropriate in producing non-monotonic behaviour of C_D consistent with its observed nature. However, all other functional forms of φ_m and φ_h produce C_D, which increases continuously with ζ from DNS to FCS.

To quantify the uncertainties involved in the simulated surface fluxes and certain near-surface variables using KY90 (Exp3) as well as other functional forms (Exp1-2 and CTRL simulation), model simulations have been compared against the observations. Figure 6 compares the model-simulated (a) u_*^2 (m^2 s^{-2}) (representative of momentum flux), (b) SHF (W m^{-2}) (sensible heat flux), (c) U_{10} (m s^{-1}) (10-m wind speed), and (d) T_{2m} (K) (2-m temperature) with the observed data obtained from the flux tower at Ranchi (23.412N, 85.440E), India. The model output was extracted at a single grid point closest to the flux tower to allow a consistent comparison. In Figure 7, a Taylor diagram is displayed along with the normalized standard deviations and correlations of considered variables. Figure 8 shows the scatter plot between CC vs. RMSE for considered variables simulated using different experiments. In case of u_*^2, Exp1 and Exp2 are found to be comparable to the CTRL simulation, while Exp3 considerably improved the simulation of u_*^2 (Figures 6a, 7 and 8). Exp3 reduced MAE (RMSE) from 0.088 (0.156) m^2 s^{-2} to 0.082 (0.144) m^2 s^{-2} (Table 2; Figures 7 and 8) and improved the CC (0.742) and IOA (0.843) for u_*^2 (Table 2). A Q-Q plot is shown in Figure S2a (supplementary material) suggesting that Exp3 (KY90 functions) is found to be slightly better than all other experiments and CTRL simulation for u_*^2. For SHF, all the experiments are comparable to the CTRL simulation; however, Exp3 shows less scatter than other experiments (Figure 6a).

In case of U_{10}, Exp3 shows less scatter and appears to be closer to the observations than other experiments (Figure 6c). Exp3 noticeably improved the simulation of U_{10} by reducing MAE (RMSE) from 1.198 (1.543) m s^{-2} to 1.164 (1.466) m s^{-2} and MB up to 5 % (Figures 6c, and 7; Table 2). It considerably improved the CC (IOA) for U_{10} from 0.659 (0.729) to 0.681 (0.751) (Figure 7 and Table 2). A Q-Q plot (Figure S2b: supplementary material) reveals that Exp3 is observed to be better than all other experiments and CTRL simulation for U_{10}. Thus, the KY90 functions in the surface layer scheme of the WRF model considerably improve the model in simulating U_{10} (Figures. 6c, 7, 8, and S2b) at the location of the flux tower. Further, in case of T_{2m}, Figures 7 and 8 exhibit that all the experiments are found to be comparable with the CTRL simulation.

4.2.2 Evaluation of mean spatial distribution of simulated variables against ERA5-Land reanalysis data during daytime

In this section, mean spatial distribution of simulated variables from different experiments as well as CTRL simulation averaged during daytime (04:00-12:00 UTC) for entire simulation period, is compared with the ERA5-Land reanalysis data. Figure 9 depicts the mean spatial patterns of simulated $\zeta \left(=\frac{z}{L}\right)$ (a1 − 4), C_D (c1-c4), and C_H (e1-4) from CTRL simulation and other experiments, as well as their differences with respect to CTRL simulation. It is observed that the absolute value of ζ simulated in Exp3 (KY90 functions) is much lower than CTRL simulation (Figure 9b3) across the whole domain, which is consistent with Figure 5a and offline simulations presented in Figure 4(a1-3). This could be because the magnitude of KY90 functions (φ_m and φ_h) are smaller than the functions employed in default scheme (CTRL simulation).

On the other hand, Exp1 also provides slightly smaller absolute values of ζ (Figure 9b1), while Exp2 is almost comparable to the CTRL simulation (Figure 9b2). Model simulated C_D is found to be smaller in Exp3 than CTRL simulation (Figure 9d3), while Exp1 and Exp2 provide comparable values of C_D to CTRL simulation (Figure 9d1-2). In the case of C_H, the simulated values from different experiments are observed to be comparable to the CTRL simulation over whole study domain (Figure 9f1-3). These large differences between C_D simulated from different experiments may be related to the fact that only φ_m functions are involved in the computation of C_D (Eqn. A8 in Appendix A), and the differences between φ_m are comparatively more than φ_h, so are the differences in C_D. The hatched regions in Figure 9 shows the differences between simulated variables from different experiments with respect to CTRL simulation are statistically significant at 95% confidence level.

The differences in C_D reflected further in the simulated u_*^2 m^2 s^{-2} (a measure of momentum flux) in Exp3 (Figure 10b3). Exp3 significantly reduced the simulated values compared to the CTRL simulation over some parts of the domain (Figure 10b3), while in Exp1 and Exp2 values are comparable with the CTRL simulation (Figure 10b1-2). In case of SHF and LHF, the mean spatial distribution from all the experiments is found to be consistent with the ERA5-Land reanalysis data, and the magnitude of differences between model simulation and ERA5-Land data is comparable for all the experiments (Table S1; supplementary material).

For T_{2m} (upper panel of Figure 11), T_S (middle panel of Figure 11), and U_{10} (lower panel of Figure 11), mean spatial distribution from different experiments and CTRL simulation agreed well with slightly varying magnitude to the ERA5-Land reanalysis data. A warm bias up to 2 K (3 K) was observed for T_{2m} (T_S) simulated from different experiments and CTRL simulation over most of the domain. For T_{2m}, bias, RMSE, and PCC between different experiments together with CTRL simulation and ERA5-Land reanalysis data are found to be comparable (Table S1; supplementary material). However, Exp3 slightly improved the PCC from 0.503 to 0.512 for T_S (Table S1; supplementary material). Further, in the case of U_{10}, all the simulations exhibit overprediction over the whole domain (lower panel of Figure 11: b1-4) and Exp3 is observed to be slightly better than all other experiments as well as CTRL simulation as it reduced bias% (RMSE) from 32.283 (0.544) m s^{-2} to 32.057 (0.539) m s^{-2} and improved the PCC from 0.899 to 0.911 (Table S1: supplementary material).

4.2.3 Evaluation of incorporated functions during strong unstable conditions with respect to ERA5-Land reanalysis data

This section describes the impacts of utilizing different similarity functions (φ_m and φ_h) on simulated variables during highly convective regime (i.e., $\zeta < -10$) with respect to the ERA5-Land reanalysis dataset. Since the functional forms of ψ_m and ψ_h are identical in near neutral to moderately unstable conditions, however, in strong unstable conditions, the differences between different functional forms are more pronounced. Thus, the corresponding differences in the simulated values of considered variables are expected to be more pronounced during highly convective regimes. For this purpose, the model output has been extracted for those hours in daytime which show ζ smaller than -10 over most of the domain and compared with the respective hours of ERA5-Land reanalysis data.

Figure S3 (Supplementary material) depicts the mean spatial distribution of ζ (a1-4), C_D (c1-4), and C_H (e1-4) as well as their deviations from CTRL simulation. Notice that the magnitude of differences for all variables (ζ, C_D, and C_H) in this case are found to be larger than the case of mean spatial patterns averaged during the whole daytime (section 6.2.2). It is evident from Figure S3b3 (supplementary material) that Exp3 produce large absolute values of ζ and smaller values of C_D and C_H (Figures S3b3, d3 and f3: supplementary material) than all other experiments and the CTRL simulation. While Exp1 and Exp2 are found to be comparable to the CTRL simulation for both C_D and C_H (Figures S3d1-2 and f1-2).

The model simulations for T_{2m} and T_S do not capture the spatial patterns well in comparison to ERA5-Land data (Figures S4a1-5 and S5a1-5: supplementary material). All experiments, as well as the CTRL simulation, exhibit overprediction across the whole domain (Figures S4b1-4 and S5b1-4). We wish to highlight that the differences between various experiments and CTRL simulation are seen up to 0.5 K for T_{2m} (Figure S4c1-3) as well as T_S (Figure S5c1-3) which is slightly higher than the case of mean spatial patterns averaged over whole daytime (upper and middle panels of Figure 11). For T_{2m}, it is evident from Figure S4 (supplementary material) and Table 3 that Exp3 noticeably reduced the bias% (RMSE) from 0.635 (2.133) K to 0.623 (2.102) K and improved the PCC from 0.435 to 0.461 (approximately 6%). In case of T_S as well, Exp3 slightly improved the PCC and reduced the bias% (RMSE) from 1.259 (4.013) K to 1.243 (3.972) K (Table 3 and Figure 12).

For U_{10}, the mean spatial patterns simulated using different experiments agreed well with the ERA5-Land reanalysis data (Figure S6a1-5: supplementary material) and the magnitude of biases is found to be up to 1 m s^{-1}. Exp3 outperformed all other experiments and the CTRL simulation by lowering the bias% from -4.962 to -0.284 m s^{-1} and improved the PCC from 0.343 to 0.364 with comparable RMSE values (Figures S6 and 12; Table 3).

5 Summary and concluding remarks

In the present study, the revised MM5 surface layer scheme of the WRFv4.2.2 model has been modified to incorporate φ_m and φ_h suggested by Kader and Yaglom (1990) to make it consistent in producing the transfer coefficient for moemntum (C_D) in line with its observed behaviour. The revised MM5 scheme is modified in such a way that it contains all commonly used φ_m and φ_h under convective conditions instead of a single functional form. Various alternatives of φ_m and φ_h in the modified scheme can be controlled by a flag (psimhu_opt) that has been introduced in the physics section of the namelist file. The impacts of utilizing different functional forms of φ_m and φ_h in the proposed scheme have been evaluated using offline simulations (with bulk flux algorithm) as well as real-case simulations with WRFv4.2.2 model. The model-simulated surface turbulent fluxes and certain near-surface variables have been compared with observational data from a flux tower at Ranchi (23.412N, 85.440E; India), and the spatial patterns have been evaluated with the ERA5-Land reanalysis dataset.

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Offline simulations indicate that at nearly neutral to moderately unstable conditions, ζ simulated using various functional forms of φ_m and φ_h is comparable, and as the instability grows (free convective conditions), the differences between different experiments become more pronounced. This might be connected to the corresponding variations between different functional forms of similarity functions in the respective regimes. Similarly, for simulated C_D, Exp3 (KY90 functions) demonstrates nonmonotonic behaviour with $-\zeta$ across all three surface types (representing smooth, transition, and rough surfaces), which is consistent with its observed behaviour. However, all other experiments and CTRL simulation indicate continuously increasing C_D with $-\zeta$ from near neutral to free convective conditions over all three surface types, which is inconsistent with its observed behaviour over the study domain. The non-monotonic behaviour of C_D in Exp3 (KY90 functions) may be associated to the analogous non-monotonic behaviour of the corresponding ψ_m in the respective regime.

In real-case simulations, the model simulated ζ, C_D and C_H are found to be consistent with the offline simulations. The variation of C_D in Exp3 (KY90 functions) with $-\zeta$ is observed to be nonmonotonic, as reported in offline simulations and found to be consistent with its observed behaviour. This indicates that the KY90 functions in the surface layer scheme of the WRF model make it compatible in producing C_D consistent with its observed behaviour over Indian land. As compared with the observations over Ranchi (India), the simulations using KY90 (Exp3) functions are found to perform better for most of the considered variables compared to all other experiments. Further, in the mean spatial distribution averaged during daytime (04:00–12:00 UTC) over the entire simulation period, the significant increase in absolute value of ζ from Exp3 resulted in a noticeable reduction in the values of C_D and C_H, which further impacted the simulated values of T_S, T_{2m}, and U_{10}. When compared with the ERA5-Land reanalysis data, the spatial patterns for T_{2m}, T_S, and U_{10} from Exp3 (KY90 functions) provided more consistent results. A reduction has been observed in bias (%) and RMSE values for T_S, and U_{10}. Moreover, in case of highly convective regime ($\zeta < -10$), Exp3 (KY90 functions) slightly improved the performance of the model by reducing the bias (%) and RMSE for T_{2m}, T_S, and U_{10} and increasing the correlation to some extent.

Thus, it is concluded that the similarity functions proposed by Kader and Yaglom (1990) (KY90 functions; Exp3) are found to be more appropriate for use in the WRF model as they can simulate C_D consistent with its observed behaviour and improve the simulation for most of the considered variables over the study domain. However, due to the limited spatial coverage of the domain considered in this study and the limited availability of observational data, KY90 functional forms need to be further evaluated in the WRF modeling framework utilizing observations from other sites. The modified surface layer scheme proposed in this study could enhance the potential applicability of the WRF modeling framework for the community in investigating the role of different functional forms of similarity functions under convective conditions for selected events/case studies such as extreme weather events, heat waves during summer, cyclonic storms, and fog predictions using the WRF model.

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Appendix A

This section consists of a brief description of the computation of surface turbulent fluxes in the revised MM5 surface layer scheme. In a homogeneous surface layer, the dimensionless wind and temperature gradients are defined as

$$\frac{kz}{u_*}\frac{\partial U}{\partial z} = \varphi_m(\zeta), \tag{A1}$$

$$\frac{kz}{\theta_*}\frac{\partial \theta}{\partial z} = \varphi_h(\zeta). \tag{A2}$$

where L denotes the Obukhov length scale and U is the wind speed at height z; k represents the von Karman constant and its value is taken as 0.4. Integrating Eqns. (A1) and (A2) with respect to z leads to

$$U=\frac{u_*}{k}\left[\ln\left(\frac{z}{z_0}\right)-\left\{\psi_m(\zeta)-\psi_m\left(\frac{z_0}{L}\right)\right\}\right], \tag{A3}$$

$$(\theta_a-\theta_g)=\frac{\theta_*}{k}\left[\ln\left(\frac{z}{z_h}\right)-\left\{\psi_h(\zeta)-\psi_h\left(\frac{z_h}{L}\right)\right\}\right] \tag{A4}$$

in which ψ_m and ψ_h denote the integrated form of similarity functions φ_m and φ_h. The roughness lengths for momentum and heat are denoted by z_0 and z_h, respectively. ψ_m and ψ_h can be calculated from the following expression (e.g., Panofsky, 1963):

$$\psi_m(\zeta)=\psi_h(\zeta)=\int_0^{\zeta}\frac{1-\varphi_{m,h,q}(\zeta')}{\zeta'}d\zeta' \tag{A5}$$

The bulk Richardson number (Ri_B) is given by:

$$Ri_B=\frac{g}{\bar{\theta}}\frac{(\theta_a-\theta_g)(z-z_0)^2}{U^2(z-z_h)} \tag{A6}$$

Substituting the values of U and $(\theta_a-\theta_g)$ from Eqns. (A3) and (A4) in Eqn. (A6), one gets

$$Ri_B=\zeta\left[\frac{\left(1-\frac{z_0}{z}\right)^2}{\left(1-\frac{z_h}{z}\right)}\right]\frac{\left[\ln\left(\frac{z}{z_h}\right)-\left\{\psi_h(\zeta)-\psi_h\left(\zeta\frac{z_h}{z}\right)\right\}\right]}{\left[\ln\left(\frac{z}{z_0}\right)-\left\{\psi_m(\zeta)-\psi_m\left(\zeta\frac{z_0}{z}\right)\right\}\right]^2} \tag{A7}$$

Note that Eqn. (A7) is a transcendental equation, and for a given value of Ri_B, the corresponding ζ value can be calculated using any iterative method.

The bulk transfer coefficient for momentum (C_D) and heat (C_H) are defined as:

$$C_D=k^2\left[\ln\left(\frac{z+z_0}{z_0}\right)-\left\{\psi_m\left(\frac{z+z_0}{L}\right)-\psi_m\left(\frac{z_0}{L}\right)\right\}\right]^{-2} \tag{A8}$$

$$C_H=k^2\left[\ln\left(\frac{z+z_0}{z_0}\right)-\left\{\psi_m\left(\frac{z+z_0}{L}\right)-\psi_m\left(\frac{z_0}{L}\right)\right\}\right]^{-1}\left[\ln\left(\frac{z+z_h}{z_h}\right)-\left\{\psi_h\left(\frac{z+z_h}{L}\right)-\psi_h\left(\frac{z_h}{L}\right)\right\}\right]^{-1} \tag{A9}$$

Once we get C_D and C_H, then the momentum (τ), and sensible heat (H) fluxes are calculated using the following expressions:

$$\tau=\rho C_D U^2 \tag{A10}$$

$$H=-\rho c_p C_H U(\theta_a-\theta_g), \tag{A11}$$

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Appendix B

Here, the detailed description of the commonly used similarity functions (φ_m and φ_h) in numerical models under convective conditions is provided.

Based on Businger (1966) and A. J. Dyer [1965, unpublished work; see Businger (1988) for details] the expressions for φ_m and φ_h are as follows:

$$\varphi_m = (1 - \gamma_m \zeta)^{-\frac{1}{4}} \tag{B1}$$

$$\varphi_h = Pr_t (1 - \gamma_h \zeta)^{-\frac{1}{2}} \tag{B2}$$

in which $\gamma_m = 15$, $\gamma_h = 9$, and $Pr_t = 0.74$ is the turbulent Prandtl number. Note that in case of Dyer (1974) the values of $\gamma_m = \gamma_h = 16$ and $Pr_t = 1.0$. These functions commonly known as Businger-Dyer similarity (BD) functions and do not satisfy the classical free convection limit (Srivastava et al. 2021).

The similarity functions proposed by Carl et al. (1973) under convective conditions are applicable for the range $-10 \le \zeta \le 0$. The expressions for φ_m and φ_h suggested by Carl et al. (1973) are:

$$\varphi_m = (1 - \beta_m \zeta)^{-\frac{1}{3}} \tag{B3}$$

$$\varphi_h = (1 - \beta_h \zeta)^{-\frac{1}{3}} \tag{B4}$$

in which $\beta_m = \beta_h = 15$. However, based on various studies reported in the literature β_m and β_h can take different values. For example, Delage and Girard (1992) proposed $\beta_m = \beta_h = 40$, on the other hand, Fairall et al. (1996) suggested that $\beta_m = \beta_h = 12.87$.

Fairall et al. (1996, 2003) proposed an interpolation function applicable for the entire range of atmospheric instability, which was based on BD functions and functions suggested by Carl et al. (1973). This interpolation function does not have the gradient form (φ_m and φ_h), as they have interpolated the integrated forms of the functions. We wish to highlight that the revised MM5 surface layer scheme of Weather Research and Forecasting Model version 4.2.2 utilized the interpolation functions suggested by Fairall et al. (1996).

Kader and Yaglom (1990) proposed a three-sublayer model under convective conditions. According to three sublayer model, in the Dynamic sub-layer (DNS) ($-\frac{1}{40} < \zeta < 0$), $\varphi_m = 1$ and $\varphi_h = Pr_t$. While in the dynamic convective sublayer (DCS) ($-0.4 < \zeta < -\frac{1}{40}$), both φ_m and φ_h varies as a $-1/3$ power law as

$$\varphi_m(\zeta) = A_u (-\zeta)^{-\frac{1}{3}} \tag{B5}$$

$$\varphi_h(\zeta) = A_T (-\zeta)^{-\frac{1}{3}} \tag{B6}$$

in which A_u and A_T are constants.

For free convective sublayer ($\zeta < -2$), the theory suggests that φ_m varies as a $1/3$ power law while φ_h varies as a $-1/3$ power law as follows:

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$$\varphi_m(\zeta) = B_u(-\zeta)^{\frac{1}{3}} \tag{B7}$$

$$\varphi_h(\zeta) = B_T(-\zeta)^{-\frac{1}{3}} \tag{B8}$$

in which B_u and B_T are constants.

Thus, under unstable conditions, φ_m exhibits a nonmonotonic behaviour with respect to $-\zeta$ as the three sublayer theory suggested that for sufficiently large values of $-\zeta$, φ_m varies as the $+1/3$ power of ζ, in contrast to the case of the free convection limit, where both φ_m and φ_h follow the $-1/3$ power law. In the literature, various expressions for φ_m and φ_h are available based on the Kader and Yaglom (1990) three-sublayer model. However, the present study employs φ_m and φ_h based on the expressions implemented in the surface layer scheme (CLM4.0) of NCAR-CAM5 (Zeng et al., 1998) model. The expressions for φ_m and φ_h utilized in this study are as follows:

$$\varphi_m = \begin{cases} (1-16\zeta)^{-\frac{1}{4}}, & -1.574 \le \zeta \le 0 \\ 0.7k^{\frac{2}{3}}(-\zeta)^{\frac{1}{3}}, & \zeta \le -1.574 \end{cases} \tag{B9}$$

and

$$\varphi_h = \begin{cases} (1-16\zeta)^{-\frac{1}{2}}, & -0.465 \le \zeta \le 0 \\ 0.9k^{\frac{4}{3}}(-\zeta)^{-\frac{1}{3}}, & \zeta \le -0.465 \end{cases} \tag{B10}$$

Srivastava and Sharan (2021) classified these commonly used similarity functions stated above into four different classes based on the exponents appearing in the expressions of φ_m and φ_h. The classification is as follows:

Class 1. This class consists of functions having the exponents of φ_m and φ_h as $-1/4$ and $-1/2$ (as in Eqns. B1 and B2), respectively from near-neutral to strong unstable conditions. φ_m and φ_h proposed by Businger (1971) and Hogstrom (1996) are the examples of class 1 functions.

Class 2. In this class, the similarity functions (φ_m and φ_h) having exponents of φ_m and φ_h as $-1/3$ for the entire range from near-neutral to moderately unstable conditions (as in Eqns. B3 and B4), respectively are included. The functional forms suggested by Carl et al. (1973) are the example of class 2 functions.

Class 3. φ_m and φ_h having exponents as $-1/4$ and $-1/2$, respectively in near neutral conditions while $-1/3$ in strong unstable conditions are included in this class. φ_m and φ_h based on Fairall et al. (1996), Grachev et al. (2000) and Fairall et al. 2003 are some examples of class 3 functions.

Class 4. Functional forms of φ_m and φ_h having the exponents as $-1/4$ and $-1/2$, respectively in near neutral conditions however, $1/3$ for φ_m and $-1/3$ for φ_h in strong unstable conditions are classified in this class (as in Eqns. B9 and B10). The

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three-sublayer model for φ_m and φ_h suggested by Kader and Yaglom (1990) (Zeng et al. 1998) is one of the examples of functions in this class.

Appendix C

In this section, the details of various physical parameterizations utilized in the real-case simulations using WRFv4.2.2 model and the different statistical indicators used for model evaluation.

The real-case simulations with the WRFv4.2.2 model utilised the Purdue Lin microphysics scheme (Lin et al., 1983); YSU (Hong, Noh, and Dudhia, 2006) PBL scheme; Kain-Fritsch (Kain and John, 2004) cumulus scheme; Dudhia (Dudhia, 1989) shortwave scheme; RRTM (Mlawer et al., 1997) longwave scheme; Noah-MP land surface model (Niu et al., 2011); and revised MM5 surface layer scheme (Jimenez et al., 2012).

In the present study, different statistical indicators have been used for the model evaluation with respect to observations/reanalysis datasets. Statistical parameters such as mean absolute error (MAE), root mean square error (RMSE), mean bias (MB), index of agreement (IOA), and correlation coefficient (CC) are defined as:

1. Mean absolute error:

$$MAE = \frac{\sum_{i=1}^{n} |p_i - o_i|}{n}$$

2. Root mean square error:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (p_i - o_i)^2}{n}}$$

3. Mean bias

$$MB = (\bar{p} - \bar{o})$$

4. Index of agreement

$$IOA = 1 - \frac{\sum_{i=1}^{n} (o_i - p_i)^2}{\sum_{i=1}^{n} (|p_i - \bar{o}| + |o_i - \bar{o}|)^2}$$

5. Correlation coefficient

$$\mathrm{CC} = \frac{\sum_{\mathrm{i}=1}^{\mathrm{n}} (\mathrm{p_i} - \bar{\mathrm{p}})\,(\mathrm{o_i} - \bar{\mathrm{o}})}{\sqrt{\sum_{\mathrm{i}=1}^{\mathrm{n}} (\mathrm{p_i} - \bar{\mathrm{p}})^2}\sqrt{\sum_{\mathrm{i}=1}^{\mathrm{n}} (\mathrm{o_i} - \bar{\mathrm{o}})^2}}$$

   in which p_i and o_i represent the predicted and observed time series, respectively, while and $\bar{p}$ and $\bar{o}$ are the predicted and observed mean for a considered variable, respectively.

6. Taylor diagram: It exhibits how well patterns match each other in terms of their correlation, ratio of their variances, and root mean square differences (Taylor, 2001).
7. Q-Q plot: It is a graphical technique used to compare the overall distribution of predicted and observed values for a variable (Venkatram, 1999)

The error or deviation between observed and simulated values is measured by MAE, RMSE, and MB. On the other hand, IOA is used to assess the trend relationship, or how closely the magnitudes and signs of the observed values are related to the projected values (Schlunzen and Sokhi 2008). In order to evaluate the spatial patterns with ERA5-Land reanalysis dataset, statistical metrics such as mean bias (%), RMSE, and pattern correlation (PCC) have been used.

Code and data availability: Weather Research and Forecasting Model version 4.2.2 (WRFv4.2.2) is an open source model and can be downloaded from https://www2.mmm.ucar.edu/wrf/users/download/get_source.html. The model output at the location of the flux tower at Ranchi (23.412N, 85.440E)**,** India is openly available at https://doi.org/10.5281/zenodo.10435513**.** The raw observational data derived from the flux tower at Ranchi (23.412N, 85.440E; India) utilized in the present study can be obtained from the Indian National Centre for Ocean Information Service upon request (http://www.incois.gov.in/portal/datainfo/ctczdata.jsp). Hourly ERA5-Land reanalysis data utilized in this study can be found in its official website https://cds.climate.copernicus.eu/cdsapp#!/dataset/reanalysis-era5-land?tab=form.

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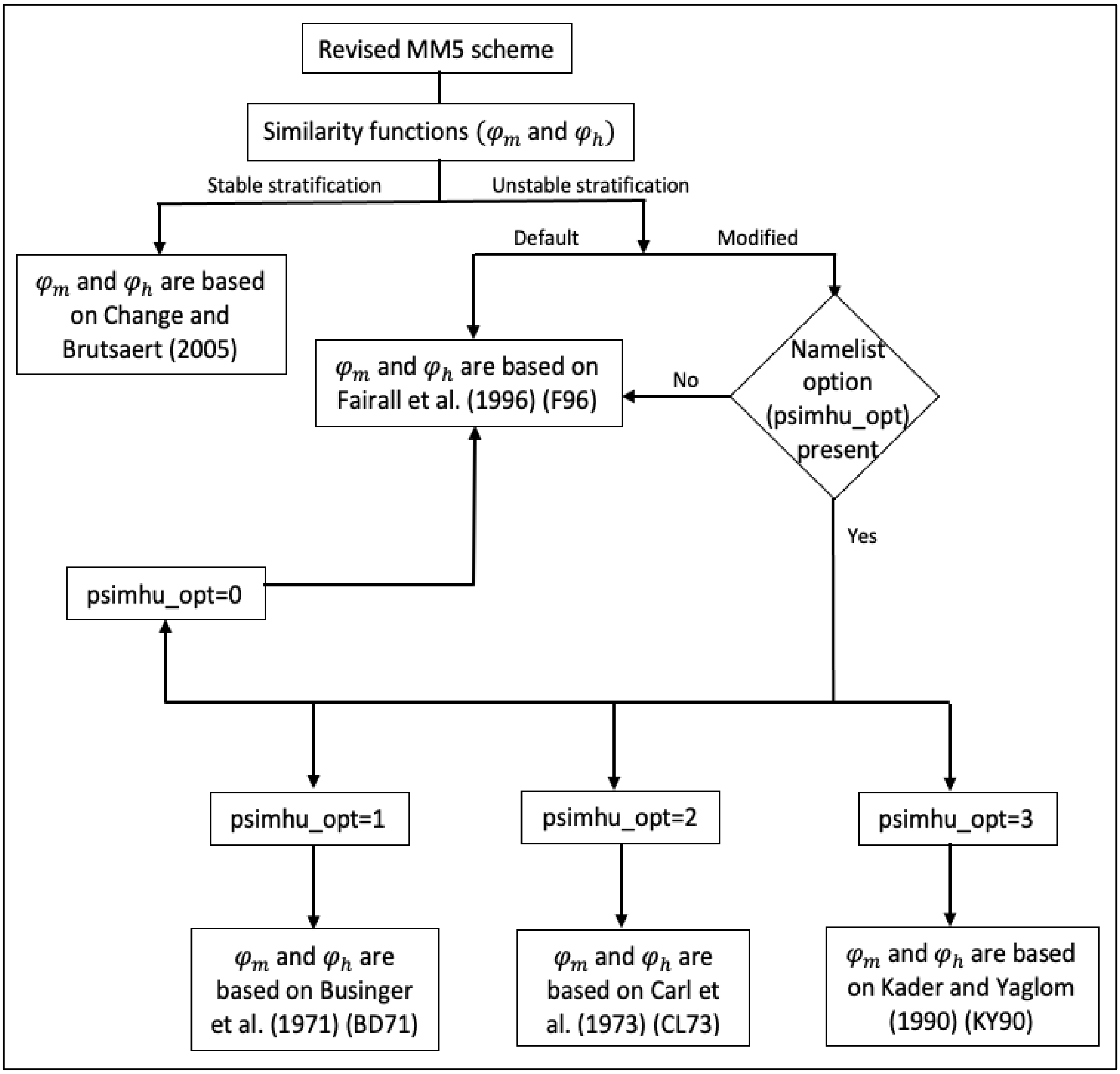

Figure 1: Flowchart to provide a brief description of different options for similarity functions in the modified surface layer scheme that can be controlled by namelist variable psimhu_opt.

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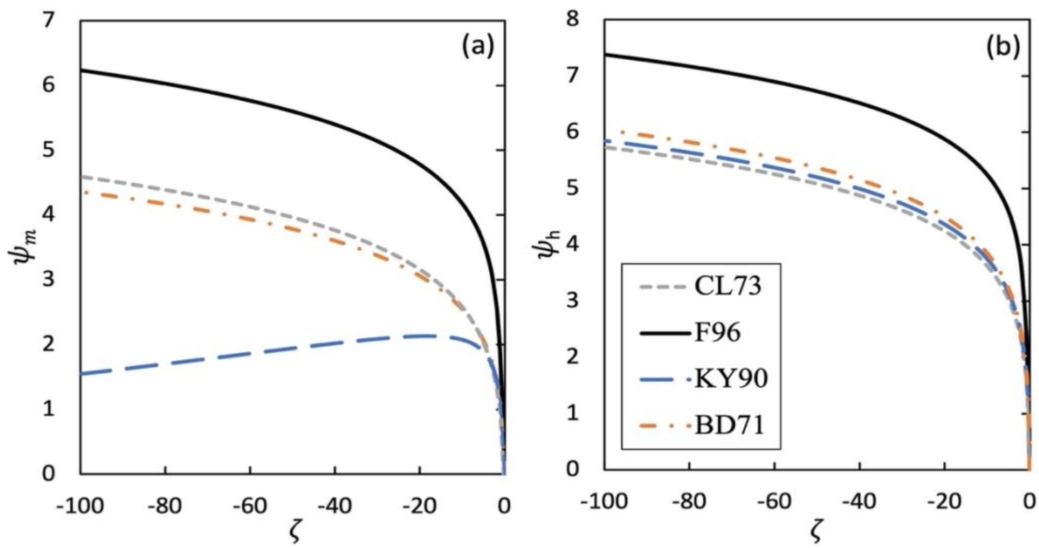

Figure 2: Integrated similarity functions $\psi_{m,h}(\zeta)$ for momentum and heat for default and incorporated functions for unstable atmospheric surface layer.

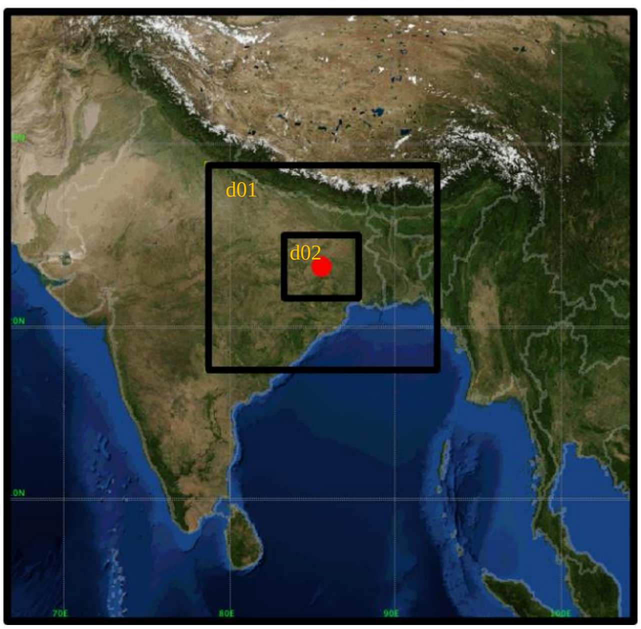

Figure 3: Spatial distribution of domain used for the simulations using WRF model. The spatial resolution for domains d01 and d02 is 6 × 6 km and 2 × 2 km, respectively. The domain d02 covers 446 × 392 km^2 area around the centre point.

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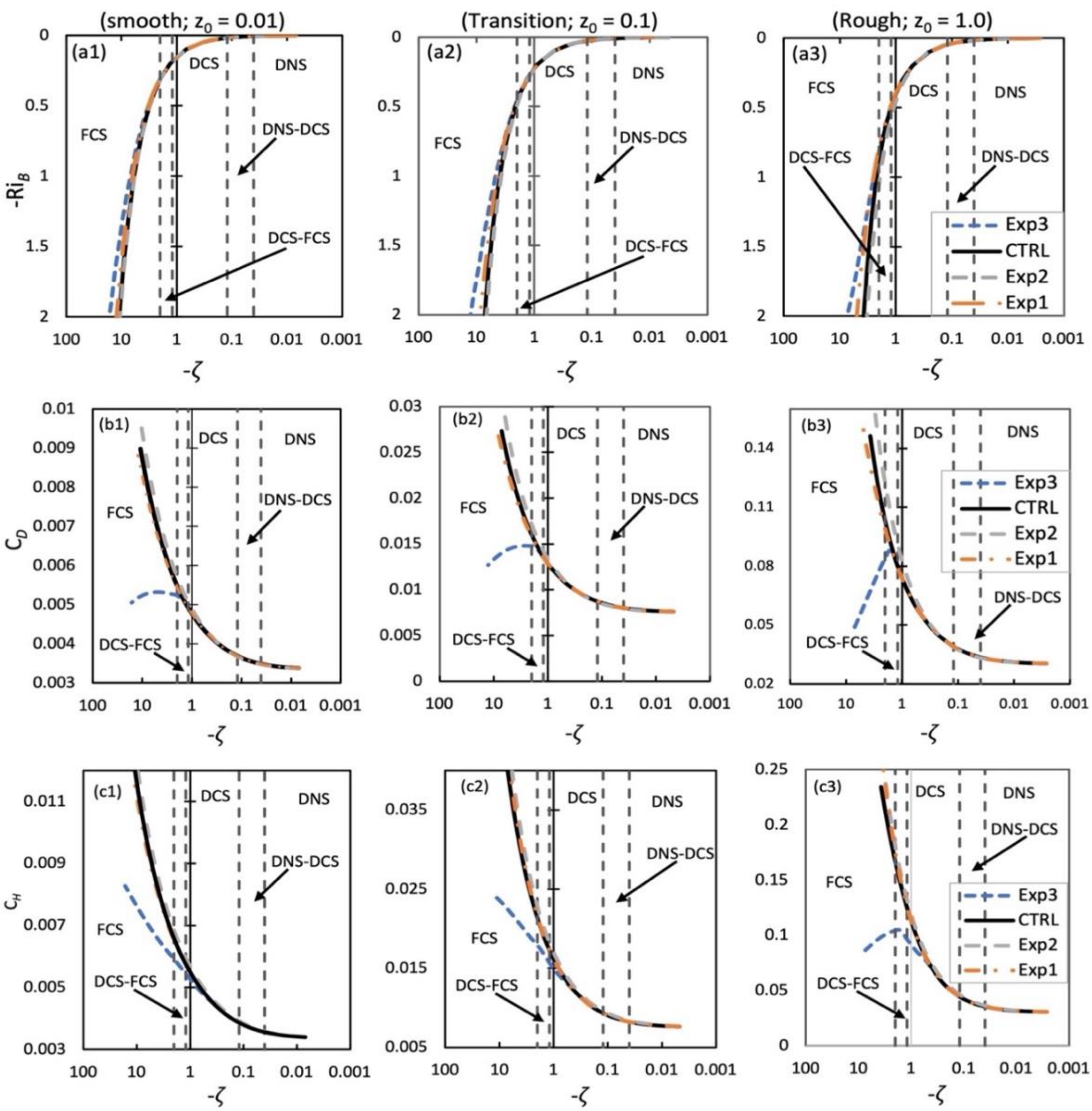

Figure 4: Variation of ζ with Ri_B (upper panel), C_D (middle panel) and C_H (lower panel) with ζ calculated from bulk flux algorithm (offline simulation) for different experiments corresponding to different functional forms of ψ_m and ψ_h together with the CTRL simulation for smooth ($z_0 = 0.01$ m; 1st column), transition ($z_0 = 0.1$ m; second column), and rough ($z_0 = 1.0$ m; third column) surfaces. The dotted lines separate different sublayer within the convective regime.

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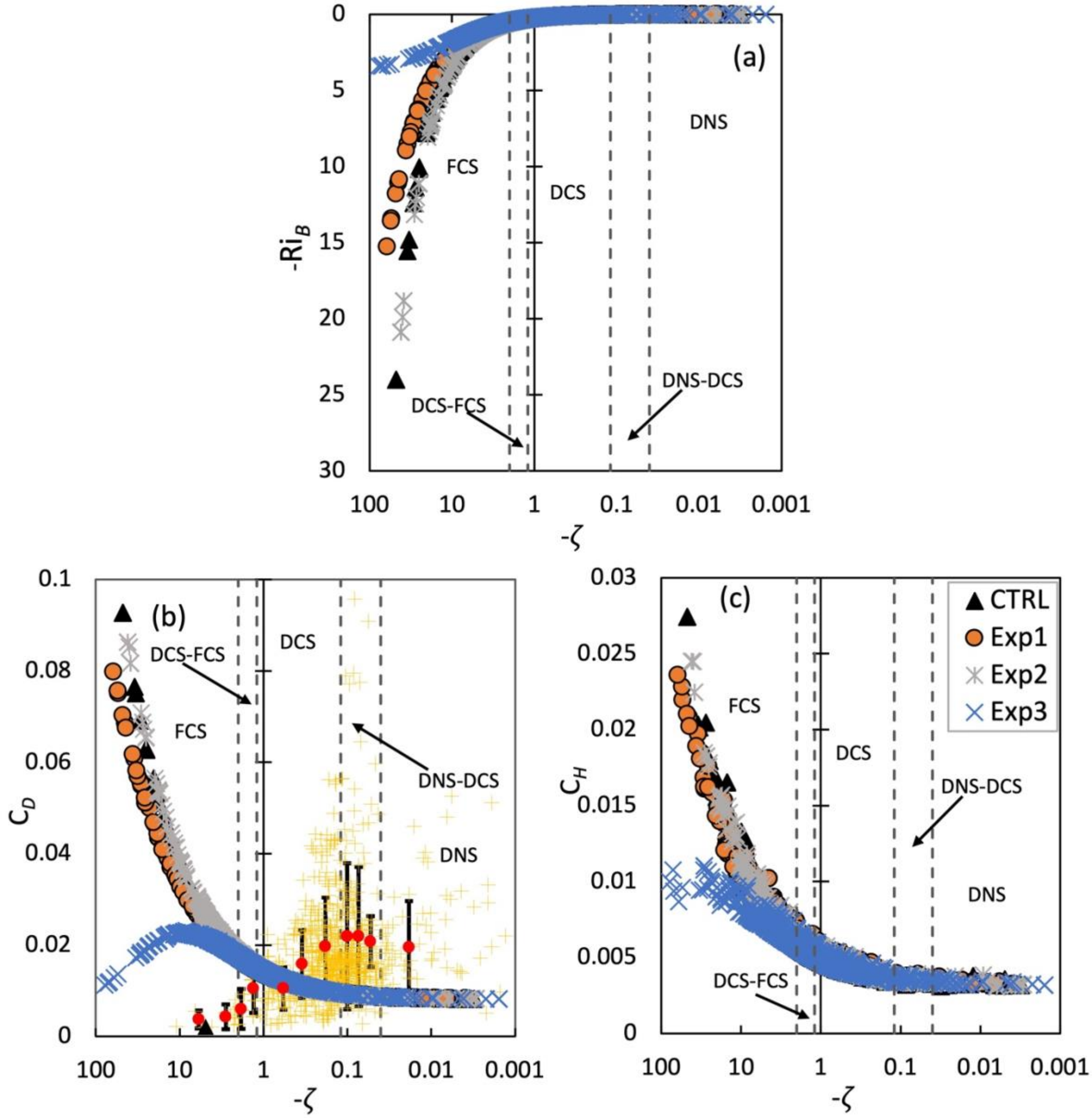

Figure 5: Variation of model simulated (a) ζ with Ri_B, (b) C_D and (c) C_H with ζ from different experiments using different ψ_m and ψ_h corresponding to F96 (CTRL), BD71 (Exp1), CL73 (Exp2), and KY90 (Exp3) under convective conditions. The yellow markers (+) in (b) denote the observed C_D with ζ at the location of flux tower. The dotted lines separate different sublayer within the convective regime. The mean values of observed C_D in each sublayer are shown with red dots along with standard deviations in the form of error bars. Depending upon the data availability, two or three bins of equal width are chosen in each sublayer.

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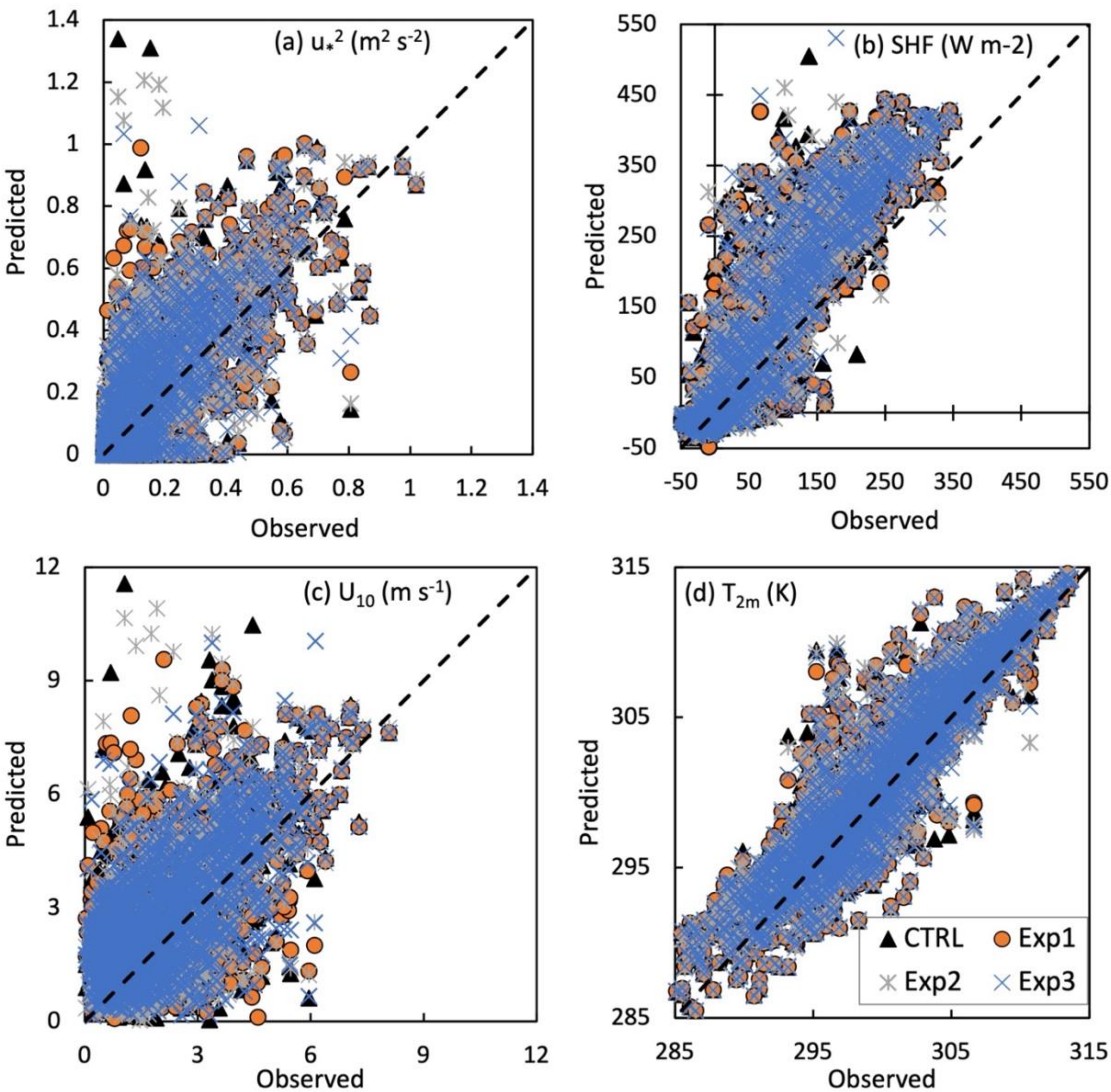

Figure 6: Scatter plot of model simulated (a) u_*^2 ($m^2 s^{-2}$) (representative of momentum flux), (b) SHF ($W m^{-2}$) (sensible heat flux), (c) U_{10} ($m s^{-1}$) (wind speed at 10 m height), and (d) T_{2m} (K) (temperature at 2 m height) vs observed values at the location of flux tower at Ranchi (23.412oN, 85.440oE), India (centre point of the domain) during pre-monsoon season (MAM).

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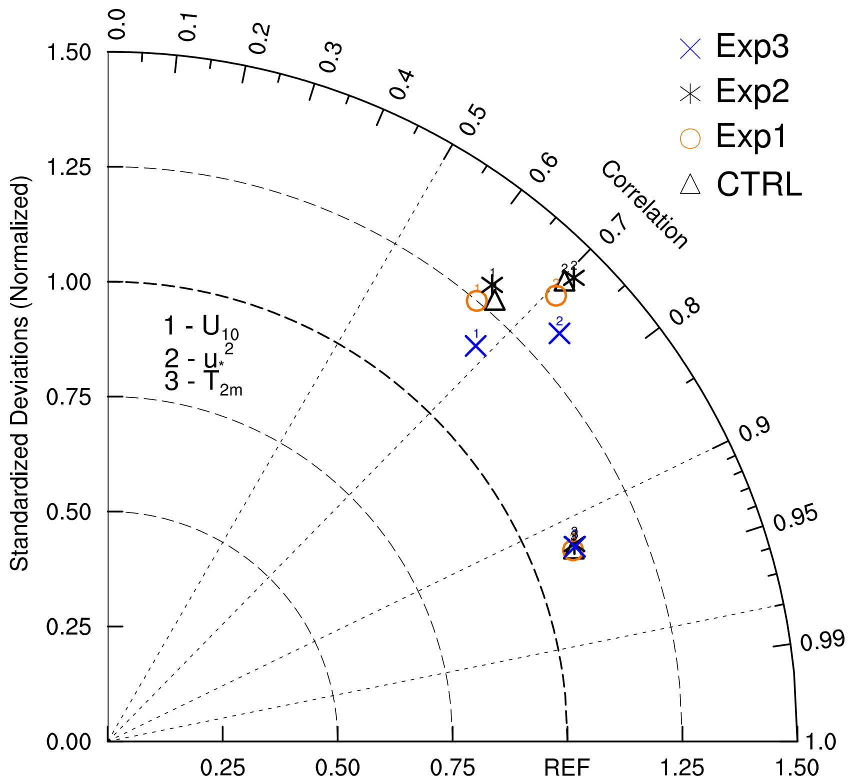

Figure 7: Taylor diagram showing the correlation coefficient, normalized standard deviations for U_{10}, u_*^2, and T_{2m} from different experiments together with CTRL simulation with respect to observations derived from flux tower installed at Ranchi (23.412ºN, 85.440ºE), India.

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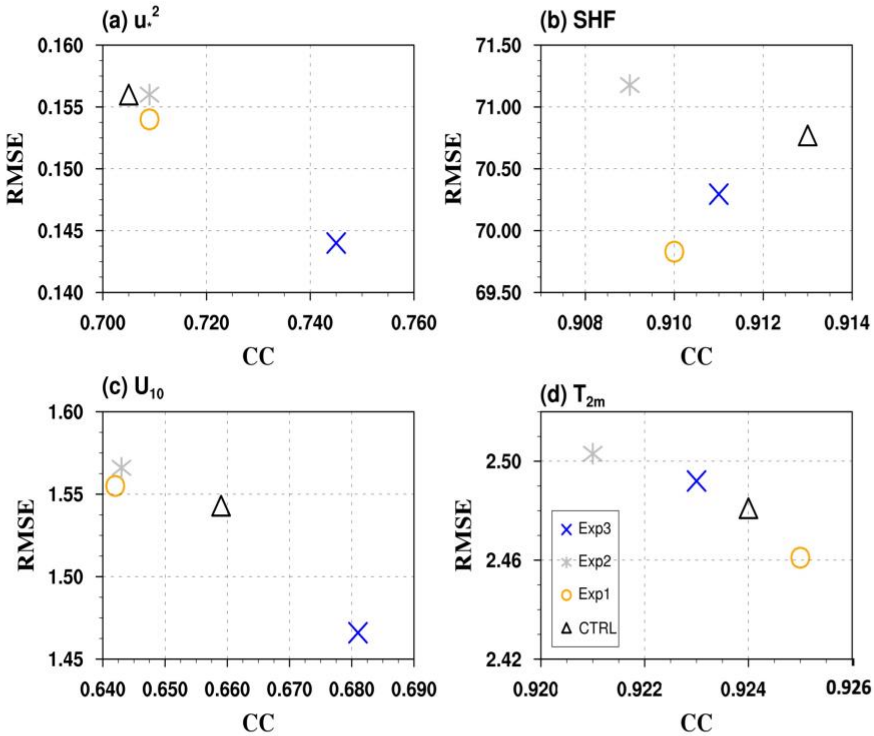

Figure 8: Scatter plot between correlation coefficient (CC) and root mean square error (RMSE) for (a) u_*^2, (b) SHF, (c) U_{10}, and (d) T_{2m} simulated by various experiments (Exp1-3) together with CTRL simulation for pre-monsoon season (MAM; 2009) at the location of the flux tower (23.412°N, 85.440°E).

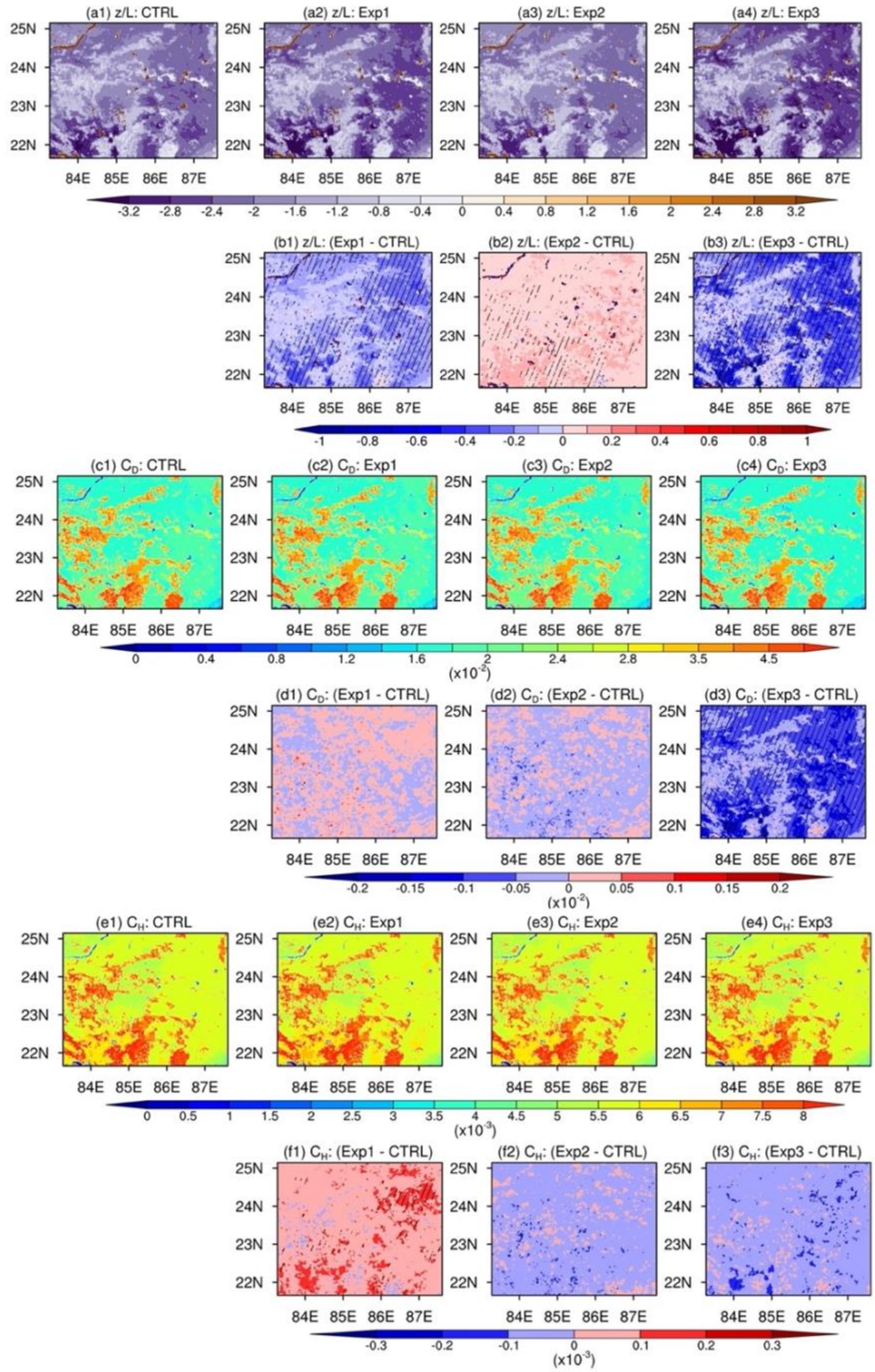

Figure 9: Mean spatial distribution of model simulated ζ (1^{st} row), C_D (3^{rd} row) and C_H (5^{th} row) from different experiments and their differences with respect to CTRL simulation averaged during daytime for whole simulation period. Hatched regions show significant differences at 95% confidence level in experiments with respect to CTRL simulation.

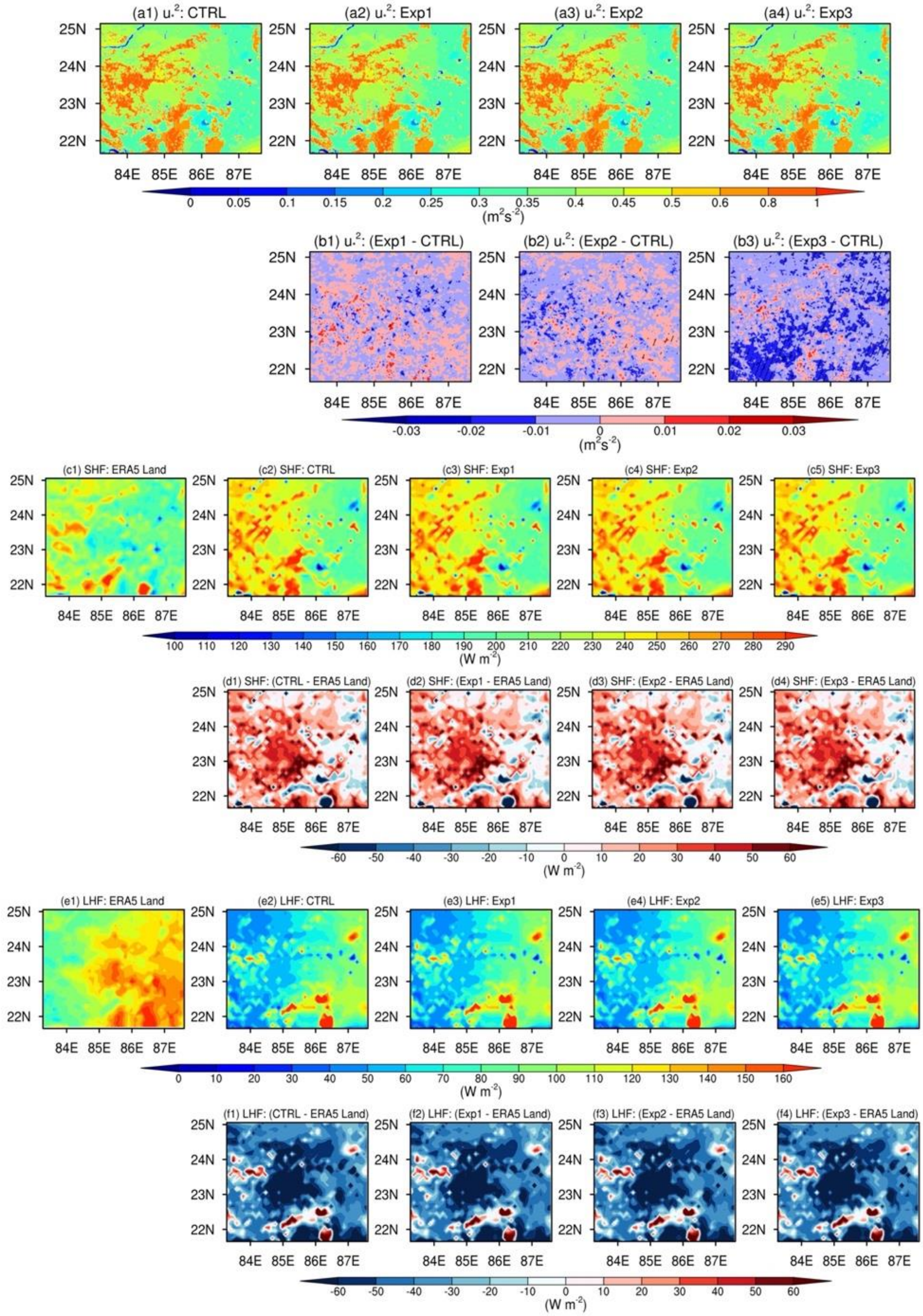

Figure 10: Mean spatial distribution of simulated u_*^2 (1st row) from different experiments and their differences (2nd row) with respect to CTRL simulation. SHF and LHF from ERA5-Land reanalysis and simulated using various experiments and their differences with respect to ERA5-Land data averaged during daytime for the whole simulation period are shown. Hatched regions show significant differences at 95% confidence level in experiments with respect to CTRL simulation.

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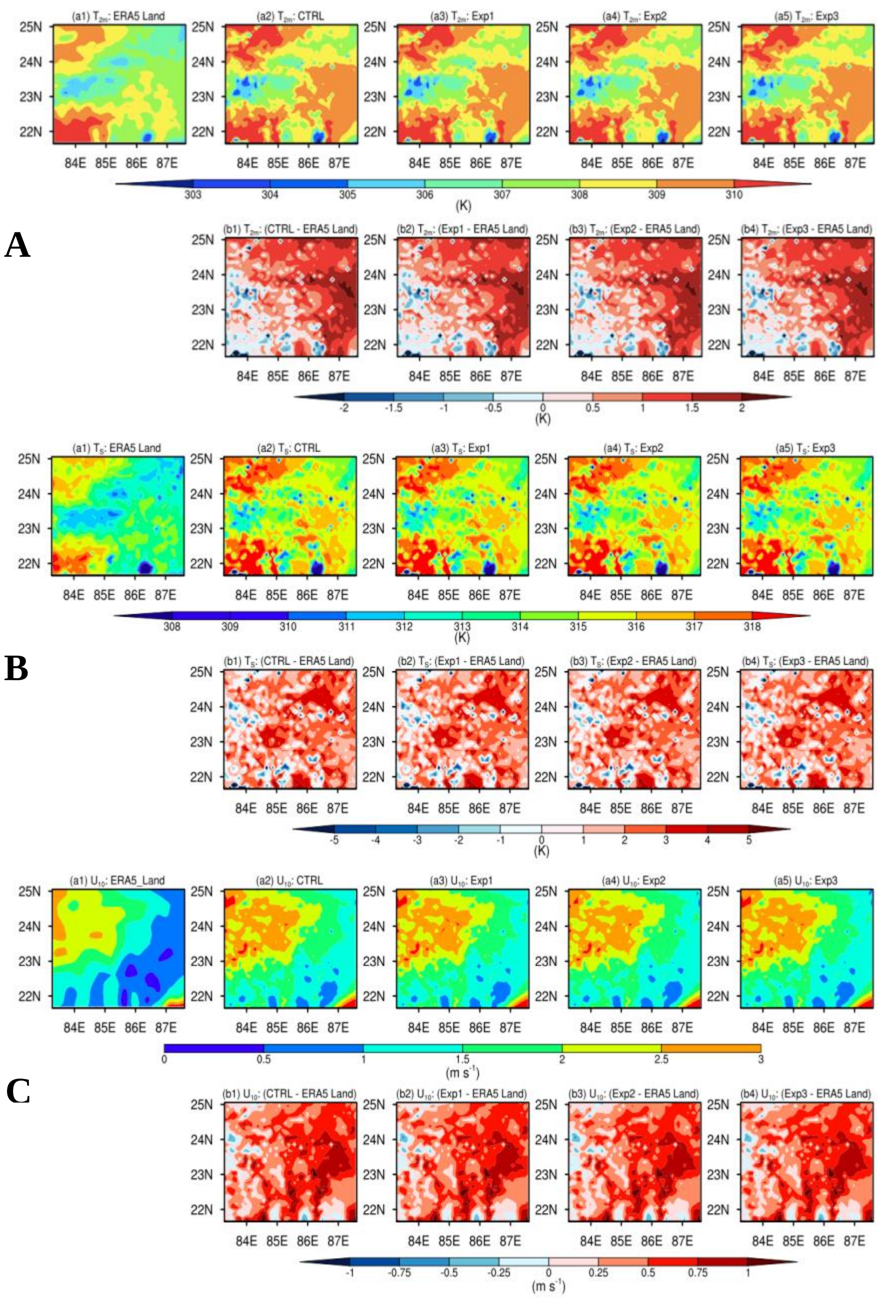

Figure 11: In upper panel (A), mean spatial distribution of T_{2m} from ERA5-Land reanalysis (a1) and simulated using different experiments (a2-a5) and their differences with respect to ERA5-Land reanalysis (b1-b4) averaged during daytime for the whole simulation period. Middle (Lower) panel is same as the upper panel but for T_S (U_{10}).

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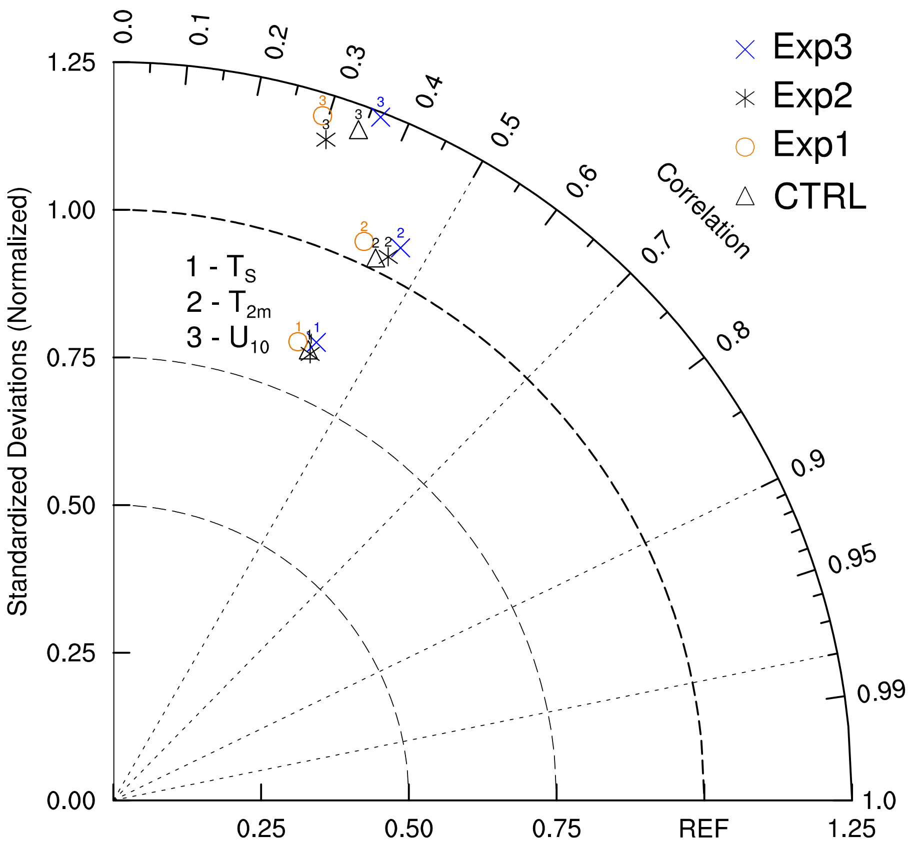

Figure 12: Taylor diagram showing the correlation coefficient, normalized standard deviations for T_S (K), T_{2m} (K), and U_{10} (m s^{-1}) from different experiments together with CTRL simulation with respect to ERA5-Land reanalysis dataset averaged during strong convective conditions (hours during daytime in which ζ is smaller than -10) for whole simulation period.

Experiments	Description
CTRL	Simulation using default surface layer scheme with F96 functions
Exp1	Simulation using surface layer scheme with BD71 functions
Exp2	Simulation using surface layer scheme with CL73 functions
Exp3	Simulation using surface layer scheme with incorporated KY90 functions

Table 1. Description of various simulations conducted in this study.

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MAM		u_*^2 (m² s⁻²)	SHF (W m⁻²)	U_{10} (m s⁻¹)	T_{2m} (K)
CTRL	**MAE**	0.088	43.456	1.198	1.815
	RMSE	0.156	70.770	1.543	2.481
	MB	0.034	34.876	0.825	0.926
	IOA	0.818	0.896	0.729	0.954
	CC	0.705	0.913	0.659	0.924
Exp1	**MAE**	0.086	**42.719**	1.207	**1.807**
	RMSE	0.154	**69.830**	1.555	**2.461**
	MB	0.031	**33.064**	0.812	0.896
	IOA	0.823	0.898	0.720	**0.955**
	CC	0.709	0.910	0.642	**0.925**
Exp2	**MAE**	0.088	43.547	1.200	1.835
	RMSE	0.156	71.177	1.566	2.503
	MB	0.032	34.486	0.812	**0.873**
	IOA	0.822	0.894	0.721	0.954
	CC	0.709	0.909	0.643	0.921
Exp3	**MAE**	**0.082**	42.960	**1.164**	1.833
	RMSE	**0.144**	70.295	**1.466**	2.492
	MB	**0.026**	33.472	**0.782**	0.908
	IOA	**0.843**	0.897	**0.751**	0.954
	CC	**0.742**	0.911	**0.681**	0.923

Table 2: Comparison statistics for u_*^2 (m^2 s^{-2}), SHF (W m^{-2}), U_{10} (m s^{-1}), and T_{2m} (K) simulated using different experiments together with CTRL simulation with respect to observations derived from flux tower at Ranchi (India) for MAM season. The mean absolute error (MAE), root mean square error (RMSE), mean bias (MB), index of agreement (IOA), and correlation coefficient (CC) are shown.

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MAM	T_S (K)			T_{2m} (K)			U_{10} (m s^{-1})		
	Bias (%)	**RMSE**	**PCC**	**Bias (%)**	**RMSE**	**PCC**	**Bias (%)**	**RMSE**	**PCC**
CTRL	1.259	4.013	0.397	0.635	2.133	0.435	-4.962	0.438	0.343
Exp1	1.261	4.030	0.373	0.638	2.157	0.409	-4.430	0.454	0.292
Exp2	1.252	3.989	0.403	0.626	2.103	0.451	-5.386	0.442	0.306
Exp3	**1.243**	**3.972**	**0.405**	**0.623**	**2.102**	**0.461**	**-0.284**	0.474	**0.364**

Table 3: Comparison statistics for T_{2m} (K), T_S (K), and U_{10} (m s^{-1}) simulated using different experiments together with CTRL simulation with respect to ERA5-Land reanalysis data averaged during strong unstable stratification (hours during daytime in which ζ is smaller than -10) for whole simulation period. The percent mean bias (Bias %), pattern correlation coefficient (PCC), and root mean square error (RMSE) are shown.