An Updated Parameterization of the Unstable Atmospheric Surface Layer in the 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 the commonly used similarity 13 functions for momentum (φ_m) and heat (φ_b) under convective conditions instead of the existing single functional form. The 14 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, 2021). The study suggests that the updated surface layerscheme performs well in simulating the surface transfer coefficients and could be potentially utilized for parameterization of surface fluxes under convective conditions in the WRF 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 27 functions of momentum (φ_m) and heat (φ_b) 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. 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, 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 37 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 the 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.

48 Srivastava and Sharan (2015) analyzed the observed behaviour of C_D over an Indian land surface and suggested that 49 the observed C_D shows non-monotonic behaviour with $-\zeta$, unlike the behaviour of predicted C_D from MOST based 50 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) 52 is able to predict C_D consistent with its observed non-monotonic behaviour. Note that the three-sublayer model has not yet been newly installed and evaluated in the 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 57 functional forms of φ_m and φ_h under convective conditions. To quantify the impacts of different functional forms, they 58 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) 59 functional forms having the exponents of φ_m and φ_h as $-1/4$ and $-1/2$, respectively (Businger et al. 1971; Hogstrom 1996). 60 (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 61 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 62 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 $-1/2$, 63 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 65 bulk flux algorithm results in a large deviation in the values of estimated fluxes. The detailed description of different functional 66 forms for φ_m and φ_h considered in different classes are given in Appendix A. We wish to highlight that all available functional 67 forms for φ_m and φ_h under convective conditions fall in one of the classes stated above.

68 The revised MM5 surface layer scheme of the WRF model version 4.2.2 (WRFv4.2.2) employed φ_m and φ_h based 69 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 the 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 75 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.

79 **2 Methodology and data**

80 **2.1 Surface flux computation in the WRF modeling system**

81 The Monin-Obukhov similarity theory serves as the foundation for the surface layer parameterization (revised MM5 scheme) 82 in the WRF model, and the surface turbulent fluxes are calculated based on the bulk approach using bulk transfer coefficients 83 for momentum (C_D) and heat (C_H) (Namdev et al., 2024; Srivastava et al., 2021; Srivastava and Sharan, 2021). Following 84 MOST they are formulated as follows: $C_{\rm D} = k^2 \left[\ln \left(\frac{z + z_0}{z} \right) \right]$ $\left(\frac{z+z_0}{z_0}\right) - \left\{\psi_m\left(\frac{z+z_0}{L}\right) - \psi_m\left(\frac{z_0}{L}\right)\right\}$ -2 85 $C_D = k^2 \left[\ln \left(\frac{\mu_0 - \mu_0}{\mu_0} \right) - \frac{1}{2} \ln \left(\frac{\mu_0 - \mu_0}{\mu_0} \right) \right]$ (1)

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

87 in which k is the von Karmann constant; z_0 and z_h are the roughness lengths for momentum and heat, respectively; ψ_m and 88 ψ_h are the integrated similarity functions for momentum and heat, respectively; and L is the Obukhov length scale.

89 Their determination based on MOST using integrated forms of the similarity functions is explained in Appendix B. In the 90 following, the default similarity functions used in WRF are explained and other functions are introduced in Section 2.2.

91 The default version of the revised MM5 scheme in the WRF model utilizes similarity functions suggested by Cheng 92 and Brutsaert (2005) under stable atmospheric conditions ($\zeta > 0$), which are developed using the CASES-99 dataset. The 93 integrated forms of functions proposed by Cheng and Brutsaert are

94
$$
\psi_m(\zeta) = -a \ln \left(\zeta + \left[1 + \zeta^b \right]^{1/b} \right), \qquad \zeta > 0
$$
 (3)

95
$$
\psi_h(\zeta) = -c \ln \left(\zeta + \left[1 + \zeta^d \right]^{1/d} \right), \qquad \zeta > 0
$$
 (4)

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

97 On the other hand, the similarity functions for unstable atmospheric surface layer (ζ < 0) are those proposed by 98 Fairall et al. (1996; F96). The corresponding integrated functional forms ψ_m and ψ_h are defined as:

99
$$
\psi_{\alpha}(\zeta) = \frac{\psi_{\alpha_{\text{BD}}}(\zeta) + \zeta^2 \psi_{\alpha_{\text{conv}}}(\zeta)}{1 + \zeta^2}, \quad \alpha = m, h.
$$
 (5)

100 where $\psi_{\alpha_{BD}}$ and $\psi_{\alpha_{CDIV}}$ denote the integrated functional forms based on Businger and Dyer, and Carl et al. (1973), 101 respectively. The expressions for $\psi_{\alpha_{BD}}$ and $\psi_{\alpha_{\text{conv}}}$ are

102
$$
\psi_{\text{m}_{BD}}(\zeta) = 2 \ln \left(\frac{1+x}{2} \right) + \ln \left(\frac{1+x^2}{2} \right) - 2 \tan^{-1} x + \frac{\pi}{2},
$$
 (6)

$$
103 \quad \psi_{\rm h_{BD}}(\zeta) = 2 \ln \left(\frac{1 + x^2}{2} \right),\tag{7}
$$

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

105
$$
\psi_{\alpha_{\text{conv}}} = \frac{3}{2} \ln(y^2 + y + 1/3) - \sqrt{3} \tan^{-1} (2y + 1/\sqrt{3}) + \frac{\pi}{\sqrt{3}}
$$
(8)

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

107 **2.2 Implementation of different similarity functions**

108 In this section, we briefly describe the implementation of different similarity functions for unstable stratification in the surface

109 layer parameterization of WRFv4.2.2. Note that two sets of functional forms, namely those suggested by Carl et al. (1973) and

- 110 the three sub-layer model proposed by Kader and Yaglom (1990) for convective conditions have not been included and tested
- 111 in the surface layer scheme of the WRF modeling framework.

112 **2.2.1 Functions by Businger et al. (1971) (BD71)**

113 Similarity functions suggested by Businger et al. (1971) are based on the KANSAS dataset (Izumi, 1971). These functions do

114 not satisfy the classical free convection limit as predicted by the MOST. They are already implemented in the old version of

- 115 the MM5 surface layer scheme (Grell et al., 1994) in the WRF model. The integrated functional forms (ψ_m and ψ_b) for φ_m
- 116 and φ_h stated in Eqns. (A1) and (A2) (Appendix A) are given in Eqns. (6) and (7).

117 **2.2.2 Functions by Carl et al. (1973) (CL73)**

118 Carl et al. (1973) proposed an expression of similarity functions φ_m and φ_b valid for the stability range −10 ≤ ζ ≤ 0. The

119 expressions for φ_m and φ_b are given in Eqns. (A3) and (A4) (Appendix A). The similarity functions proposed by Carl et al.

120 (1973) have not been analyzed in the surface layer scheme of the WRF model. The integrated forms (ψ_m and ψ_h) of similarity

121 functions $φ_m$ and $φ_h$ are given by Eqn. (8).

122 **2.2.3 Functions by Kader and Yaglom (1990) (KY90)**

123 Kader and Yaglom (1990) introduced a three-sublayer model for convective conditions. The three sublayers are categorized 124 based on ζ values as (1) the dynamic sublayer which corresponds to near-neutral conditions, (2) the dynamic convective 125 sublayer which corresponds to moderately unstable conditions and (3) the free convective conditions. The present study 126 utilized φ_m and φ_h expressions given in Eqns. (A9), and (A10) (Appendix A) that are being used in the surface layer scheme 127 (CLM4.0; Zeng et al. 1998) of NCAR-CAM5 model. The corresponding integrated forms for $φ_m$ and $φ_h$ are

128
$$
\psi_{m}(\zeta) = \begin{cases} \psi_{m1}(\zeta_{m}) + \ln \frac{\zeta}{\zeta_{m}} - 1.14[(-\zeta)^{1/3} - (-\zeta_{m})^{1/3}], & \zeta \le -1.574 (= \zeta_{m}) \\ \psi_{m1}(\zeta) = 2\ln \left(\frac{1+x}{2}\right) + \ln \left(\frac{1+x^{2}}{2}\right) - 2\tan^{-1} x + \frac{\pi}{2}, & -1.574 < \zeta < 0 \end{cases}
$$
(9)

129
$$
\psi_{h}(\zeta) = \begin{cases} \psi_{h1}(\zeta_{h}) + \ln \frac{\zeta}{\zeta_{h}} - 0.8[(-\zeta)^{-1/3} - (-\zeta_{h})^{-1/3}], & \zeta \le -0.465 (= \zeta_{h}) \\ \psi_{h1}(\zeta) = 2 \ln \left(\frac{1 + x^{2}}{2} \right), & -0.465 < \zeta < 0 \end{cases}
$$
(10)

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

 Note that all the functions stated above have been newly installed 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 133 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 136 structure and different choices for psimhu_opt based on newly installed and default functional forms of φ_m and φ_h in the default and modified revised MM5 scheme are shown in Figure 1.

138 **2.3 Characteristics of default and newly installed similarity functions**

139 The expressions of φ_m and φ_h for different functional forms utilized in this study are stated in Appendix A. Figure S1 140 (supplementary material) shows the variation of different (a) φ_m and (b) φ_h under moderately to strongly unstable conditions. 141 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 142 moderately unstable conditions (up to $\zeta = -0.1$ approximately). However, at higher instabilities one can expect noticeable 143 differences between different functional forms of φ_m and φ_h . Note that the functional forms for φ_m corresponding to BD71 144 and CL73 decrease continuously on increasing instability; however, φ_m corresponding to KY90 functional forms show 145 decreasing behaviour in near-neutral to moderately unstable conditions and attain a minimum at $\zeta = -1.574$, and, as the 146 instability further increases, it starts increasing with $-\zeta$ (Figure S1a). This implies that φ_m based on class 4 functions shows 147 non-monotonic behaviour which contradicts the classical MOST prediction. On the other hand, in case of φ_b , all the functional 148 forms provide continuously decreasing behaviour of φ_h from near-neutral to moderately unstable conditions (Figure S1b).

149 Figure 2 illustrates the variation of default (F96) and newly installed integrated similarity functions $ψ_m$ and $ψ_h$ 150 (BD71, CL73, and KY90) with respect to $-\zeta$. One can see from Figure 2a that ψ_m corresponding to F96, BD71, and CL73 151 functional forms increases continuously with − in moderately to strongly unstable conditions. However, a non-monotonic 152 behaviour has been found for ψ_m corresponding to the KY90 functions implying it first increases with −ζ and reaches a 153 maximum at $\zeta = -1.574$ and then starts decreasing as instability further grows. On the other hand, ψ_h corresponding to all 154 the considered functional forms increases continuously in near-neutral to strong unstable conditions. However, the rate of 155 increase is slightly higher for F96 in comparison to the other three functions (BD71, CL73, and KY90), whose results are very 156 similar to each other (Fig. 2b).

157 **2.4 Observational data for model evaluation**

 For the evaluation of different simulations corresponding to newly installed similarity functions, 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) with an average elevation of 609 m above sea level in a tropical region. The site has a few buildings in between east and northwest; agriculture land in between northwest and west; and residential area, and dense trees in between southeast and east. The site also has a relatively flat area in between southeast and west which is free from any obstacle (Srivastava and Sharan, 2015). 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. We have utilized

- 169 hourly data for considered variables. Apart from this we have also utilized the ERA5-Land reanalysis dataset available at
- $170 \quad 0.10^{\circ} \times 0.10^{\circ}$ spatial resolution to evaluate the spatial distribution of the model simulated near surface atmospheric variables.
- 171 For consistency, we have regridded the model output to the same grid resolution of reanalysis/observed dataset.

172 **3 Numerical simulations**

173 To analyze the impacts of newly installed similarity functions together with the existing functional forms in the surface layer 174 scheme of WRFv4.2.2, the performance of the default and newly installed similarity functions is investigated in two steps. The 175 first one is independent of the WRF model. Namely, we apply Eqn. $(B8)$ (Appendix B) to iteratively determine C_D and C_H as 176 a function of ζ by prescribing the bulk Richardson number (Ri_B) and surface roughness parameters for momentum (z₀) and 177 heat (z_h) . The value of ζ is estimated by calculating the root of least magnitude of Eqn. (B8) for a given value of Ri_B. Once ζ 178 is calculated then utilizing it in Eqns. (B9) and (B10), the values of C_D and C_H can be estimated. We call this in the following 179 offline simulation. 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 180 carried out over three different surface types by considering surface roughness (z_0) to be 0.01 m (smooth surface), 0.1 m 181 (transition surface) and 1 m (rough surface) to analyze the impact of roughness of underlying surface on the simulation of ζ, 182 C_D and C_H .

 The second step is to apply all the parameterizations of the similarity functions in the WRF model version 4.2.2 over an Indian land site whose output is compared then with the observations 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 186 micrometeorological tower installed at Ranchi (23.412°N, 85.44°E), India (Figure 3). Domain d01 (6 \times 6 \times m²) consists of 233 187 east-west and 210 north-south grid points and domain d02 (2×2 km²) consists of 223 east-west and 196 north-south grid 188 points which covers 1398×1260 km² and 446×392 km² 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 $0.25^{\circ} \times 0.25^{\circ}$ 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.

Note that the revised MM5 surface layer scheme has lower limits on the values of $u_*(> 0.001 \text{ m s}^{-1})$ and $U(> 0.1 \text{ m s}^{-1})$ 196 $\,$ s⁻¹) that allow nocturnal values of u_{*} at night and control Ri_B values to be inordinately high, respectively (Jimenez et al., 2012). 197 However, the stability parameter ζ or R_{1B} is not restricted in the revised MM5 surface layer scheme, which gives complete 198 freedom to the WRF model to show its sensitivity to the tested similarity functions (Jimenez et al., 2012). Moreover, some of 199 the LES studies reported in the literature suggest that the friction velocity cannot be zero when the mean wind drops to zero,

i.e., there should be a minimum friction velocity that is proportional to the w∗ (Schumann, 1980). For this purpose, the existing 201 version of the revised MM5 scheme sets 0.001 m s⁻¹ as the minimum value of u_{*} based on the recommendations by Jimenez et al. (2012). Thus, to avoid the complexity that arises when mean wind drops to zero, the updated revised MM5 scheme 203 proposed in the present study also utilizes a minimum value of $u_* (> 0.001$ m s⁻¹) as suggested by Jimenez et al. (2012) in the 204 existing version of the revised MM5 scheme. Moreover, the scheme uses constant values of z_0 , while the values of z_h are 205 calculated from the expression suggested by Brutsaert (1982).

 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 the first 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. A brief description of the performance indicators for validation utilized in the present study is given in Appendix C.

4 Results

4.1 Offline simulations

216 To analyze the functional dependence of ζ , C_D and C_H on the utilized forms of similarity functions, the offline simulations independent of the WRF model have been conducted utilizing newly installed functions (BD71, CL73, and KY90) together with F96 functions existing in the default version of the surface layer scheme of the WRF model for three different roughness 219 lengths for momentum (z_0) , which are representative of smooth $(z_0 = 0.01 \text{ m})$, transition $(z_0 = 0.1 \text{ m})$, and rough $(z_0 = 1.0 \text{ m})$ surfaces. The results for ζ (Figure 4a, b, and c) with Ri_B, C_D (Figure 4d, e, and f) and C_H (Figure 4g, h, and i) with ζ across various surface types and sublayers have been analyzed. 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). Note 224 that the sublayers DNS ($-0.04 \le \zeta \le 0$) and DNS-DCS transition ($-0.12 \le \zeta < -0.04$) are corresponding to weakly to 225 moderately unstable conditions, while sublayers DCS (−1.20 ≤ ζ < −0.12), DCS-FCS (−2.0 ≤ ζ < −1.20), and FCS (ζ < −2.0) belong to moderately to strongly convective conditions (Srivastava and Sharan, 2015).

227 It is found that the simulated values of ζ at smaller values of Ri_B (i.e., in DNS to DCS) from different forms of 228 similarity functions are found to be almost identical to the F96 functional forms (Figure 4a-c). Moreover, results from the 229 BD71, CL73, and F96 functions are even similar at higher instabilities (i.e., the whole range of ζ values), while they differ

- 230 strongly from values obtained using the KY90 functions (Figure 4a-c). Notably, BD71, CL73, and F96 functional forms predict 231 relatively smaller absolute values of ζ for a given value of Ri_B. However, KY90 functions are found to produce a relatively 232 larger magnitude of ζ for a given value of Ri_B. This behaviour is found to be consistent for all ratios z/z_0 (Figures 4a-c) 233 representative of smooth, transition, and rough surfaces. A relatively larger magnitude of ζ for a given value of Ri_B and the 234 smaller values of ψ_m and ψ_b (Figure 2) in KY90 functional forms implies that the momentum and heat fluxes predicted using 235 KY90 functions will be smaller than those anticipated in BD71, CL73, and F96 functional forms.
- 236 Figure 4d-f shows the variation of C_p with ζ estimated using BD71, CL73, KY90, and F96 functional forms over 237 different surfaces. Notice that the C_D values calculated from BD71, CL73, and F96 forms of functions are relatively higher 238 than those produced by KY90 functional forms and continue to rise as instability progresses from DCS to FCS. It is important 239 to highlight that C_p estimated using KY90 functions shows a non-monotonic behaviour, which is consistent with the observed 240 behaviour of C_D over the Indian region reported in the literature (Srivastava and Sharan, 2019; 2021). Note that this non-241 monotonic behaviour is consistent for all three cases of different roughness lengths (Figure 4d-f).
- 242 On the other hand, across all three surfaces, one can see that the values of C_H estimated from all four functional forms 243 increase with increasing instability (Figure 4g-i), while the rate of increase of C_H in KY90 functions is relatively slower. 244 Moreover, BD71, CL73, and F96 functions predict almost similar values over all three types of surfaces. Noticeably, C_H 245 estimated using KY90 functions also exhibits non-monotonic behaviour with ζ over rough surfaces, which contradicts the 246 predictions of the other three functional forms. In addition, it is important to note that C_D and C_H predicted by KY90 functional 247 forms are found to bound by twice their near-neutral values, while the other functional forms predict continuously increasing 248 values of C_D and C_H on increasing instability.
- 249 Note that the error caused by different values of z_0 can be so large that the stability dependence of using different 250 forms of similarity functions is less important in the computation of C_p and C_H . As a result, three different values of z_0 have 251 been chosen, similar to a recent study by Srivastava and Sharan (2021), which are representative of smooth ($z_0 = 0.01$ m), 252 transition ($z_0 = 0.1$ m), and rough ($z_0 = 1.0$ m) surfaces to account for the impacts of using different z_0 on the estimation of 253 C_D and C_H from different functional forms of similarity functions in offline simulations.
- 254 Moreover, Figure 4 depicts the offline simulations with equal values of z_0 and z_h . While in the revised MM5 surface 255 layer scheme available in the WRF model, the values of z_0 and z_h are not the same. Thus, we have also attempted to discuss 256 the results from the offline simulations with different values of z_h , assuming $z_0 = 0.1$ m. Figure S2 (supplementary material) 257 shows the variation of ζ with Ri_B, C_D, and C_H with ζ calculated from the bulk flux algorithm using similarity functions 258 corresponding to BD71, CL73, KY90, and F96 with different values of z_h while z_0 is fixed. The values of z_h are taken such 259 that the ratio ln(z_0/z_h) assumes 0.1, 1, 2, 3, and 4. Figure S2 clearly shows that the estimated values of ζ are similar in near-260 neutral to moderately unstable conditions for all values of z_h ; however, relatively smaller values have been found as the ratio 261 $ln(z_0/z_0)$ increases for each form of similarity function. Since the computation of C_p does not involve the values of z_0 (Eqn. 262 B9), the estimated values of C_D for each form of similarity function are found to be approximately the same for different values

263 of z_b . However, in the case of C_H, differences are clearly visible if one uses different values of z_b . The estimated C_H using

264 various similarity functions behaves similarly for different values of z_h , while the magnitude decreases as the ratio $ln(z_0/z_h)$

265 increases.

266 Hence, it is evident that the BD71, CL73, and F96 functional forms predict values of ζ , C_D , and C_H that are almost 267 same over all the three different surface types. However, using KY90 functions compared to other commonly used φ_m and 268 φ _h, one can expect a significant reduction in the estimated values of transfer coefficients in moderately to strongly unstable 269 stratification.

270 **4.2 Results of the WRF model using different sets of integrated similarity functions**

 In this section, observational and reanalysis datasets have been used to analyze the simulations performed with WRFv4.2.2 272 utilizing newly installed and default φ_m and φ_h . The model simulated output has been extracted at the location of the 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 newly installed functions under free convective conditions, the mean 276 spatial patterns of considered variables averaged across strong convective conditions (hours in which ζ < −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.

279 **4.2.1 Evaluation against observations derived from flux tower installed at Ranchi (India)**

280 Figure 5 depicts the variation of (a) ζ with Ri_B, (b) C_p, and (c) C_H at the first model level with ζ from different experiments 281 (Exp1, Exp2, and Exp3) and CTRL simulation. Although the absolute values of the parameters differ from each other due to 282 the different prescribed roughnesses, the variation of ζ with Ri_B, C_D and C_H with ζ is very similar to the offline results. Note 283 that, at the moment, due to the inaccessibility of long-term data on detailed surface properties such as vegetation structure 284 needed to quantify the roughness length, we do not have an access to the precise values of z_0 and z_h at the Ranchi station. 285 Moreover, the values of z_0 and z_h do not directly involve in the estimation of C_p , C_H , and the surface fluxes from the 286 observational data, while they are important in computing these variables using the MOST framework. Thus, the default value 287 of z_0 is used in the revised MM5 surface layer scheme available in the WRF model, which is found to be approximately in the 288 range $0.1 - 0.2$ m at the Ranchi station. We wish to highlight that the z_0 used in the WRF model simulations at the Ranchi 289 station is nearly similar to the case of $z_0 = 0.1$ m presented in Figure 4, and the offline simulations also indicate that the 290 behaviour of the estimated C_D and C_H with ζ remains almost the same for different values of z_0 with slightly varying 291 magnitudes. Thus, one can interpret the results of C_D and C_H shown in Figures 4 and 5 from the offline simulations and the 292 WRF model, respectively, and can compare the WRF model simulated C_D with the observed one at the Ranchi station. 293 Although the model simulations and observed data may have a different z_0 , the comparison of model simulated variables with

294 the Ranchi data allows for an impression of the structural behaviour of model results as a function of stratification compared

295 with measurements.

296 It is clear from Figure 5 that the values of simulated variables are found to be almost identical in DNS to DCS 297 sublayers for all the experiments. Moreover, in FCS, the results obtained from Exp1, 2 and CTRL simulation are found to be 298 nearly similar however, relatively strong differences have been found in results from Exp 3 (Figure 5a, b, and c). Simulated ζ 299 for a given Ri*B* in Exp2 and CTRL simulation are similar and found to be relatively smaller in magnitude than Exp1 and Exp3 300 in FCS. However, the absolute values of ζ in Exp3 (KY90 functions) are relatively higher in FCS than in all other experiments. 301 Figure 5b shows the variation of simulated C_p with ζ from different experiments. Purple circles denote the variation 302 of observed C_D with ζ at the location of flux tower (Figure 5b). It is found that the observed C_D increases as the instability 303 increases from DNS to DCS and has the maximum value in the DCS (at $\zeta = -0.1$ approx.) and then starts to decrease as 304 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) 305 exhibits non-monotonic behaviour (Figure 5b), which is consistent with the observed behaviour of C_{D} (Srivastava and Sharan, 306 2015; 2021). The magnitude of C_p predicted in Exp3 is significantly smaller than that simulated from other experiments as 307 well as CTRL simulation, specifically in FCS. This may be due to the large differences between the KY90 functional forms of 308 ψ_m and ψ_h and other forms of functions. On the other hand, C_D simulated using ϕ_m and ϕ_h based on the first three classes

309 (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) show large disagreement 311 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. As a result, the study also highlighted the necessity of fine-tuning the original KY90 functional forms and evaluating their performance in the WRF model with additional observational datasets from various land sites and seasons.

 Note that 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 318 seasons.

319 Further, we would like to point out that currently no observational datasets are available which show a better 320 agreement with the KY90 functions over Indian land. However, it is desirable to further validate these functional forms over 321 Indian land once such observational datasets become available.

322 We wish to highlight that utilizing KY90 (Exp3) functions in the revised MM5 scheme of the WRF model makes it 323 consistent in predicting C_p with its observed non-monotonic behaviour over the Indian region.

324 The variation of simulated C_H with ζ from different experiments is shown in Figure 5c. C_H simulated from Exp1-3 as 325 well as CTRL simulation shows continuously increasing behaviour with ζ . The magnitude of simulated C $_H$ from CTRL

- 326 simulation and Exp1-2 is relatively higher than that of Exp3 in FCS beyond $\zeta < -10$ (approximately). It is also evident that 327 at higher instabilities, even C_H shows non-monotonic behaviour with ζ (Figure 5c). We wish to point out that a relatively larger 328 scatter has been found in the values of C_H than C_D. As the WRF model utilizes constant values for z_0 , while z_h is calculated 329 using expression suggested by Brutsaert (1982). The relatively large scatter in the values of C_H simulated from the WRF model 330 can be due to the parameterization of the ratio of momentum and scalar roughness lengths in the model.
- 331 Note that the transfer coefficients C_D and C_H shown in Figure 5 are at the reference height corresponding to the lowest 332 model grid level, which is ~12 m in the present study. However, we have also analyzed the behaviour of C_D and C_H at 10 m 333 height with ζ and found that they behave similarly to those presented in Figure 5.
- 334 The analysis presented here indicates that the KY90 functions in the revised MM5 surface layer scheme are found to 335 be appropriate in producing non-monotonic behaviour of C_D consistent with its observed nature. However, all other functional 336 forms of φ_m and φ_b produce C_D, which increases continuously with ζ from DNS to FCS.
- 337 To quantify the uncertainties involved in the simulated surface fluxes and certain near-surface variables using KY90 338 (Exp3) as well as other functional forms (Exp1-2 and CTRL simulation), model simulations have been compared against the 339 observations. Figure 6 compares the model-simulated (a) u_*^2 (m^2 s⁻²) (representative of momentum flux), (b) SHF (W m⁻²) 340 (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 341 from the flux tower at Ranchi (23.412N, 85.440E), India. The model output was extracted at a single grid point closest to the 342 flux tower to allow a consistent comparison. In Figure 7, a Taylor diagram is displayed along with the normalized standard 343 deviations and correlations of considered variables. Figure 8 shows the scatter plot between CC vs. RMSE for considered 344 variables simulated using different experiments. In case of u^2 , Exp1 and Exp2 are found to be comparable to the CTRL 345 simulation, while Exp3 considerably improved the simulation of u^2 (Figures 6a, 7 and 8). Exp3 reduced MAE (RMSE) from 346 0.09 (0.16) m² s⁻² to 0.08 (0.14) m² s⁻² (Table 2; Figures 7 and 8) and improved the CC (0.74) and IOA (0.84) for u_*^2 (Table 2). 347 A Q-Q plot is shown in Figure S3a (supplementary material) suggesting that Exp3 (KY90 functions) is found to be slightly 348 better than all other experiments and CTRL simulation for u^2 . For SHF, all the experiments are comparable to the CTRL 349 simulation; however, Exp3 shows less scatter than other experiments (Figure 6a).
- 350 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 1.20 (1.54) m s⁻² to 1.16 (1.47) m s⁻² and 352 MB up to 5 % (Figures 6c, and 7; Table 2). It considerably improved the CC (IOA) for U₁₀ from 0.66 (0.73) to 0.68 (0.75) 353 (Figure 7 and Table 2). A Q-Q plot (Figure S3b: supplementary material) reveals that Exp3 is found to be better than all other 354 experiments and CTRL simulation for U10. Thus, the KY90 functions in the surface layer scheme of the WRF model 355 considerably improve the model in simulating U_{10} (Figures. 6c, 7, 8, and S2b) at the location of the flux tower. Further, in case 356 of T_{2m} , Figures 7 and 8 exhibit that all the experiments are found to be comparable with the CTRL simulation.
- 357 Note that earlier studies, especially the ones done in the GABLS model intercomparison projects, have studied the 358 impacts of the similarity functions on the modelled profiles and fluxes (though mostly for stable conditions). However, they 359 learnt that applying different stability functions in the surface and boundary layer parameterizations may trigger unnatural

360 kinks in the model simulated wind speed and temperature profiles. Here, we have analyzed the profiles of U_{10} and T_{2m} simulated 361 from WRF model using different similarity functions in the surface layer scheme for the occurrence of unnatural kinks in their 362 values. One can see that the U₁₀ predicted from CTRL simulation, as well as different experiments corresponding to different 363 similarity functions at certain hours goes higher than that of its observed maximum value (approx. 8 m s^{-1}) (Figure S4: 364 supplementary material). These relatively higher magnitudes may be linked with some localised weather phenomenon 365 characterized by rapid changes in weather including strong wind, lightning and thunderstorms and are justifiable. However, 366 the simulated T_{2m} from different similarity functions are found to be in line with the observed values across the whole 367 simulation period (Figure S5: supplementary material). This suggests that the values of U_{10} and T_{2m} predicted from WRF 368 model are found to be in justifiable range and no unnatural kinks have been found.

369 **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. 372 Figure 9 depicts the mean spatial patterns of simulated ζ $\left(=\frac{z}{L}\right)$ (a1 – 4), C_D (c1-c4), and C_H (e1-4) from CTRL simulation 373 and other experiments, as well as their differences with respect to CTRL simulation. It is found that the absolute value of ζ simulated in Exp3 (KY90 functions) is relatively smaller than CTRL simulation (Figure 9b3) across the whole domain, which is consistent with Figure 5a, and offline simulations presented in Figure 4(a-c). This could be because the magnitude of KY90 376 functions (φ_m and φ_b) (Figure S1: supplementary material) is relatively smaller than the functions employed in default scheme (CTRL simulation).

378 On the other hand, Exp1 also provides slightly smaller absolute values of ζ (Figure 9b1), while Exp2 is almost 379 comparable to the CTRL simulation (Figure 9b2). Model simulated C_D is found to be relatively smaller in Exp3 than CTRL 380 simulation (Figure 9d3), while Exp1 and Exp2 provide comparable values of C_D to CTRL simulation (Figure 9d1-2). In the 381 case of CH, the simulated values from different experiments are comparable to the CTRL simulation over the whole study 382 domain (Figure 9f1-3). Note that simulated C_H is found to be comparable in all the experiments while one can see slight 383 differences in C_D in Exp3 than all other experiments which may be related to the fact that only φ_m functions are involved in 384 the computation of C_D (Eqn. 1), and the differences between φ_m corresponding to Exp3 are relatively more than φ_h , so are 385 the differences in C_D. The hatched regions in Figure 9 shows the differences between simulated variables from different 386 experiments with respect to CTRL simulation are statistically significant at 95% confidence level.

387 The slight differences in C_D in Exp3 reflected further in the simulated u_*^2 m² s⁻² (a measure of momentum flux) (Figure 388 10b3). A slight reduction has been found in simulated u² in Exp3 compared to the CTRL simulation over some parts of the 389 domain (Figure 10b3), while in Exp1 and Exp2 values are comparable with the CTRL simulation (Figure 10b1-2). In case of 390 SHF and LHF, the mean spatial distribution from all the experiments is found to be consistent with the ERA5-Land reanalysis

391 data, and the magnitude of differences between model simulation and ERA5-Land data is comparable for all the experiments

392 (Table S1: supplementary material).

393 For T_{2m} (upper panel of Figure 11), Ts (middle panel of Figure 11), and U_{10} (lower panel of Figure 11), mean spatial 394 distribution from different experiments and CTRL simulation agreed well with slightly varying magnitude to the ERA5-Land 395 reanalysis data. One can see a warm bias up to 2 K (3 K) for T_{2m} (Ts) simulated from different experiments and CTRL 396 simulation over most of the domain. For T_{2m} , bias, RMSE, and PCC between different experiments together with CTRL 397 simulation and ERA5-Land reanalysis data are found to be comparable (Table S1: supplementary material). However, Exp3 398 slightly improved the PCC from 0.50 to 0.51 for Ts (Table S1: supplementary material). Further, in the case of U_{10} , all the 399 simulations exhibit overprediction over the whole domain (lower panel of Figure 11: b1-4) and Exp3 is found to be slightly 400 better than all other experiments as well as CTRL simulation as it reduced bias% (RMSE) from 32.28 (0.54) m $s²$ to 32.06 401 (0.53) m s⁻² and improved the PCC from 0.89 to 0.91 (Table S1: supplementary material).

402 **4.2.3 Evaluation of newly installed functions during strong unstable conditions with respect to ERA5-Land reanalysis** 403 **data**

404 This section describes the impacts of utilizing different similarity functions (φ_m and φ_b) on simulated variables during highly 405 convective regime (i.e., $\zeta < -10$) with respect to the ERA5-Land reanalysis dataset. Since the functional forms of ψ_m and ψ_b are almost 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.

411 Figure S6 (Supplementary material) depicts the mean spatial distribution of ζ (a1-4), C_D (c1-4), and C_H (e1-4) as well 412 as their deviations from CTRL simulation. Notice that the magnitude of differences for all variables (ζ , C_D , and C_H) in this 413 case are found to be larger than the case of mean spatial patterns averaged during the whole daytime (section 6.2.2). It is 414 evident from Figure S6b3 (supplementary material) that Exp3 produce large absolute values of ζ and smaller values of C_p and 415 C_H (Figures S6b3, d3 and f3: supplementary material) than all other experiments and the CTRL simulation. While Exp1 and 416 Exp2 are found to be comparable to the CTRL simulation for both C_D and C_H (Figures S6d1-2 and f1-2).

417 The model simulations for T_{2m} and T_s do not capture the spatial patterns well in comparison to ERA5-Land data 418 (Figures S7a1-5 and S8a1-5: supplementary material). All experiments, as well as the CTRL simulation, exhibit overprediction 419 across the whole domain (Figures S7b1-4 and S8b1-4). We wish to highlight that the differences between various experiments 420 and CTRL simulation are seen up to 0.5 K for T_{2m} (Figure S7c1-3: supplementary material) as well as T_S (Figure S8c1-3) 421 which is slightly higher than the case of mean spatial patterns averaged over whole daytime (upper and middle panels of Figure 422 11). For T_{2m} , it is evident from Figure S7 (supplementary material) and Table 3 that Exp3 noticeably reduced the bias% 423 (RMSE) from 0.64 (2.13) K to 0.62 (2.10) K and improved the PCC from 0.43 to 0.46 (approximately 6%). In case of Ts as 424 well, Exp3 slightly improved the PCC and reduced the bias% (RMSE) from 1.25 (4.01) K to 1.24 (3.97) K (Table 3 and Figure 425 12).

 426 For U₁₀, the mean spatial patterns simulated using different experiments agreed well with the ERA5-Land reanalysis 427 data (Figure S9a1-5: supplementary material) and the magnitude of biases is found to be up to 1 m s⁻¹. Exp3 outperformed all 428 other experiments and the CTRL simulation by lowering the bias% from -4.96 to -0.28 m s⁻¹ and improved the PCC from 0.34 429 to 0.36 with comparable RMSE values (Figures S9 and 12; Table 3).

 The results presented so far suggest that the changes corresponding to different functional forms of similarity functions in the surface layer parameterization of the WRF model are more pronounced in convective conditions during daytime hours. For the number of grid points over the study domain that are being affected by the changed similarity functions, 433 no fixed pattern was found; however, the changes depend on the considered variable and similarity functions. Furthermore, we observe that the changes are more pronounced in grids that experience strong instability during the daytime.

435 **5 Summary and concluding remarks**

436 In the present study, the revised MM5 surface layer scheme of the WRFv4.2.2 model has been modified to incorporate φ_m 437 and φ_h suggested by Kader and Yaglom (1990) to make it consistent in producing the transfer coefficient for momentum (C_D) 438 in line with its observed behaviour. The revised MM5 scheme is modified in such a way that it contains all commonly used 439 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 440 scheme can be controlled by a flag (psimhu opt) that has been introduced in the physics section of the namelist file. The 441 impacts of utilizing different functional forms of φ_m and φ_h in the proposed scheme have been evaluated using offline 442 simulations (with bulk flux algorithm) as well as real-case simulations with WRFv4.2.2 model. The model-simulated surface 443 turbulent fluxes and certain near-surface variables have been compared with observational data from a flux tower at Ranchi 444 (23.412N, 85.440E; India), and the spatial patterns have been evaluated with the ERA5-Land reanalysis dataset.

445 Offline simulations indicate that at nearly neutral to moderately unstable conditions, ζ simulated using various 446 functional forms of φ_m and φ_h is comparable, and as the instability grows (free convective conditions), the differences 447 between different experiments become more pronounced. This might be connected to the corresponding variations between 448 different functional forms of similarity functions in the respective regimes. Similarly, for simulated C_D , $Exp3$ (KY90 functions) 449 demonstrates nonmonotonic behaviour with −ζ across all three surface types (representing smooth, transition, and rough 450 surfaces), which is consistent with its observed behaviour. However, all other experiments and CTRL simulation indicate 451 continuously increasing C_D with $-\zeta$ from near-neutral to free convective conditions over all three surface types, which is 452 inconsistent with its observed behaviour over the study domain. The non-monotonic behaviour of C_D in Exp3 (KY90 functions) 453 may be associated to the analogous non-monotonic behaviour of the corresponding ψ_m in the respective regime.

454 In real-case simulations, the model simulated ζ , C_D and C_H are found to be consistent with the offline simulations. 455 One can see that the variation of C_D in Exp3 (KY90 functions) with $-\zeta$ is nonmonotonic, as reported in offline simulations 456 and found to be consistent with its observed behaviour. This indicates that the KY90 functions in the surface layer scheme of 457 the WRF model make it compatible in producing C_D consistent with its observed behaviour over Indian land. As compared 458 with the observations over Ranchi (India), the simulations using KY90 (Exp3) functions are found to perform better for most 459 of the considered variables compared to all other experiments. Further, in the mean spatial distribution averaged during daytime 460 (04:00–12:00 UTC) over the entire simulation period, the significant increase in absolute value of ζ from Exp3 resulted in a 461 noticeable reduction in the values of C_D and C_H , which further impacted the simulated values of Ts, T_{2m} , and U_{10} . When 462 compared with the ERA5-Land reanalysis data, the spatial patterns for T_{2m} , T_s, and U_{10} from Exp3 (KY90 functions) provided 463 more consistent results. A reduction has been found in bias $\%$ and RMSE values for T_s, and U₁₀. Moreover, in case of highly 464 convective regime ($\zeta < -10$), Exp3 (KY90 functions) slightly improved the performance of the model by reducing the bias 465 (%) 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 467 found to be more appropriate for use in the WRF model as they can simulate C_D consistent with its observed behaviour and 468 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.

475 **Appendix A**

476 Here, the detailed description of commonly used functions (φ_m and φ_b) in numerical models under convective conditons is 477 provided.

478 Based on Businger (1966) and A. J. Dyer [1965, unpublished work; see Businger (1988) for details] the expressions 479 for φ_m and φ_h are as follows:

$$
480 \quad \varphi_m = (1 - \gamma_m \zeta)^{-\frac{1}{4}} \tag{A1}
$$

$$
481 \quad \varphi_h = Pr_t (1 - \gamma_h \zeta)^{-\frac{1}{2}} \tag{A2}
$$

482 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 483 $\gamma_m = \gamma_h = 16$ and $Pr_t = 1.0$. These functions commonly known as Businger-Dyer similarity (BD) functions and do not 484 satisfy the classical free convection limit (Srivastava et al. 2021).

485 The similarity functions proposed by Carl et al. (1973) under convective conditions are applicable for the range 486 −10 ≤ ζ ≤ 0. The expressions for φ_m and φ_h suggested by Carl et al. (1973) are:

$$
487 \quad \varphi_m = (1 - \beta_m \zeta)^{-\frac{1}{3}} \tag{A3}
$$

$$
488 \quad \varphi_h = (1 - \beta_h \zeta)^{-\frac{1}{3}} \tag{A4}
$$

489 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 490 example, Delage and Girard (1992) proposed $\beta_m = \beta_h = 40$, on the other hand, Fairall et al. (1996) suggested that $\beta_m = \beta_h =$ 491 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 494 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. The dynamic sublayer 498 corresponds to near-neutral conditions in which $\varphi_m = 1$ and $\varphi_h = Pr_t$. Further, in the dynamic convective sublayer, mechanical energy is in the x direction, while buoyancy-induced energy is in the z direction. Thus, in this sublayer, the functional forms for similarity functions, as determined by dimensional analysis, are

501
$$
\varphi_m(\zeta) = A_u(-\zeta)^{-\frac{1}{3}}
$$
 (A5)

502
$$
\varphi_h(\zeta) = A_T(-\zeta)^{-\frac{1}{3}}
$$
 (A6)

503 in which A_u and A_T are constants.

504 Moreover, in the free-convective sublayer, buoyancy dominates the mechanical production of energy, and the 505 pressure redistribution term feeds the buoyant energy in the vertical direction into the horizontal direction (Kader and Yaglom, 506 1990). Thus, in this case, the dimensional analysis suggests

507
$$
\varphi_m(\zeta) = B_u(-\zeta)^{\frac{1}{3}}
$$
 (A7)

508
$$
\varphi_h(\zeta) = B_T(-\zeta)^{-\frac{1}{3}}
$$
 (A8)

509 in which B_u and B_T are constants.

510 Thus, under unstable conditions, φ_m exhibits a nonmonotonic behaviour with respect to − ζ as the three sublayer 511 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 512 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 513 available based on the Kader and Yaglom (1990) three-sublayer model. However, the present study employs φ_m and φ_h based 514 on the expressions implemented in the surface layer scheme (CLM4.0) of NCAR-CAM5 (Zeng et al., 1998) model. The 515 expressions for φ_m and φ_h utilized in this study are as follows:

516
$$
\varphi_m = \begin{cases} (1 - 16\zeta)^{-\frac{1}{4}}, & -1.574 \le \zeta \le 0 \\ 0.7k^{\frac{2}{3}}(-\zeta)^{\frac{1}{3}}, & \zeta \le -1.574 \end{cases}
$$
(A9)

517 and

518
$$
\varphi_h = \begin{cases} (1 - 16\zeta)^{-\frac{1}{2}}, & -0.465 \le \zeta \le 0 \\ 0.9k^{\frac{4}{3}}(-\zeta)^{-\frac{1}{3}}, & \zeta \le -0.465 \end{cases}
$$
(A10)

519

520 Srivastava and Sharan (2021) classified these commonly used similarity functions stated above into four different classes based 521 on the exponents appearing in the expressions of φ_m and φ_h . The classification is as follows:

522

523 **Class 1.** This class consists of functions having the exponents of φ_m and φ_b as $-1/4$ and $-1/2$ (as in Eqns. A1 and A2), 524 respectively from near-neutral to strong unstable conditions. $φ_m$ and $φ_h$ proposed by Businger (1971) and Hogstrom (1996) 525 are the examples of class 1 functions.

526

527 **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 528 near-neutral to moderately unstable conditions (as in Eqns. A3 and A4), respectively are included. The functional forms 529 suggested by Carl et al. (1973) are the example of class 2 functions.

530

531 **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 532 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. 533 2003 are some examples of class 3 functions.

534

535 **Class 4.** Functional forms of φ_m and φ_h having the exponents as $-1/4$ and $-1/2$, respectively in near-neutral conditions 536 however, 1/3 for φ_m and $-1/3$ for φ_h in strong unstable conditions are classified in this class (as in Eqns. A9 and A10). The 537 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 538 functions in this class.

539 **Appendix B**

540 This section consists of a brief description of the computation of surface turbulent fluxes in the revised MM5 surface layer 541 scheme. In a homogeneous surface layer, the dimensionless wind and temperature gradients are defined as

$$
542 \quad \frac{kz}{u_*} \frac{\partial U}{\partial z} = \varphi_m(\zeta),\tag{B1}
$$

$$
543 \quad \frac{\text{K2 }00}{\theta_* \partial z} = \varphi_h(\zeta). \tag{B2}
$$

544 where L denotes the Obukhov length scale and U is the wind speed at height z ; k represents the von Karman constant and its 545 value is taken as 0.4. Integrating Eqns. $(B1)$ and $(B2)$ with respect to z leads to

$$
546 \quad \mathbf{U} = \frac{\mathbf{u} \cdot \mathbf{u}}{\mathbf{k}} \left[\ln \left(\frac{\mathbf{z}}{\mathbf{z}_0} \right) - \left\{ \psi_m(\zeta) - \psi_m\left(\frac{\mathbf{z}_0}{\mathbf{L}} \right) \right\} \right],\tag{B3}
$$

$$
547 \quad \left(\theta_a - \theta_g\right) = \frac{\theta_*}{k} \left[\ln\left(\frac{z}{z_h}\right) - \left\{\psi_h(\zeta) - \psi_h\left(\frac{z_h}{L}\right)\right\} \right] \tag{B4}
$$

548 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 549 heat are denoted by z_0 and z_h , respectively. The ground and surface air potential temperature are denoted by θ_g and θ_a , 550 respectively. $\zeta = \frac{z}{L}$ is the stability parameter and is defined as

$$
551 \quad \zeta = \frac{\text{kgz}}{\theta_a} \frac{\theta_*}{u_*^2} \tag{B5}
$$

552 ψ_m and ψ_h can be calculated from the following expression (e.g., Panofsky, 1963):

553
$$
\psi_{m}(\zeta) = \psi_{h}(\zeta) = \int_{0}^{\zeta} \frac{1 - \phi_{m,h,q}(\zeta')}{\zeta'} d\zeta'
$$
 (B6)

554 The bulk Richardson number (Ri_B) is given by:

555
$$
Ri_B = \frac{g}{\theta} \frac{(\theta_a - \theta_g)(z - z_0)^2}{U^2(z - z_h)}
$$
(B7)

556 Substituting the values of U and $(\theta_a - \theta_a)$ from Eqns. (B3) and (B4) in Eqn. (B7), one gets

$$
557 \quad Ri_B = \zeta \left[\frac{\left(1 - \frac{z_0}{z}\right)^2}{\left(1 - \frac{z_h}{z}\right)} \right] \left[\ln \left(\frac{z}{z_0}\right) - \left\{\psi_h(\zeta) - \psi_h\left(\zeta \frac{z_h}{z}\right)\right\} \right] \tag{B8}
$$

558 Note that Eqn. (B8) is a transcendental equation, and for a given value of Ri_B , the corresponding ζ value can be calculated 559 using any iterative method.

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

561
$$
C_D = k^2 \left[ln \left(\frac{z + z_0}{z_0} \right) - \left\{ \psi_m \left(\frac{z + z_0}{L} \right) - \psi_m \left(\frac{z_0}{L} \right) \right\} \right]^{-2}
$$
 (B9)

$$
562 \quad C_H = k^2 \left[\ln \left(\frac{z + z_0}{z_0} \right) - \left\{ \psi_m \left(\frac{z + z_0}{L} \right) - \psi_m \left(\frac{z_0}{L} \right) \right\} \right]^{-1} \left[\ln \left(\frac{z + z_h}{z_h} \right) - \left\{ \psi_h \left(\frac{z + z_h}{L} \right) - \psi_h \left(\frac{z_h}{L} \right) \right\} \right]^{-1} \tag{B10}
$$

563 Once we get C_D and C_H, then the momentum (τ), and sensible heat (H) fluxes are calculated using the following expressions:\n
$$
f(x) = \frac{1}{2} \int_{-\infty}^{\infty} f(x) \, dx
$$

$$
564 \quad \tau = \rho C_D U^2 \tag{B11}
$$

$$
565 \quad H = -\rho c_p C_H U (\theta_a - \theta_g), \tag{B12}
$$

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:

577
$$
MAE = \frac{\sum_{i=1}^{n} |p_i - o_i|}{n}
$$

2. Root mean square error:

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

3. Mean bias

$$
MB = \overline{(p_i - o_i)}
$$

4. Index of agreement

583
$$
IOA = 1 - \frac{\sum_{i=1}^{n} (o_i - p_i)^2}{\sum_{i=1}^{n} (|p_i - \bar{o}| + |o_i - \bar{o}|)^2}
$$

5. Correlation coefficient

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

586 in which p_i and σ_i represent the predicted and observed time series, respectively, while and \bar{p} and $\bar{\sigma}$ 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)
-

593 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.

 Author contribution: All authors contributed to the design of the study, analysis, and writing of the manuscript. PN carried out the computations as well as the analysis of the model output.

Competing interests: The authors have declared that they have no conflict of interest.

Acknowledgements:

 We would like to thank Dr. Manoj Kumar for providing observational data at Ranchi. The authors acknowledge the use of NCAR-NCL and ERA5-Land reanalysis dataset for this study. The use of supercomputing facility (HPC) provided by IIT Delhi is gratefully acknowledged. This work is partially supported by INSA, DST, DST-INSPIRE, and YES Foundation. We wish to thank the reviewers for their helpful comments and suggestions, which have significantly enhanced the quality of this paper.

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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.

 Figure 3: Spatial distribution of domain used for the simulations using the WRF model. The spatial resolution for domains d01 and 736 **d02 is 6** \times **6 km and 2** \times **2 km, respectively. The domain d02 covers 446** \times **392 km² area around the centre point.**

*T*39 **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 *740* (offline simulation) for different functional forms of ψ_m a 740 (offline simulation) for different functional forms of ψ_m and ψ_h corresponding to BD71, CL73, KY90, and F96 forms for smooth $z_0 = 0.01$ m; 1st column), transition $(z_0 = 0.1$ m; 2nd column), and rough $(z_0 =$ ($\mathbf{z}_0 = 0.01 \text{ m}$; 1st column), transition ($\mathbf{z}_0 = 0.1 \text{ m}$; 2^{nd} column), and rough ($\mathbf{z}_0 = 1.0 \text{ m}$; 3^{rd} column) surfaces. The background

($\mathbf{z}_0 = 742$ colour corresponds to different sublav colour corresponds to different sublayers in convective conditions (Kader and Yaglom 1990), from the dynamic sublayer ($0 \ge \zeta$) 743 -0.04 ; light grey) to the free convective sublayer ($\zeta < -2$; dark grey).

 $a)$ $\boldsymbol{0}$ 5 10 $\ddot{\mathbf{g}}_\text{B}$ 15 Δ 20 25 30 10^2 10^{-2} $10¹$ 10^{-1} $10⁰$ 10^{-3} $-\zeta$ $b)$ C 0.10 0.030 0.025 0.08 Exp3 0.020 Exp2 0.06 ပိ 0.015 ٸ Exp1 0.04 0.010 **CTR** \wedge 0.02 0.005 **AAM** 0.00 0.000 10^{-2} $10²$ $10¹$ 10^0 10^{-1} 10^{-3} $10²$ 10^{-1} 10^{-2} $10¹$ $10⁰$ 10^{-3} $-\zeta$ $\overline{\zeta}$

748 Figure 5: Variation of model simulated (a) ζ with \mathbf{R}_{B} , (b) \mathbf{C}_{D} and (c) \mathbf{C}_{H} with ζ from different experiments using different ψ_{m} and 749 ψ_{h} corresponding to F96 (749 **ψ**_h corresponding to F96 (CTRL), BD71 (Exp1), CL73 (Exp2), and KY90 (Exp3) under convective conditions. The red circles in (b) 750 denote the observed C_D with ζ at the location of flux tower. The mean val 750 denote the observed C_D with ζ at the location of flux tower. The mean values of observed C_D in each sublayer are shown with green 751 solid circles along with standard deviations in the form of error bars. D 751 **solid circles along with standard deviations in the form of error bars. Depending upon the data availability, two or three bins of** 752 **equal width are chosen in each sublayer. The background colour corresponds to different sublayers in convective conditions (Kader** 753 and Yaglom 1990), from the dynamic sublayer ($0 \ge \zeta > -0.04$; light grey) to the free convective sublayer ($\zeta < -2$; dark grey).

T60 Figure 7: Taylor diagram showing the correlation coefficient, normalized standard deviations for U₁₀, u², and T_{2m} from different

 \times Exp3

763 Figure 8: Scatter plot between correlation coefficient (CC) and root mean square error (RMSE) for (a) u², (b) SHF, (c) U₁₀, and (d)

764 **T2m simulated by various experiments (Exp1-3) together with CTRL simulation for pre-monsoon season (MAM; 2009) at the location** 765 of the flux tower (23.412^oN, 85.440^oE).

Figure 9: Mean spatial distribution of model simulated ζ **(1st row),** $C_{\rm D}$ **(3rd row) and** $C_{\rm H}$ **(5th row) from different experiments and 767 their differences with respect to CTRL simulation averaged during 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 ∗ **(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.

 Figure 11: In upper panel (A), mean spatial distribution of T2m 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 803 **simulation period. Middle (Lower) panel is same as the upper panel but for** $T_s(U_{10})$ **.**

Figure 12: Taylor diagram showing the correlation coefficient, normalized standard deviations for T_S (K), T_{2m} (**K**), and U₁₀ (m s⁻¹) 806 from different experiments together with CTRL simulation with respect to **from different experiments together with CTRL simulation with respect to ERA5-Land reanalysis dataset averaged during strong convective conditions (hours during daytime in which is smaller than** −**) for whole simulation period.**

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

Table 2: Comparison statistics for u_*^2 **(m² s⁻²), SHF (W m⁻²), U₁₀ (m s⁻¹), and T_{2m} (K) simulated using different experiments together**

842 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 co 843 **error (MAE), root mean square error (RMSE), mean bias (MB), index of agreement (IOA), and correlation coefficient (CC) are**

shown.

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Table 3: Comparison statistics for T_{2m} (K), T_S (K), and U_{10} (m s⁻¹) simulated using different experiments together with CTRL 856 simulation with respect to ERA5-Land reanalysis data averaged during strong unst

856 simulation with respect to ERA5-Land reanalysis data averaged during strong unstable stratification (hours during daytime in 857 which ζ is smaller than -10) for whole simulation period. The percent mean bias (Bias %) 857 **which is smaller than** −**) for whole simulation period. The percent mean bias (Bias %), pattern correlation coefficient (PCC),**

and root mean square error (RMSE) are shown.

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