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Title

From Deterministic to Machine Learning: A New Approach for Estimating the Atmospheric Turbulence

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Abstract

This study proposes a machine-learning (ML) replacement for the Holtslag–Boville (1993) turbulence parameterization in the BAM-1D model. An optimal multi-layer perceptron neural network was trained to reproduce eddy diffusivities and counter-gradient terms by using data from the GoAmazon experiment, achieving excellent agreement with the reference scheme, with correlations of 0.9996 for the momentum eddy diffusivity (kvm) and 0.9968 for the scalar eddy diffusivity (kvh). The ML-based turbulence driver preserved the dynamic behavior of temperature, wind components, and precipitation, showing no artificial signals or instability. Computational analysis based on 87,120 samples shows that the neural-network routine is only ~ 0.09 ms (≈ 3 — 4%) slower per call than the Holtslag–Boville scheme (2.51 ms vs. 2.42 ms), implying an expected impact below 2% on total runtime in a full BAM-3D configuration, the operational version for the National Institute for Space Research (INPE), Brazil. Overall, the results demonstrate that data-driven turbulence parameterizations can reproduce traditional closures with high accuracy and stability while remaining computationally competitive for atmospheric modeling.

Keywords: Atmospheric turbulence; parameterization by neural network; BAM-1D model.

1. Introduction

Numerical models simulate atmospheric dynamics by solving the Navier–Stokes equations (which govern fluid motion) while accounting for a wide range of physical processes (Kalnay, 2003). Many of these processes, including turbulence, cannot be explicitly resolved at model grid scales and must therefore be represented through parameterizations. Turbulence is a persistent and fundamental feature of atmospheric dynamics within the lowest part of the atmosphere, the Planetary Boundary Layer (PBL), where surface–atmosphere interactions dominate.

Turbulent mixing in the PBL is primarily driven by wind shear and thermal energy exchange with the surface. For instance, during nighttime, when the surface cools more rapidly than the overlying air, heat is transferred downward, reducing turbulent kinetic energy and establishing a stable atmospheric regime. The stability of the PBL can be diagnosed using the gradient Richardson number, which quantifies the competition between buoyancy and shear. Another widely used stability metric is the Monin–Obukhov length (LO), which represents the height at which shear production and buoyant production (or destruction) of turbulence are in balance. Negative values of LO indicate unstable conditions driven by surface heating, positive values indicate stable regimes typically associated with nighttime cooling, and large magnitudes correspond to near-neutral conditions.

In turbulent flows, the Reynolds hypothesis assumes that fluid properties can be decomposed into a mean component and a fluctuating component. Although the mean of the fluctuations tends to zero, the mean products of these fluctuations do not cancel, giving rise to the Reynolds stress tensor. These terms require parameterization and are central to most turbulence models used in atmospheric simulations, including those that employ stability functions based on Richardson number or Monin–Obukhov similarity theory.

A variety of parameterization approaches have been developed to represent turbulence, using different closure methods (Stull, 1988; Campos Velho, 2010). These approaches range from first-order schemes (e.g., Degrazia et al., 2000; Holtslag & Boville, 1993), which relate turbulent fluxes directly to mean gradients, to more complex higher-order closures (e.g., Mellor & Yamada, 1982), where higher-order turbulent fluxes are parameterized. Among these, the first-order scheme developed by Holtslag and Boville

(1993) is widely used, and it is one of the available schemes for turbulence parameterization in the operational turbulence for the Brazilian Global Atmospheric Model (BAM) (Figueroa et al., 2016), a three-dimensional model used by INPE for weather and climate prediction.

Despite their usefulness and long operational history, classical turbulence parameterizations have limitations, especially in regimes involving strong stability, rapid transitions, or nonlocal mixing (Stull, 1988; Holtslag & Boville, 1993; Mellor & Yamada, 1982). These challenges have motivated the development of hybrid or data-driven methods that exploit high-resolution simulations (e.g., LES, DNS) and advances in machine learning (ML). Neural networks offer the potential to approximate nonlinear relationships that traditional schemes struggle to represent, correct systematic biases, and provide improved estimates of turbulent fluxes and mixing coefficients.

In recent years, machine learning (ML) algorithms have been increasingly applied to atmospheric sciences, showing strong potential for capturing the evolution of complex and nonlinear boundary-layer processes when sufficiently large datasets are available (Schultz et al. 2021; Dueben and Bauer 2018). Extending these advances, several studies have explored ML approaches for representing turbulence within the PBL, including the prediction of turbulent fluxes, vertical diffusivity, and other key parameters such as PBL height (Pereira Neto et al., 2026; Stapleton et al., 2025).

Recent efforts have shown that machine-learning approaches can represent higher-order interactions between surface forcing, stratification, and vertical gradients that traditional first-order turbulence schemes struggle to capture (Rasp et al., 2018; Yuval et al., 2021; Wang et al., 2022; Canché-Cab et al., 2024). For example, studies evaluating neural networks, random forests, and gradient-boosted ensembles have shown that machine-learning algorithms can reproduce turbulent structures across stable and convective regimes, outperforming classical parameterizations in terms of bias and variance. These models also highlight the relevance of nontraditional predictors — such as soil temperature, radiative flux divergence, or near-surface moisture variability — suggesting that low-cost or sparse sensor networks may be sufficient to generate accurate PBL turbulence estimates in operational environments.

Together, these findings indicate that ML-based turbulence representations are capable not only of

approximating outputs from high-resolution simulations, but also of improving upon traditional parameterizations by reducing structural biases, capturing nonlocal mixing, and providing more realistic transitions between stability regimes.

In this context, this study proposes a machine learning–based approach for representing turbulence within the PBL. An optimal Multi-Layer Perceptron (MLP) neural network is trained to emulate and improve turbulent diffusivity and related quantities. Data from the GoAmazon experiment (Observations and Modeling of the **G**reen **O**cean **Amazon**) (Martin et al., 2016; Martin et al., 2017) were used for the learning process, MLP architecture configuration, and evaluations of the neural turbulence parameterization performance.

The methodology is evaluated through detailed comparison with the Holtslag and Boville (1993) parameterization, using vertical profiles, residual analysis, heatmaps, time series, and bias-correction procedures. Section 2 presents the machine-learning methodology, including the neural-network architecture and training strategy. Section 3 describes the BAM-1D model, and the software tools used for implementation. Section 4 discusses the results, and Section 5 provides the conclusions.

2. Machine Learning Scheme: Artificial Neural Network

ML is a specialized field within artificial intelligence and computer science that focuses on developing algorithms capable of making predictions, building non-linear regression models, and performing classification tasks based on reference datasets. Some well-established ML techniques include systems based on fuzzy logic (neuro-fuzzy), artificial neural networks, support vector machines, and decision trees (Mehryar et al. 2012). Numerous computer systems have been developed to apply these techniques across various applications. For this work, the free Gnu/Octave internet platform will be used for development.

2.1. Artificial Neural Networks

The artificial neural network (ANN) is a branch of machine learning that addresses the functioning of a computational structure made up of artificial nodes or neurons interconnected to form the network (Fig. 1b)

that is inspired by the functioning of the human brain. Artificial neurons (Fig. 1a) can recognize patterns from a data set, store values in memory, and improve their learning capacity through training (Haykin 2009).

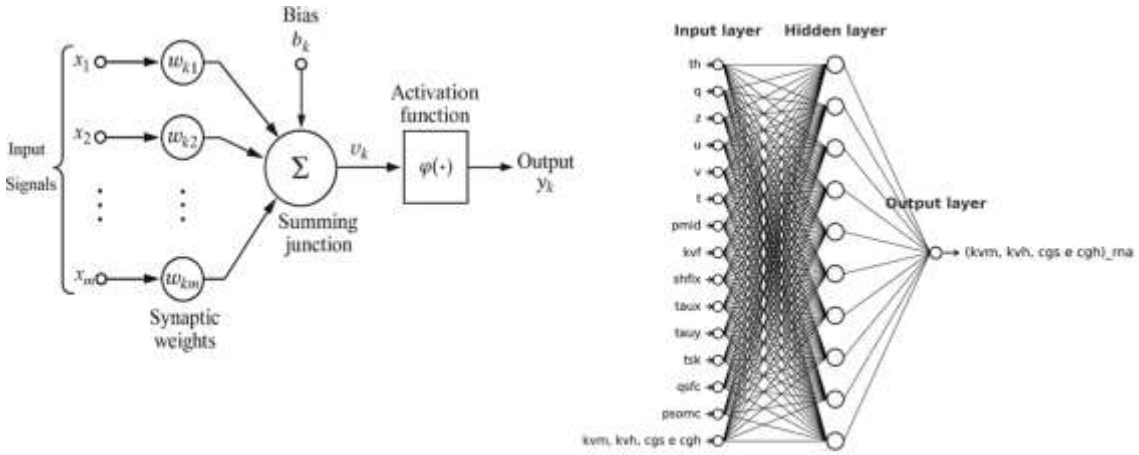


Figure 1 – Shown on the right is the layout of a general feed-forward artificial neural network with one hidden layer, comprised of 10 neurons. The design of a perceptron neuron is shown in more detail on the left (Source: Haykin 2009).

2.2. Multi-layered Perceptron (MLP)

The Multi-layer Perceptron (MLP) neural network (NN) was developed to solve non-linearly separable problems and has been applied to solve various complex problems (Haykin 2009). This is a supervised NN, with a training strategy using the error backpropagation algorithm based on the error correction learning rule (Haykin 2009). In this learning strategy, the input signals are propagated layer by layer until the output vector is obtained in the last layer. The learning process ends when the desired error is reached or when a maximum number of learning epochs is reached.

The architecture of a MLP network consists of the topological arrangement of the neuron processing units with the respective weight values associated with the connections. The synaptic weights are adjusted to bring the network's actual response closer to the desired response (Haykin 2009). The linear combination of the inputs added to a bias value is the argument of a non-linear function - the activation function, completing the processing of the artificial neural unit. In the MLP, the neural units are fully connected.

Figure 1 illustrates the architecture of the multilayer perceptron (MLP) neural network adopted in this study. The network consists of an input layer, a single intermediate (hidden) layer, and an output layer, with full connectivity between successive layers. This configuration corresponds to the neural structure effectively employed in the experiments and in the implementation of the machine-learning-based turbulence parameterization.

2.3. Learning Process

The main property of an artificial neural network (ANN) is its ability to learn from examples. The ability to acquire knowledge is one of the essential qualities of these structures, and the learning process is interactive and consists of adjustments to be applied to their synaptic weights and biases (Haykin 2009).

The learning process can be defined as a set of well-defined rules for determining the strength of the connections between neurons and producing the solution to a given problem. Various methods for training neural networks have been developed and can be grouped into supervised, semi-supervised, reinforcement, and unsupervised learning (Haykin 2009; França et al. 2023 — see Chapter 01). The supervised scheme is the most common learning method for training neural networks. An external supervisor (reference database) provides the desired reference. The aim is to adjust the network parameters to find a balanced link between the input and output pairs provided. The ANN has calculated and compared its output with the desired reference, providing information on the error of the current ANN output. The connection weights are adjusted to minimize the difference between the reference and the network estimation. The delta rule, or error correction, is the most famous example of supervised learning algorithms. The learning algorithm for the multi-layer network is the delta rule with error backpropagation (Widrow 1962).

3. Material and Method

3.1. Study Area

In the Amazon, measurements from the GoAmazon campaign were collected at Fazenda Exata, Manacapuru (AM), Brazil — approximately 66 km from Manaus — at site T3 (03°12′36″ S; 60°36′00″ W;

altitude 60 m), as shown in Figure 3. This site was the main data collection point for the GoAmazon 2014/15 "IOP" experiments (Martin et al., 2016).

The central Amazon region, where the experiment was conducted, is characterized by a humid tropical climate with high temperatures, abundant rainfall (≈ 2,300 mm year^{-1}), and a small annual temperature amplitude (~ 2.1 °C). The mean annual temperature is 26.7 °C, The central Amazon with average daily maxim of 31,2 °C and minimum of 23.7 °C (Fisch et al., 1998). The climate is strongly influenced by intense solar radiation and the large availability of moisture from forests, rivers, and lakes.

Rainfall in central Amazonia exhibits a pronounced seasonal cycle, with a minimum of approximately 50 mm in August and a maximum of about 330 mm in March. The wet season extends from September to June, characterized by relative humidity around 90 – 92% and a thermodynamic environment that is unstable and favorable to moist convection (Martin et al., 2016). In contrast, the dry season, from June to September, is marked by large-scale subsidence over the basin, reduced humidity (~ 75%), and suppressed deep convection, although isolated cumulonimbus clouds can still develop (Marengo et al. 2001; Zhuang et al. 2017).

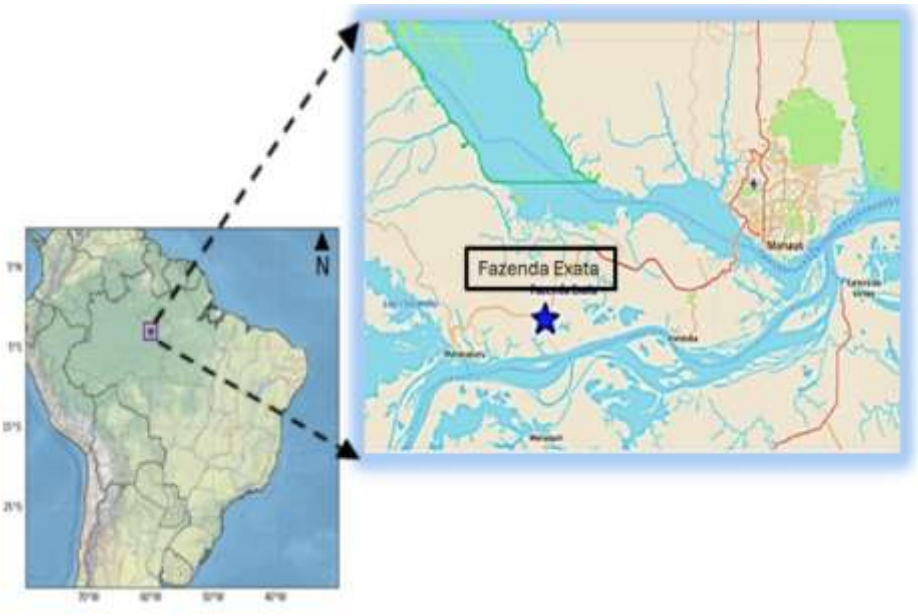


Figure 2 - Map of the location of the Exata farm (Municipality of Manacapuru-AM.

3.2. Model BAM-1D

The numerical experiments were carried out with the one-dimensional version of the Brazilian Global Atmospheric Model (BAM-1D). The model is derived from the BAM model (Figueiroa et al. 2016). BAM-1D model is a single column model, representing the vertical structure of the atmosphere at a given horizontal coordinate. The initial and boundary conditions can be provided from field experiments or global or regional model outputs. For the simulations here, data from GoAmazon project was used. Data from the ARM (Atmospheric Radiation Measurement) program (see: https://www.arm.gov/research/campaigns) were obtained from the National Institute for Space Research (INPE), Brazil.

The Atmospheric Radiation Measurement (ARM) program, funded by the U.S. Department of Energy, operates long-term and campaign-based sites that provide comprehensive atmospheric datasets. This program uses continuous measurements from the Southern Great Plains (SGP) site in Oklahoma, along with data from two field campaigns: GoAmazon in the Amazon rainforest (Manacapuru, Brazil) and CACTI in the Sierras de Córdoba, Argentina. Observations include thermodynamic profiles from radiosondes, active remote sensing of clouds (Clothiaux et al. 2000), *in-situ* surface meteorology, and surface energy fluxes from site-specific products (Tang et al. 2019).

The initial conditions for BAM-1D include temperature profiles (ºC), specific humidity (kg/kg), and the zonal and meridional wind components (m/s). The forcing data consists of trend profiles for temperature (ºC/s), humidity (1/s), vertical velocity (cb/s), and zonal and meridional wind components (m/s). Five parameterizations were chosen to represent the physical processes (Table 1).

Table 1. Parameterisations from BAM-1D were used in the study.

Physical Process	Reference
Surface process	Mellor Yamada 2.0 (1982)
Planetary boundary layer	Holtslag Boville (1993)
Deep convection	Grell & Deveny (2016)
Shallow convection	Tiedke (1983)
Long and shortwave radiation	RRTMG; Iacomo et al. (2008)

We employ standard parameterizations for the key physical processes. Surface turbulent fluxes follow the

Mellor–Yamada level 2.0 scheme (1982), with Monin–Obukhov similarity linking near-surface gradients to fluxes. The PBL is represented by the Holtslag & Boville (1993) scheme, a first order (K-theory) closure with a nonlocal counter-gradient heat flux in convective conditions, stability-dependent eddy diffusivities for momentum and heat, a PBLH diagnosed with a bulk Richardson criterion, background free-tropospheric diffusion, and a reduction to local diffusion under stable stratification. This PBL scheme is our reference paradigm in all comparisons. Deep convection follows the Grell & Dévényi (2016) ensemble cumulus approach, shallow convection uses the Tiedtke (1983) mass-flux scheme, and longwave/shortwave radiation is treated with RRTMG (Iacono et al. 2008; correlated-k).

3.3. MLP-NN for the GNU/Octave

GNU/Octave is a computational platform with its own interpreted programming language, where the artificial neural network (ANN) used in this study was implemented. Although the original MLP code was developed as part of the MPCA package (Luz et al., 2008; Anochi and Campos Velho 2014; Anochi et al. 2019), the MPCA meta-heuristic itself was not employed here. Instead, only the standalone MLP module included in the package was used. The hyperparameters adopted in this study are part of the proposed methodology, and they were defined during an exploratory phase carried out entirely in GNU/Octave. Several combinations of learning rate, momentum coefficient, number of neurons, activation functions, and stopping criteria (maximum number of epochs) were evaluated. The detailed results of these tuning experiments are not shown, as they fall outside the central scope of this paper.

The MLP-NN Fortran code was migrated to GNU/Octave, and a dedicated preprocessing script was developed to assemble and prepare the dataset before training. First, all atmospheric records from 2014 and 2015 were merged into a single continuous dataset. The last two days of each month were then removed and reserved as an independent testing subset, ensuring that the evaluation captured different seasonal and stability regimes. The remaining data were normalized to the [0, 1] interval using min–max scaling, followed by a controlled data-augmentation procedure applied to all input variables. This augmentation generated $N_AUG = 5$ synthetic realizations per profile using stochastic perturbations of amplitude $NOISE_FRAC = 0.02$, produced reproducibly with $BASE_SEED = 42$.

After normalization and augmentation, the dataset (excluding the monthly test days) was split into training and generalization subsets. The final neural-network weights for each predicted turbulence variable (kvm, kvh, cgh, and cgs) were obtained entirely within the GNU/Octave environment, where the MLP was trained using the prepared inputs and the hyperparameters defined during the exploratory phase.

Table 2 – Variables used as inputs for training the neural network and their equivalents in the HB parameterization scheme

Name variables	BAM	Name variables	BAM
Potential Temperature	th	Surface u stress	taux
Height above surface	z	Surface y stress	tauy
Windspeed x-direction	u	Surface Temperature	tsk
Windspeed y-direction	v	Surface Humidity	qsfc
Temperature (t - used for density)	t	Pressure	psomc
Midpoint pressures	pmid	Free atmospheric eddy diffusivity	kvf
Surface heat flux	shflx	Boundary-Layer height	pblh

During training, the backpropagation phase adjusts the connection weights of the multilayer perceptron neural network (MLP-NN). This phase also plays an essential role in defining the most adequate network topology. The hyperparameters to be determined include the number of hidden layers, the number of neurons in each layer, the activation function, the learning rate, the momentum term, and the maximum number of iterations (epochs).

The adopted MLP-NN architecture consisted of a single hidden layer with ten neurons. Before defining the final configuration, extensive preliminary experiments were performed for each target variable to evaluate different network topologies and hyperparameter combinations. Although the complete details of this tuning process are not presented here, these experiments guided the selection of balanced and computationally efficient architecture. Data from 2014 were used for training, and data from 2015 were reserved for testing.

Table 3 – Variables used as outputs for training the neural network and their equivalents in the HB parameterization scheme

Name variables	BAM
Eddy diffusivity for momentum	kvm
Eddy diffusivity for heat	kvh
Counter-gradient term for heat	cgh
Counter-gradient star	cgs

4. Results and Discussion

The BAM-1D model implements a non-local turbulence parameterization scheme (first-order closure with a counter-gradient term) to compute the turbulent fluxes of temperature, humidity, and momentum within the PBL, following Holtslag and Moeng (1991). This scheme is expressed as:

$$\overline{w'\chi'} = K_\chi \left(\frac{\partial \chi}{\partial z} - \Upsilon_\chi\right) \quad (1)$$

where $K\chi$ represents the eddy diffusivity for the scalar or vector component χ (specific humidity: q, potential temperature: θ, zonal or meridional wind (u,v), $\partial\chi/\partial z$ is the local vertical gradient, and γ_χ represents the non-local (*counter-gradient*) transport term related to dry convection. This term γ_χ is traditionally referred to as the *counter-gradient term* in the context of a scalar quantity flux (Troen and Mahrt, 1986; Holtslag and Boville, 1993).

$$K_\chi = \left[\kappa w_t z \left(1 - \frac{z}{h}\right)^2\right] \quad (2)$$

where z is the height over the surface, w_t represents a characteristic turbulent velocity scale, h is the height of the PBL (HPBL), and $\kappa \approx 0.4$ is the von Kármán constant. Both are applied in the formulation of turbulent diffusivity for heat, water vapor, and passive scalars. The turbulent momentum diffusivity, K_m, is defined analogously, but with w_t replaced by the momentum-specific scale w_m.

The local counter-gradient transport term γ_χ, as expressed in Equation 1, accounts for the non-local influences on turbulent mixing. Under stable atmospheric conditions, this term is typically negligible due to the suppression of large eddies. However, under unstable conditions — characterized by vigorous convective activity, most of the heat and moisture transport is carried out by large turbulent eddies that span the full depth of the boundary layer. In such cases, the counter-gradient term Y_χ is represented by the following formulation:

$$\gamma_\chi = a\frac{w_*(\overline{w'\chi'})_0}{w_m^2 h}, \tag{3}$$

where a = 7.2 and $(\overline{w'\chi'})_0$ is the kinematic flux of the scalar being transported, and w_* is the convective velocity scale. To apply this scheme, it is necessary to estimate the PBL height. In the original BAM-1D model, the height h is determined iteratively using the bulk Richardson number formulation (Troen and Mahrt, 1986):

$$h - z_1 = \frac{Ri_{cr}[(u_h-u_1)^2+(v_h-v_1)^2]}{(g/\theta_{v_h})(\theta_{v_h}-\theta_s)} \tag{4}$$

where z_1 is the height of the first model level, u_1 and v_1 are wind components at the surface, u_h and v_h at height h, θ_s is surface air temperature, θ_{vh} is virtual temperature at height h, and Ri_{cr} = 0.19 is the critical Richardson number (Beare et al., 2006). Once the Richardson number exceeds Ri_{cr}, linear interpolation between levels determines the precise height.

4.1. Sample Profiles and Diffusivity Replacement

Figure 3 summarizes the comparison between the Holtslag–Boville (HB) parameterization and the MLP-NN representation for all turbulence-related variables (kvm, kvh, cgs, cgh) using independent validation days. A statistical evaluation was performed for vertical model levels $k \geq 7$, where $k$denotes the index of the discrete vertical levels of the BAM-1D model, counted from the surface upward. This range corresponds to the dynamically active portion of the planetary boundary layer (PBL) and the lower troposphere.

The results indicate that the neural network reproduces HB behavior with remarkable fidelity for the eddy diffusivity coefficients:

- kvm: extremely high correlation (CC = 0.9996), negligible bias (−0.088), and low RMSE (0.558), indicating that the ANN captures the vertical structure and magnitude of momentum diffusivity with almost perfect agreement.
- kvh: similarly strong performance (CC = 0.9968) and RMSE = 4.80, fully consistent with the expected variability of thermal diffusivity in the BAM-1D environment.
- cgs and cgh: despite lower correlations (0.846 and 0.809), the absolute errors remain very small (MAE of 0.022 for cgs and $2.7 \times 10^{-4}$for cgh), reflecting the extremely small physical magnitude of these counter-gradient terms. Because HB frequently produces values close to zero for these variables, MAPE (Mean Absolute Percentage Error) becomes mathematically undefined and is therefore not a suitable diagnostic metric.

Figures 3a–3d illustrate representative vertical profiles under distinct atmospheric stability regimes sampled on independent days:

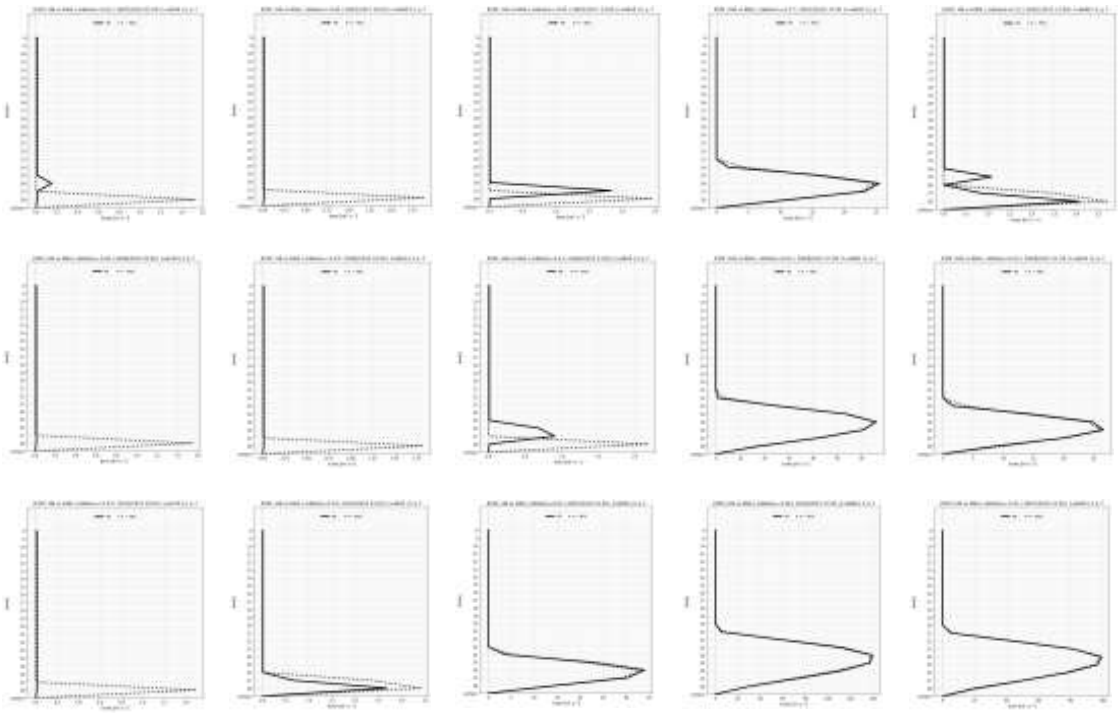
- Convective conditions (unstable PBL, daytime), typically represented by the late-afternoon profiles (e.g., February and October cases).
- In these regimes, the MLP-NN exhibits its best performance, accurately reproducing the deep mixed-layer structure, large values of kvm and kvh, and the presence of non-local transport expressed by non-zero counter-gradient terms (cgs and cgh).
- The agreement with HB is nearly exact throughout the convective layer, indicating that the neural network successfully learns the dominant turbulent mixing associated with buoyancy-driven convection.
- Neutral to weakly stable conditions (transition periods) : commonly observed during morning or evening transitions:
- The ANN maintains excellent agreement for kvm and kvh, correctly representing the gradual reduction of diffusivity with height. Minor deviations appear near the PBL top, where sharp vertical gradients occur, but these differences remain small and do not affect the overall structure

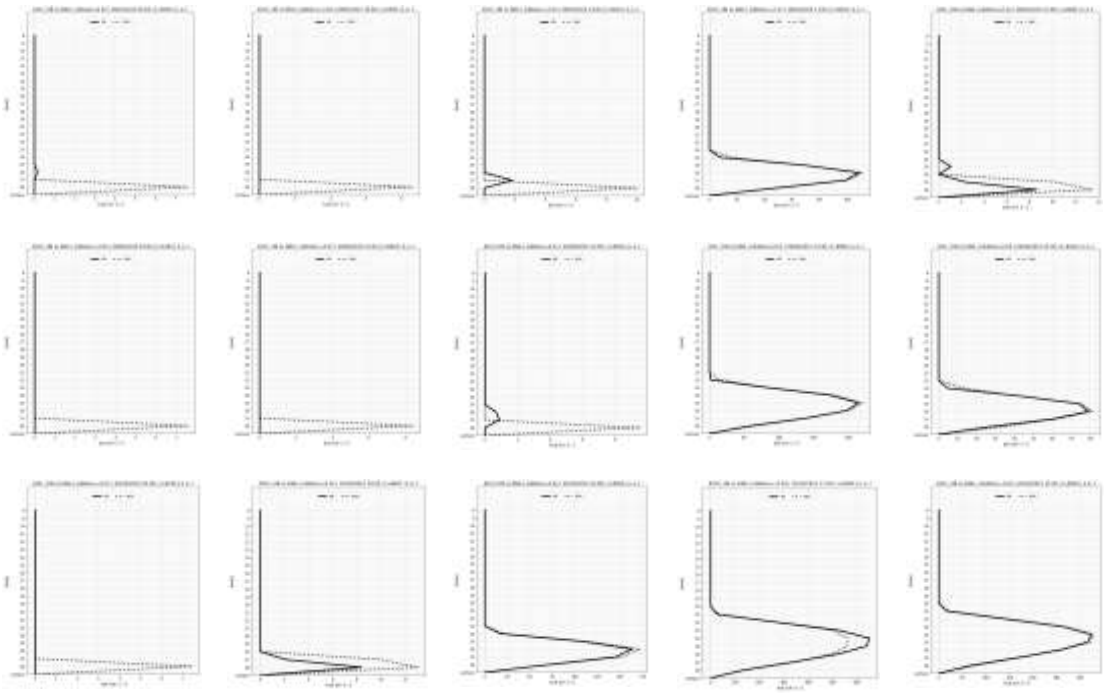
of the turbulence profiles.

- Stable conditions (nocturnal boundary layer), typically represented by wintertime or nighttime profiles (e.g., June case): The largest relative discrepancies are observed under stable stratification, particularly near the surface and close to the PBL top. In these situations, diffusivities are small and highly sensitive to local stability, which amplifies relative errors despite the small absolute magnitudes. Even so, the ANN preserves the correct order of magnitude and vertical decay of kvm and kvh, while deviations in cgs and cgh remain physically negligible.

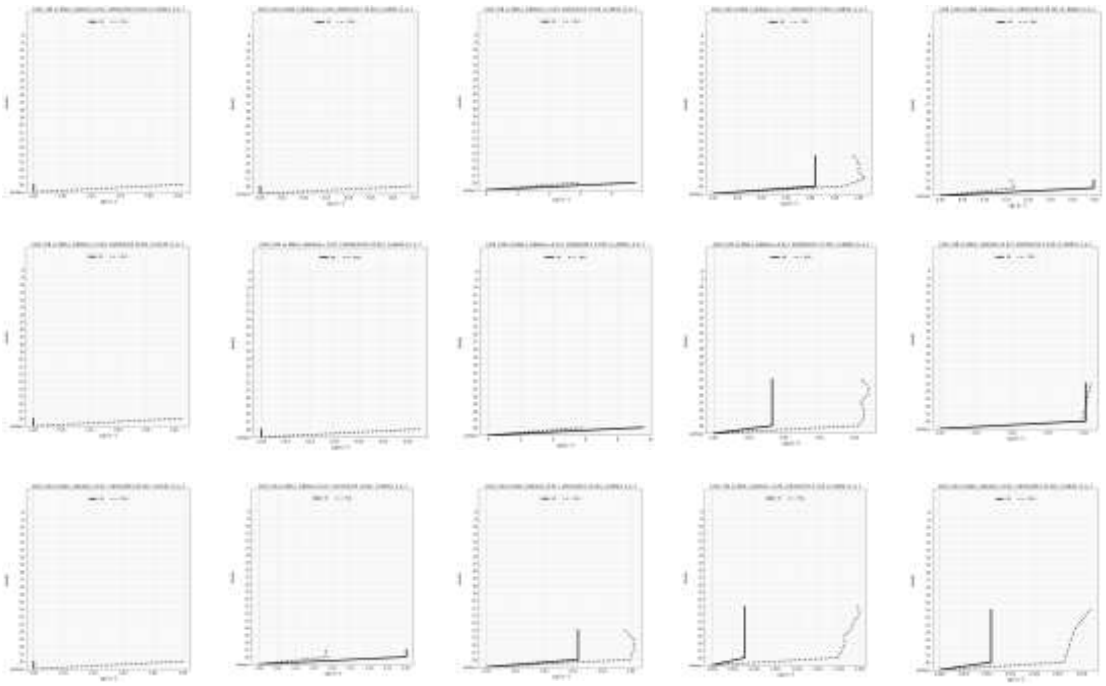
Overall, the largest errors occur under strongly stable conditions, where turbulence is intermittent and weak, while the best agreement is achieved under convective and near-neutral regimes, which dominate the energetically active portion of the PBL.

Taken together, these results confirm that the MLP-NN faithfully reproduces the behavior of the reference turbulence scheme across a wide range of stability conditions, accurately capturing both the magnitude and vertical gradients of all turbulence-related fields. The ANN-based turbulence driver is therefore physically consistent and appropriate to replace the original HB routine within BAM-1D.

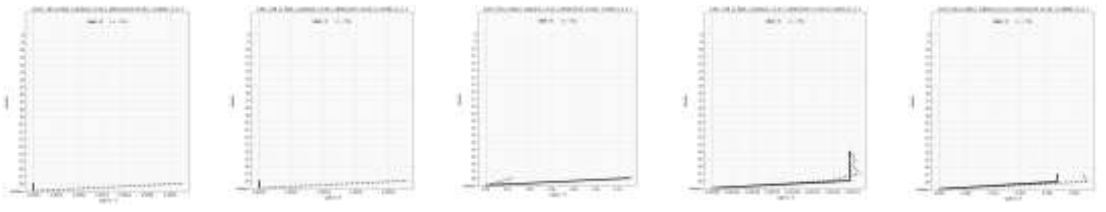




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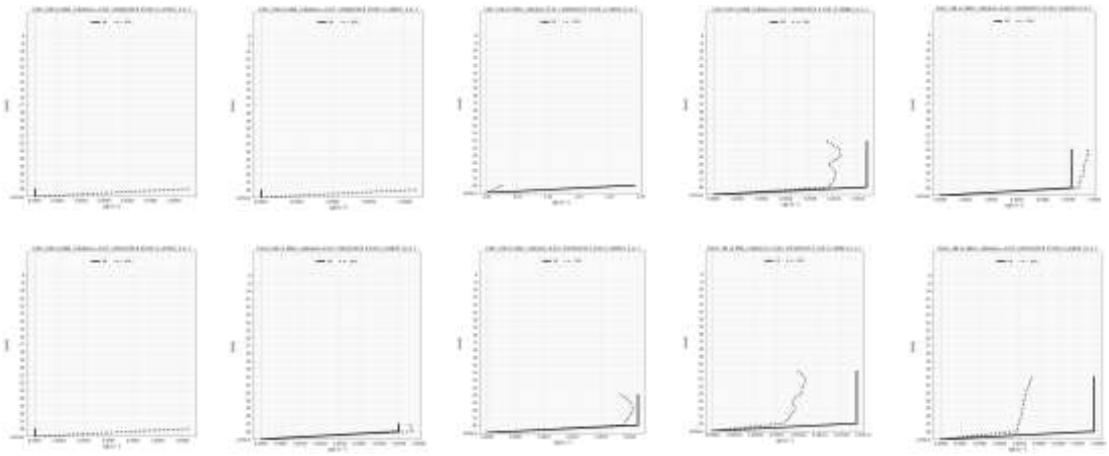


Figure 3 – Vertical profile comparisons between the HB scheme and the MLP-NN using independent validation days (28 February, 29 June, and 29 October): (a) eddy diffusivity for momentum (kvm), (b) eddy diffusivity for heat (kvh), (c) counter-gradient term for heat (cgh), and (d) counter-gradient term for moisture (cgs).

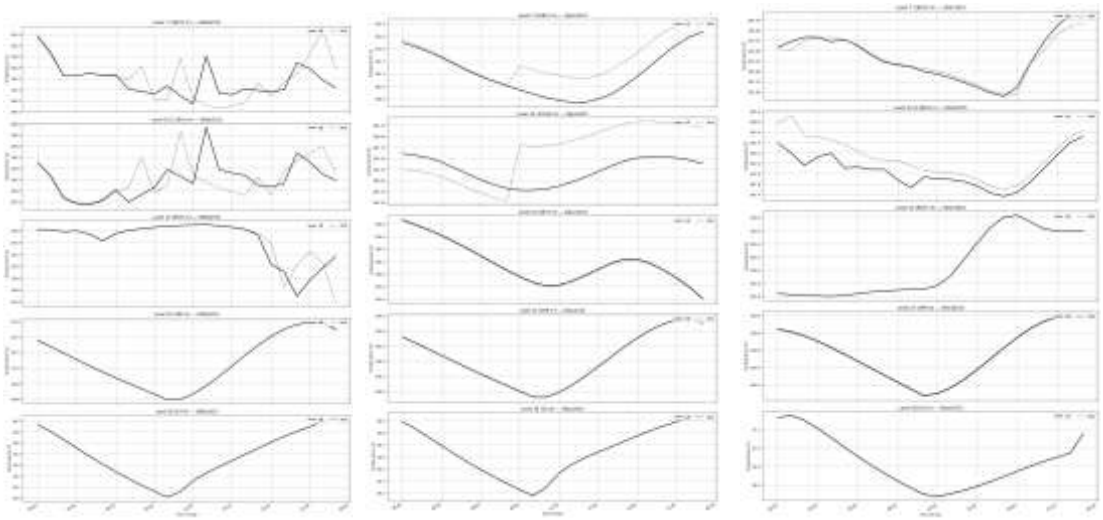
4.2. Evaluation of Temperature, Wind, and Precipitation Forecasts

The excellent agreement obtained for the turbulence variables directly translates into high-quality forecasts of temperature and wind. Figures 4a–c illustrates the vertical profiles of temperature, zonal wind, and meridional wind for the validation days (28 February, 29 June, and 29 October), showing that the MLP-NN preserves all key dynamical and thermodynamical features produced by the HB scheme.

- The extremely high correlations found for kvm (0.9996) and kvh (0.9968) explain the close match between the two schemes:
- During nighttime (02 UTC), the ANN maintains stable stratification generated by HB.
- Around 10–13 UTC, the warming and deepening of the convective boundary layer are accurately captured.
- The turning of the wind with height and regions of enhanced shear are reproduced without distortions or phase shifts.
- No spurious oscillations or artificial vertical discontinuities appear in any of the variables.

These results demonstrate that the learned turbulent mixing remains dynamically compatible with the model

and that the ANN-based scheme can sustain the realistic diurnal cycle of momentum and temperature transport.



(a) (b) (c)

Figure 4 – a) Vertical profiles of temperature (T), (b) zonal wind (u), and (c) meridional wind (v) simulated by BAM-1D using the original Holtslag–Boville (HB) parameterization and the neural-network scheme (MLP-NN) for three independent validation days: (a) 28 February 2015, (b) 30 June 2015, and (c) 29 October 2015.

4.2.1 Precipitation Response

Although BAM-1D with RNA is not a full microphysics model, the precipitation time series provides a sensitive indirect metric of changes in vertical transport. The comparison between the HB and MLP-NN schemes for the independent validation days is presented in Figure 5, which contains the precipitation forecasts for (a) 28 February, (b) 30 June, and (c) 29 November 2015.

Across the three panels in Figure 5: The neural-network precipitation closely follows the HB time series, with both schemes exhibiting nearly identical temporal variability.

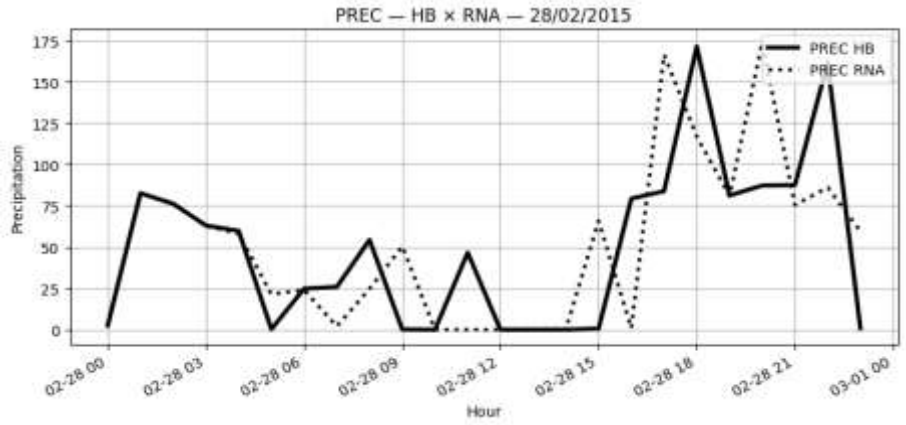
- Peaks and timing are well captured, for example, the strong late-evening peak around 21 UTC on 28 February (Fig. 5a).
- Although small differences in magnitude appear at isolated hours, the overall precipitation pattern

remains consistent.

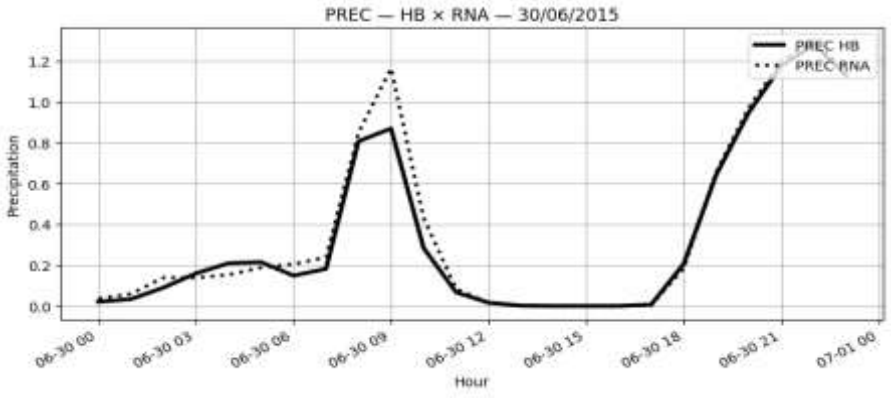
- On 29 November (Fig. 5c), even under extremely low precipitation values ($\sim 10^{-7}$), the ANN successfully reproduces the correct onset and decay timing.

Together, these results indicate that:

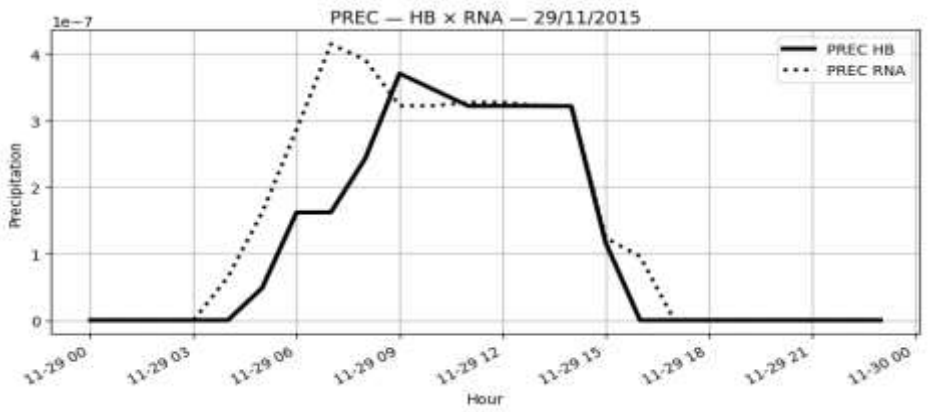
- The ANN-driven turbulent fluxes preserve the large-scale thermodynamic structure required for precipitation formation.
- No significant drift, instability, or artificial triggering of convection is introduced by the neural-network turbulence scheme.



(a)



(b)



(c)

Figure 5 - Precipitation time series simulated by BAM-1D using the original Holtslag–Boville (HB) parameterization and the neural-network turbulence scheme (MLP-NN) for the independent validation days: (a) 28 February 2015, (b) 30 June 2015, and (c) 29 November 2015.

Thus, the precipitation diagnostics presented in Figure 5 strongly support the suitability of the ANN-based turbulence driver as a robust, drop-in replacement for the Holtslag–Boville parameterization.

Vertical profiles of temperature (T), (b) zonal wind (u), and (c) meridional wind (v) simulated by BAM-1D using the original Holtslag–Boville (HB) parameterization and the neural-network scheme (MLP-NN) for three independent validation days: (a) 28 February 2015, (b) 30 June 2015, and (c) 29 October 2015.

The MLP-NN reproduces the timing and magnitude of precipitation events with high fidelity, including the evening peak observed on 28 February and the very low precipitation regime on 29 November ($\sim 10^{-7}$). Across all cases, the ANN maintains the temporal variability produced by the HB scheme, indicating that the learned turbulence representation does not introduce spurious triggering or suppression of convective processes.

4.4 – Computacional performance

Beyond accuracy, the computational cost of the neural-network scheme was evaluated in detail. Timing diagnostics were collected for the turbulence routines over the full 2015 simulation, yielding 87.120 individual samples for each configuration (Holtslag–Boville and MLP-NN). For each call to the turbulence driver, the mean wall-clock time was approximately 2.42 ms for the traditional Holtslag–Boville (pbldif) scheme and 2.51 ms for the MLP-NN implementation. The dispersion was similar in both cases (standard deviation of about 0.78 ms), and the 5 - 95% range remained within 1.5 - 4.0 ms for both methods.

The resulting difference in average cost per call is on the order of 10^{-4} s (≈ 0.09 ms), corresponding to a relative change below 5%. In other words, at the subroutine level, the neural-network turbulence scheme is computationally competitive with the original Holtslag–Boville parameterization, and the small difference falls well within the expected variability of runtime measurements. This indicates that replacing the deterministic closure with the MLP-NN does not introduce a significant computational penalty in the 1D prototype.

It is important to note that these results were obtained without exploiting specialized hardware or optimized inference strategies. In a full 3D configuration, although the iterative procedures associated with Richardson number–based formulations are not eliminated, the use of neural-network-based parameterizations can reduce their relative computational impact. When combined with batched neural inference on parallel or heterogeneous architectures (e.g., GPUs), this approach is expected to further enhance the potential runtime efficiency of machine-learning-based turbulence parameterizations.

4.4.1 – Projection of Computational Cost to a Full BAM-3D Configuration

Although the timing diagnostics were obtained in a one-dimensional environment, they allow a meaningful projection of the expected computational impact in a fully three-dimensional BAM-3D simulation. In a global model, the cost of the boundary-layer turbulence routine typically scales linearly with the number of horizontal grid columns and the number of time steps per day. Because the MLP-NN and Holtslag–Boville (HB) schemes showed nearly identical behavior in the 1D prototype,

differing by only ~ 0.09 ms per call (≈ 3 - 4%), the same relative difference is expected to hold when the routine is applied across the entire 3D grid

In operational global models, the turbulence parameterization accounts for only a fraction of the total model integration cost. Thus, even if the MLP-NN scheme were systematically ~ 4% slower per call than HB, its impact on the *total* wall-clock time of BAM-3D would likely remain below 1 ~ 2%. This makes the neural-network closure computationally feasible in a real 3D environment, particularly because no inference-specific optimizations were applied in the present study.

Furthermore, the traditional HB scheme relies on iterative procedures based on the Richardson number, which become increasingly expensive in large 3D domains due to convergence checks performed at every model column. The MLP-NN, by contrast, provides a direct non-iterative estimate of turbulent diffusivities and counter-gradient terms. When executed in batched mode or on heterogeneous hardware (e.g., GPUs, TPUs), the neural-network approach has the potential to reduce the overall turbulence cost even further. This suggests that, in a fully optimized BAM-3D implementation, the MLP-NN parameterization may offer not only physical realism but also tangible computational savings.

5. Conclusion

This study developed and evaluated a machine-learning-based replacement for the Holtslag–Boville turbulence parameterization in the BAM-1D atmospheric model. The proposed MLP-NN demonstrated outstanding skill in reproducing the vertical structure of the main turbulence-related quantities, including the eddy diffusivity coefficients (kvm, kvh), counter-gradient terms (cgs, cgh), and the overall PBL behavior.

For levels $k \geq 7$, the neural network achieved correlations of 0.9996 (kvm) and 0.9968 (kvh) with the reference scheme, with small RMSE and bias. Although cgs and cgh exhibit lower correlations due to their very small physical magnitude, the absolute errors are minimal and physically acceptable.

The ANN-based turbulence driver successfully preserved the model's internal dynamics, maintaining the fidelity of temperature, wind, and precipitation forecasts. No instability, drift, or artificial signals

were generated in any experiment. A computational analysis further revealed that the ANN implementation is as efficient as the traditional scheme in a 1D environment and is likely to offer substantial performance gains in parallel architectures.

Overall, the results demonstrate that machine-learning-based turbulence schemes can serve as accurate, stable, and computationally viable alternatives to traditional parameterizations. The successful integration of the MLP-NN into BAM-1D provides a solid foundation for future extensions to the full BAM-3D model and for broader applications in numerical weather prediction.

Future work will aim to extend this approach to replace other physical parameterizations in BAM and to evaluate scalability and performance gains in parallel operational frameworks.

Declarations

Author Contributions: All authors contributed to the study's conception and design. A.V.P.N performed material preparation, data collection, pre-processing, and analysis, did the experiments, and wrote the first draft of the manuscript. All authors commented on previous versions of the manuscript. All authors read and approved of the final manuscript.

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It is not applied

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