

Optimized Deployment of Atmospheric Models on High-Performance Computing Platforms

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Abstract. This study evaluates the performance of two atmospheric reanalysis datasets: ERA5 and NARR (NCEP / NCAR) when used as boundary conditions for the WRF model to simulate meteorological conditions over Mexicali, a rapidly urbanized city located in a semi-arid region of northwestern Mexico. Simulations were carried out over a dry, synoptically stable period to assess the sensitivity of the model to different initial and boundary conditions, while maintaining physical parameterizations fixed. Validation against in situ surface observations focused on key atmospheric variables, including 2-meter air temperature, surface heat fluxes, and 10-meter wind components. The results reveal systematic differences between the two reanalysis products: ERA5 more accurately reproduces near-surface temperature patterns and ground heat fluxes, while NARR tends to overestimate sensible and latent heat fluxes, as well as wind variability. Both

datasets exhibit biases in representing the diurnal cycle and surface energy partitioning, which have significant implications for simulating boundary layer development and urban climate processes in arid environments.

Keywords. Numerical weather prediction, WRF model, reanalysis, performance, parallel programming.

1 Introduction

In recent decades, atmospheric reanalysis datasets have become essential tools for climate studies and numerical weather modeling. These datasets combine observational data with short-term forecasts to produce continuous, spatially complete time series of meteorological variables at global and regional scales. Their

broad coverage and temporal consistency make them valuable resources for initializing and validating atmospheric models such as the Weather Research and Forecasting (WRF) model [10].

Despite their advantages, reanalysis products often exhibit biases in regions with complex surface characteristics or limited observational coverage. It is well documented that even with the use of high-quality reanalysis datasets and carefully selected physical parameterizations, certain atmospheric variables, such as precipitation, remain difficult to simulate with high accuracy [29, 24].

For this reason, arid regions such as Mexicali provide an ideal setting for evaluating reanalysis products, as the absence of significant atmospheric moisture reduces the complexity of convective processes. In addition, Mexicali represents a particularly relevant urban case study, as it is surrounded by desert terrain and experiences strong land–atmosphere interactions. Originally an agricultural region, Mexicali has experienced rapid urban expansion and industrialization, largely driven by its proximity to the U.S.–Mexico border and the economic influence of Southern California. These land use changes have significantly modified the city's surface energy balance, thermal behavior, and aerodynamic properties, directly influencing the planetary boundary layer above the urban and vegetated canopies. In this context, accurately simulating surface–atmosphere interactions is essential for developing reliable weather forecasts, climate projections, and environmental risk assessments.

The objective of this work is to investigate the performance of two distinct reanalysis datasets—ERA5, the fifth-generation atmospheric reanalysis from ECMWF, and NARR (North American Regional Reanalysis) from NCEP/NCAR—when utilized as initial and boundary conditions for WRF simulations over the Mexicali region. Focused on a dry and synoptically stable period in June 2003, during which a meteorological campaign was conducted across three distinct land use and land cover types. This study evaluates the

ability of the reanalysis datasets to accurately reproduce critical atmospheric variables, such as 2-meter air temperature, surface heat fluxes, and 10-meter wind components. Analyzing extreme hot weather events in desert regions is essential, as these areas are climatologically predisposed to intense thermal conditions such as heatwaves [9]. Although mountain regions already face challenges related to heat extremes [3], the impact in desert environments can be even more severe due to inherently higher baseline temperatures and reduced atmospheric moisture. With climate change projected to intensify both the frequency and magnitude of these events [18], developing robust, high-resolution, and well-calibrated numerical models is crucial for improving predictive capabilities and informing adaptation strategies.

This study contributes to that effort by exploring the sensitivity of WRF simulations to various initial and boundary conditions, keeping physical parameterizations fixed, and identifying the optimal input data for high-resolution modeling in semi-arid urban environments. Accurate simulation of atmospheric conditions is critical not only for improving scientific understanding but also for applications such as thermal comfort assessments, particularly for vulnerable population groups. Ultimately, this work supports the optimization of numerical weather models for urban planning, climate adaptation, and air quality management in rapidly evolving arid regions, where a reliable representation of urban microclimates is increasingly necessary.

2 Materials and Methods

2.1 Study Area

Figure 1a shows the terrain characteristics of the Mexicali region. The western boundary is defined by the Sierra Juárez, while the southeastern limit is marked by the Laguna Salada basin. Mexicali is located in the northeastern region of Baja California, Mexico (32°33' N, 115°28' W) at an altitude of approximately 4 meters above sea level.

Figure 2 presents the climatological characteristics of Mexicali, illustrating the

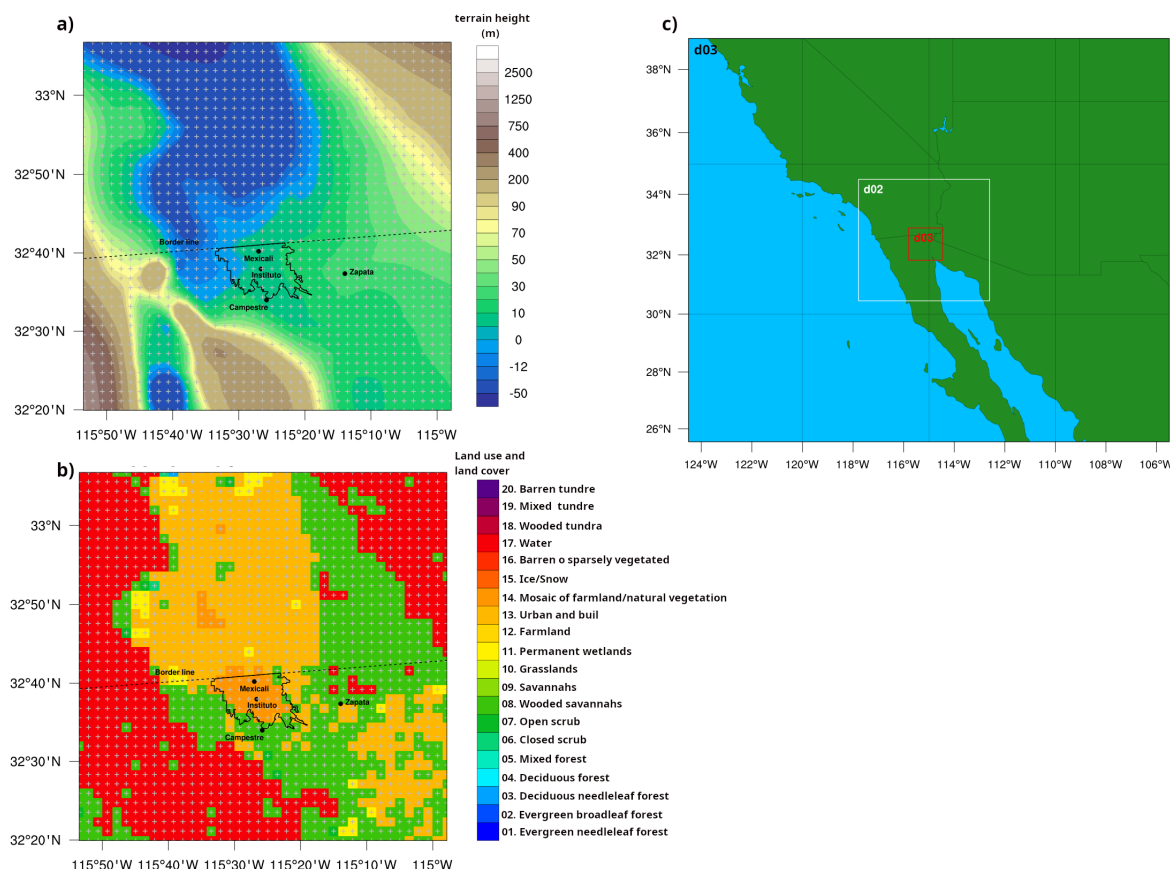


Fig. 1. a) The topography of the Mexicali contours in meters. The black dots represents the campaign sites location. Mexicali station belonged to the Mexico's National Meteorological Service (SMN). The black outline indicates the Mexico-US border line. b) The land use and land cover of Mexicali include urban area, farmland, pasture with predominant barren LULC associated to (orangered pixels). Light orange pixels represent the extent of the current urban area covered by Mexicali B.C. c) Shown the three nested configuration domains in the experiments

monthly average maximum, minimum and mean temperatures, together with monthly precipitation based on 30-year climatological observations, downloaded from the link in the footnote¹.

The climograph clearly reflects the arid nature of the region, with extremely high temperatures during the summer months (peaking above 40 °C) and very limited rainfall, particularly from April to June, which are characterized by nearly zero precipitation.

¹<https://smn.conagua.gob.mx/es/climatologia/informacion-climatologica/climogramas-1981-2010> (accessed on April 10, 2025)

Total annual precipitation is 75 mm which is a typical value for desert areas at this latitude.

These conditions support the selection of Mexicali as an ideal study area to evaluate the performance of atmospheric models and reanalysis datasets.

The absence of convective precipitation and the dominance of thermal forcing during this period provide a simplified yet challenging environment to assess the sensitivity of model configurations, especially for boundary layer processes and surface-atmosphere interactions under extreme heat.

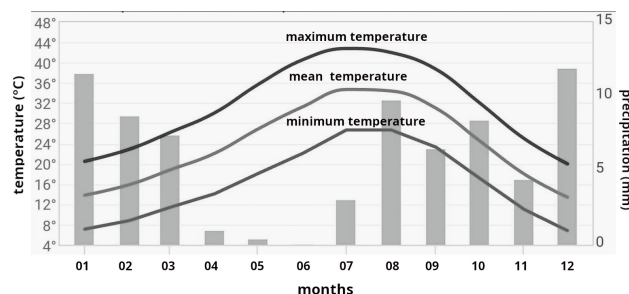


Fig. 2. Climograph, bars and lines represents monthly precipitation and temperature for the Mexicali climatology 1981-2010

2.2 Meteorological Data and UABC-2003 Field Campaign

We used surface data to evaluate the performance of the WRF 4.1.2 model (see Figure 1a). The data used in this study were obtained from a field campaign conducted over different land use and land cover types in and around Mexicali. The campaign took place from 15 to 24 June 2003, organized by the Applied Climatology group of the Engineering Institute of the Autonomous University of Baja California (hereafter UABC) [11]. This research group engages in operational, educational, and scientific activities, including preparing daily regional weather forecasts and monitoring of atmospheric variables, among other tasks.

Table 1 shows the four surface stations: three corresponding to the meteorological field campaign managed by the UABC and the Mexicali station managed by the SMN.

The station network outside Mexicali records temperature at 2m, wind direction, and wind speed every twenty minutes. The Mexicali station, on the other hand, has the same set of data but as hourly averages. We, therefore, create a homogeneous database for every hourly data with a basic quality control that removes erroneous data, outliers and missing data [2].

We also recorded turbulent surface fluxes, including sensible heat flux (SHF), latent heat flux (LHF), and ground heat storage at the surface (GHF) across three classifications of land use and land cover.

The measurement of surface fluxes across different land use and land cover types enables a detailed characterization of atmosphere–surface interactions, offering valuable insights into the energy exchange processes within the study area.

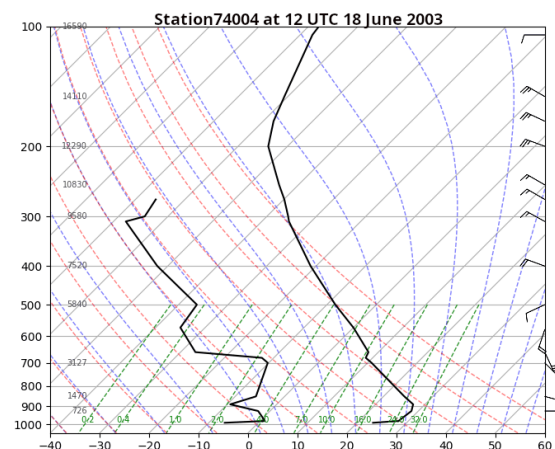


Fig. 3. The Skew-T diagram presents the meteorological sounding for Tucson, Arizona (station code 74004). The temperature profiles indicate stable atmospheric conditions, which are representative of the meteorological characteristics during the study period

It is important to note that urban expansion is a dynamic process, which can significantly influence surface-atmosphere exchanges over time [20, 23].

However, given that the length of the observational period spans only 10 days for the flux measurements and 30 days for the meteorological data collection, we extract the land use land cover information for the innermost computational domain from MODIS 2001 as the most representative of the Mexicali region for the month of June [5].

Nevertheless, the study's objective does not focus on analyzing land surface heterogeneity but rather on evaluating the representation of reanalysis input data within the Mexicali region.

To further assess the prevailing meteorological conditions in the vertical, we use radiosonde profiles from the nearest launching site in Tucson, Arizona (<https://weather.uwyo.edu/upperair/sounding.shtml>, accessed on March 25, 2025). The corresponding analysis of the Skew-T diagram reveals westerly

winds throughout the entire atmospheric column. The significant separation between the environmental temperature and the dew point temperature indicates a dry and stable atmosphere.

Therefore, the meteorological campaign was conducted under suitable synoptic conditions, allowing for a clear assessment of local meteorological processes (Figure 3).

2.3 The Weather Research and Forecasting System Model (WRF v4.1.2)

The WRF model is a state-of-the-art, non-hydrostatic atmospheric model designed for both operational forecasting and atmospheric research. It solves the governing equations using prognostic variables including horizontal and vertical wind components (u , v , w), perturbation potential temperature, geopotential, and dry-air surface pressure [27].

WRF employs a terrain-following, mass-based hybrid sigma-pressure vertical coordinate, allowing grid stretching, with the model top set at a constant pressure level. It uses Arakawa C-grid horizontal staggering and supports second- to sixth-order advection schemes for spatial discretization. Time integration is performed using a time-split Runge-Kutta scheme (second or third order), with a reduced timestep for acoustic and gravity waves [30].

The model includes advanced treatments for sub-grid scale turbulence, divergence damping, and filtering of external modes, enabling accurate simulations of complex atmospheric dynamics [27]. WRF model is a system composed of several steps for conducting numerical atmospheric experiments. The process begins by obtaining the initial and boundary conditions, which are used to initialize the model and provide the necessary meteorological variables to drive the numerical core dynamics. Once the model is executed, it generates output files in NetCDF (Network Common Data Format) format, which can then be post-processed and visualized to analyze fine-scale meteorological data (see Figure 4).

2.3.1 WRF Parameterizations

As part of the computational design, a standardized set of physical parameterizations was implemented across all WRF simulations to ensure consistency and reliability in model outputs. The RRTMG (Rapid Radiative Transfer Model for GCMs) was selected to simulate both shortwave and longwave radiation, providing accurate radiative forcing [17]. For cumulus convection, the Kain-Fritsch scheme was applied exclusively in the outermost (coarse) domain, while it was deactivated in the inner domains to allow explicit resolution of convective processes [21]. Land-atmosphere interactions were represented using the Noah Land Surface Model (LSM), which simulates soil moisture, subsurface temperature, and hydrological fluxes [6].

To capture vertical mixing and turbulent diffusion within the boundary layer, the Yonsei University (YSU) scheme was used as the planetary boundary layer (PBL) parameterization [16, 15, 14]. This was coupled with the Revised Monin-Obukhov Similarity (01) surface layer scheme, which estimates turbulent surface fluxes of energy, moisture, and momentum based on similarity theory [19]. Given that the study period was characterized by dry, synoptically stable conditions without precipitation, the microphysics scheme was turned off, reducing computational demand while remaining physically consistent with the atmospheric setup. The parameterization are detailed by domain in table 2.

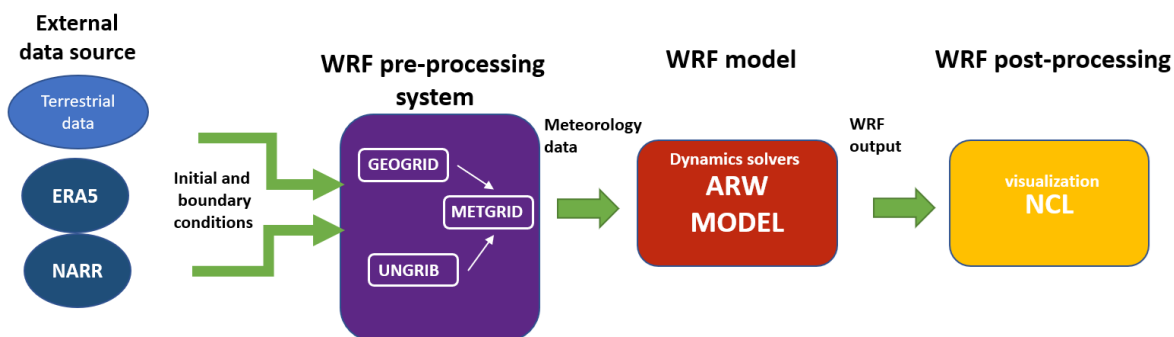
To conduct the case study, the experiments were initialized on June 1st at 00:00 Local Standard Time (LST) (where LST = GMT – 6 hours) and concluded on June 30th at 23:00 LST, with model outputs generated every hour.

The first 24 hours of simulation were discarded to allow for model spin-up, enabling the adjustment of dynamic and thermodynamic fields and ensuring more realistic results and eliminate the spurious simulations.

The WRF source code, written in Fortran and C, was compiled using Intel® Fortran and C compilers version 19 and parallelized with Message Passing Interface (MPI) [1]. All simulations were executed on the Tlaloc supercomputer, housed at the

Table 1. Stations position: ID, Institution (Inst), latitude (Lat), longitude (Lon) and altitude (Alt) of stations

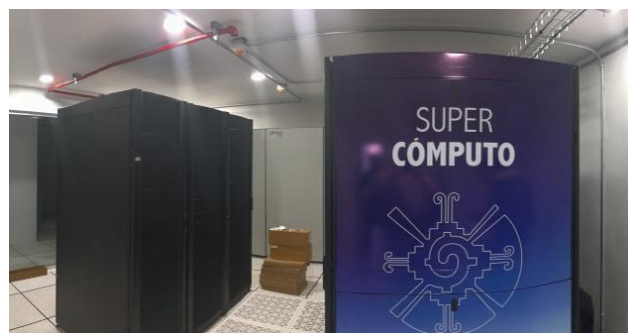
ID	Inst	Lat(°N)	Lon(°W)	Alt(m amsl)	Name
01	UABC	32.62	115.43	10	INSTITUTO
02	UABC	32.57	115.43	08	CAMPESTRE
03	UABC	32.55	115.53	29	ZAPATA
04	SMN	32.67	115.45	14	MEXICALI

**Fig. 4.** Flux diagram of the parameterizations of WRF model, <https://www.mmm.ucar.edu/models/wrf>

Institute of Atmospheric Sciences and Climate Change and managed by the Computing and High-Performance Unit (Fig. 5). Tlaloc features a 40 Gb/s Mellanox® InfiniBand network connecting eleven heterogeneous nodes. For this study, experiments were conducted on a single node equipped with four Intel® Xeon® Gold 6252 CPUs @ 2.10 GHz, providing 24 physical cores (single-threaded) and 500 GB of RAM.

To optimize performance, the WRF binary utilizes a two-level domain decomposition strategy: the model domain is first divided into patches (assigned to processing nodes), and each patch is further subdivided into tiles (assigned to individual processor cores). All simulations were performed using 36 processors. A fixed time step of 2 seconds was applied for the outermost domain, with a nesting time step ratio of 3 for the internal domains, ensuring numerical stability [12].

Simulation outputs were stored and processed on the ST00 computing cluster, managed by the Tropical Hydroclimatology Research Group. Each experimental configuration required approximately 180 GB of memory for storage and processing.

**Fig. 5.** Tlaloc, as part of the supercomputer processing at the Institute of Atmospheric and Climate Change, generates and processes weather forecasts, air and biological quality, storm surges, ocean waves, and ash dispersal

2.3.2 Reanalysis Data as the Driver of WRF

Atmospheric reanalysis products are comprehensive simulations of the atmosphere that combine historical observational data with global numerical weather prediction models to produce gridded, spatially and temporally consistent datasets.

Table 2. WRF Parameterizations

Process - PBL scheme option	Details
Radiation - RRTMG (Rapid Radiative Transfer Model for GCMs)	Longwave and shortwave radiation
Cumulus Convection - Kain-Fritsch	Enabled only in outer domain
Land Surface Model (LSM) - Noah LSM	Simulates soil and surface interactions
Planetary Boundary Layer - Yonsei University	Vertical mixing and entrainment
Surface Layer (SL) - Revised Monin-Obukhov Similarity (01)	Computes turbulent surface fluxes
Microphysics - Disabled	Not used due to dry, non-precipitating

These datasets reconstruct past atmospheric conditions, providing temperature, wind, humidity, and pressure data as solutions for the governing equations and boundary conditions at the model's top and bottom [26].

Reanalysis products are particularly valuable for initializing and validating weather and climate models, offering a reliable and consistent foundation for simulations, model calibration, and long-term environmental studies. Their broad spatial coverage and temporal continuity make them essential tools for improving forecast accuracy, climate trend analysis, and model performance assessment in both research and operational applications. For this study, two sets of numerical experiments were conducted using different sources of initial and lateral boundary conditions: the ERA5 global reanalysis and the North American Regional Reanalysis (NARR) from NCEP/NCAR [4].

The ERA5 reanalysis dataset, developed by the European Centre for Medium-Range Weather Forecasts (ECMWF), provides global meteorological fields on a regular $0.25^\circ \times 0.25^\circ$ grid ($\approx 30 \text{ km} \times 30 \text{ km}$) with hourly resolution, starting in 1979. ERA5 data were accessed through the Research Data Archive (RDA) maintained by the Computational and Information Systems Laboratory (CISL) at the National Center for Atmospheric Research (NCAR) [13].

The NARR–NCEP reanalysis, developed by the National Centers for Environmental Prediction (NCEP) and distributed by NOAA, provides high-resolution data over North America with a 32-km spatial resolution and 3-hourly temporal

resolution. NARR assimilates a large volume of regional observations and is particularly useful for evaluating boundary-layer processes and land–atmosphere interactions over complex terrain [22]. WRF utilizes reanalysis data for its most external computational domain at the four lateral computational walls. The required variables are temperature, zonal and meridional wind components, specific humidity, and geopotential height defined at those walls.

2.4 Modeling Configurations and Experiments

The methodology begins by identifying the optimal reanalysis dataset to provide initial and boundary conditions (IBC) for WRF simulations [8]. This selection is based on a quantitative evaluation of pattern correlation with observational data, using established statistical methods [28] on multiple candidate reanalysis datasets. Only datasets offering sub-daily temporal resolution for the study region were considered. Sources with longer time intervals (e.g., monthly outputs) or coarse spatial resolutions (greater than 32 km) were excluded from the analysis. An additional selection criterion was the compatibility of the dataset format with the WRF preprocessing system (see Figure 4), following practices adopted in other studies [25].

Once the best-performing dataset is identified, the full model configuration is established using the planetary boundary layer (PBL) scheme previously determined to be the most appropriate for the study area, according to the findings of [1].

Furthermore, a direct comparison between two reanalysis products ERA5 and NARR–NCEP is conducted to assess their ability to accurately

represent the regional atmospheric state. This step ensures that the WRF model is initialized with the most reliable large-scale information, thereby improving the fidelity of the subsequent high-resolution simulations.

Experimental setups use one-way nested grid configurations. Figure 1c shows the computational domain extent, designed to capture orographically forced local phenomena from Sierra Juárez west of Mexicali and avoid potential computational instabilities associated with steep mountain regions in proximity to the model's lateral walls.

The outer domain d01 encompasses a broad area covering the northwestern region of Mexico and the southwestern United States, extending approximately from 26°N to 38°N latitude and 106°W to 124°W longitude. This domain captures large-scale synoptic features influencing the regional climate. Nested within the d02 domain is the high-resolution inner domain (d03), centered over Mexicali, Baja California, and its surroundings. Domain d03 is specifically configured to resolve the finer-scale atmospheric processes over the study area, including strong land-atmosphere interactions and urban thermal effects. The refined domain covers the northwestern part of Baja California and adjacent areas of southern California and western Arizona, where the dominant geographic features include desert terrain, limited topographic variation, and proximity to the Gulf of California.

By employing this two-domain nesting approach, the model simulates regional-scale dynamics while delivering detailed spatial resolutions of 2 and 6 km over the Mexicali region. This fine resolution is crucial for accurately capturing surface-atmosphere exchanges during extreme heat events. The dimensions of the mesh are provided in Table 3.

To achieve realistic simulations of atmospheric processes both near the surface and aloft within the planetary boundary layer (PBL), the model configuration employs 76 vertical levels, distributed as follows: 20 levels between the surface and 2.25 km, 30 levels from 2.25 km to 6 km, and 26 levels from 6 km up to 16 km, which represents the top of the computational domain. A higher concentration of vertical levels near the surface

Table 3. Default configuration of WRF model. The resolution (res) is the distance between each node of the mesh, and the dimensions (dim) are the number of points of the grid domain

Dynamics		Details
Nested domains		3
Horizontal grid		Arakawa C-grid
Time integration		3 rd order Runge-Kutta
Res - dim d01		18 - 99,83
Res - dim d02		06 - 81,75
Res - dim d03		02 - 63,60
Map projection		Mercator
Vertical coordinate		terrain-following
Vertical levels		76 eta lev

is necessary to accurately resolve turbulent fluxes of mass, energy, and momentum associated with surface-atmosphere interactions.

As previously noted, the Yonsei University (YSU) PBL scheme was selected, as it is commonly used in mesoscale urban meteorology studies [24]. The YSU PBL scheme is coupled with the Revised Monin-Obukhov similarity surface layer scheme to compute surface fluxes.

This specific configuration has been successfully tested in previous studies over complex terrain regions in Mexico, demonstrating adequate performance in simulating surface and boundary layer processes [2].

2.5 Evaluation Protocol

The performance of the WRF simulations is evaluated by comparing the model outputs with observations from four meteorological stations recorded during 2003 (Table 2), using the values from the nearest model grid point [25]. In this section, we define a set of evaluation metrics designed to identify the statistical deviations of the reanalysis input among all the experiments described in previous sections.

We employ four statistical measures to define the model error [28]. Each statistical measure and its corresponding equation are defined and numbered

according to the order presented: (1) the Pearson correlation coefficient (P):

$$P = \frac{1}{n-1} \sum_{i=1}^n \left(\frac{Mv_i - \mu_M}{\sigma_M} \right) \left(\frac{Ov_i - \mu_O}{\sigma_O} \right), \quad (1)$$

(2) the normalized root mean square error (RMSE), calculated by normalizing RMSE with the observed standard deviation:

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (Mv_i - Ov_i)^2}{n\sigma_{Ov}^2}}, \quad (2)$$

(3) the standard deviation ratio (SDR), representing the ratio of the model standard deviation to that of the observations, and:

$$SDR = \frac{\sigma_{Mv}}{\sigma_{Ov}}, \quad (3)$$

(4) the bias (B), defined as the mean difference between modeled and observed values:

$$B = \frac{1}{n} \sum_{i=1}^n (Mv_i - Ov_i), \quad (4)$$

where Mv_i and Ov_i correspond to the modeling and observation variables, respectively. In the case of modeling data, it refers to the closest grid point to the i_{th} observational site, and n is the total number of observational sites. The μ 's and σ 's are the mean and standard deviations of the corresponding model and observed variable, respectively.

Previous studies have used execution time (ET) as the primary indicator of computational performance, focusing on how ET responds to different selections of physical parameterizations [1, 12]. In this work, the execution time remains consistent across experiments, since the physical parameterizations were kept static, and only minor adjustments were made to the WRF preprocessing system, specifically during the running of metgrid step of WRF input files [27]. The number of processors and the execution time were maintained constant throughout all simulations, ensuring that any observed differences in model outputs are attributable solely to the model physics running different reanalyses rather than computational variability [7].

3 Results

The simulations were executed in a high-performance computing cluster, allowing parallel processing in multiple domains and configurations. Each set of simulations required approximately 960 core-minutes, reflecting the significant computational demand associated with regional modeling studies at high spatial resolution.

The temporal evolution of the simulation series is presented below, based on the use of two different reanalysis datasets: NCEP-NARR and ERA5.

3.1 Temporal Comparison of Modeled Meteorological Variables under Different Initial and Boundary Condition Datasets

Figure 6a shows the evolution of 2-meter air temperature over ten days during June 2003 in Mexicali, Baja California, comparing observational data (OBS) with two reanalysis products: ERA5 and NARR. The results reveal a well-defined diurnal cycle, characterized by a large diurnal temperature range of about 20 °C between day and night, consistent with the arid desert climate of the region.

Across the time series, observed temperatures (OBS) exhibit sharper daily cycles, with lower nighttime minima between 17 °C and 23 °C, while daytime maxima vary between 34 °C and 42 °C, which may reflect localized surface effects, including soil moisture and land cover, not fully resolved in the reanalysis datasets.

Except for a couple of days (June 18 and 19, which correspond to an interval of 48 simulation hours), ERA5 systematically overestimates the daytime maxima, from 1 °C to 5 °C, indicating a warmer bias during daylight hours. This may be attributed to its coarser representation of land surface processes or urban parameterizations. NARR tracks the observed temperature more closely, especially during the nighttime, though it still shows a tendency to overestimate peak values during the hottest part of the day. Both reanalyses successfully reproduce the phase and frequency of the diurnal cycle, demonstrating their capacity to resolve synoptic and mesoscale atmospheric variability in this region.

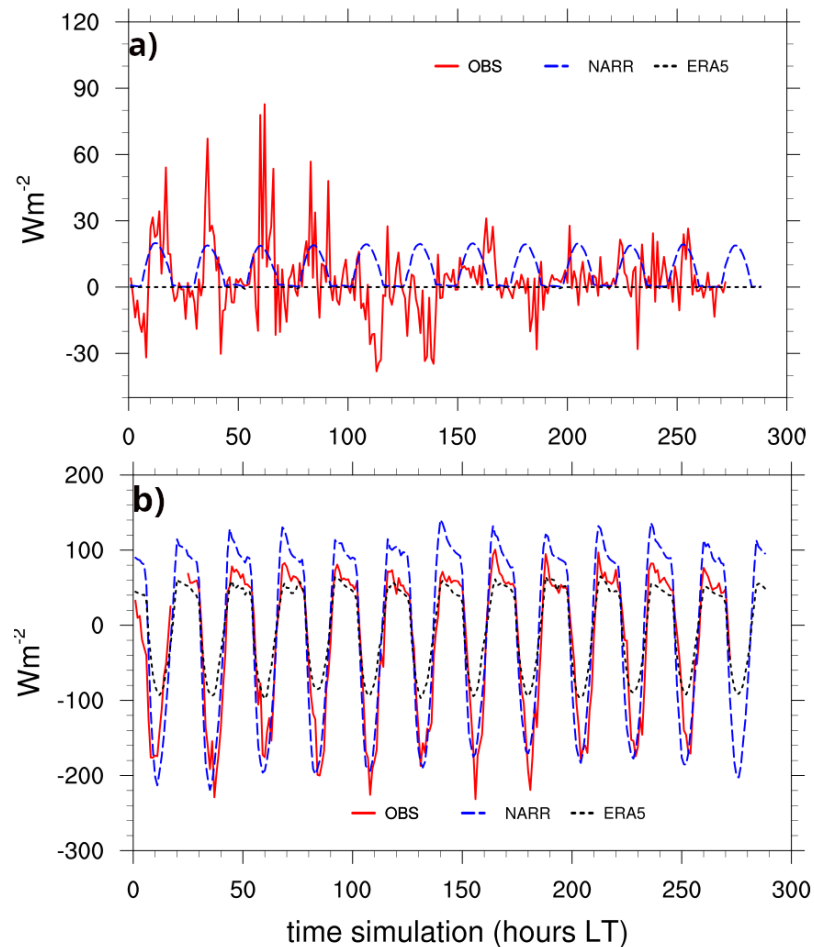


Fig. 6. Data series are presented for a) 2-meter temperature and b) sensible heat flux. The red, blue, and black curves represent the observations, WRF model outputs using NARR, and WRF model outputs using ERA5, respectively. The observational data correspond to the period from June 15 to June 24, 2003

Figure 6b shows the temporal comparison of observations and modeled surface heat flux (SHF) over the campaign days. All three datasets show a strong diurnal cycle, with positive daytime peaks corresponding to surface heating and near-zero or slightly negative values during nighttime, when surface cooling occurs.

The observed sensible heat flux (OBS) ranges mostly between 0 and 300 W m^{-2} , with a consistent daily pattern of sharp rises during the day and drops at night. NARR significantly overestimates the daytime sensible heat flux compared to observations and ERA5, frequently

exceeding 400 W m^{-2} , suggesting that the surface-atmosphere heat exchange is too strong, possibly due to biases in surface properties (e.g., albedo, soil moisture, land cover).

ERA5 generally follows the shape and timing of the observed diurnal cycle more closely than NARR, although it tends to underestimate peak fluxes and shows greater nighttime variability, occasionally dropping below 0 W m^{-2} .

Table 4 presents the statistical evaluation of the WRF simulations initialized with NARR and ERA5 datasets against surface observations for critical meteorological variables: 2-meter temperature

Table 4. Statistical measures used to evaluate the experiments comparing observations of temperature, surface fluxes, and wind components against WRF simulations initialized with NARR and ERA5 datasets. P represents the Pearson correlation coefficient, R is the root mean square error, SDR is the standard deviation ratio relative to observations, and B denotes the bias with respect to the observed values

	OBS vs NARR				OBS vs ERA5			
EX	P	RMSE	SDR	BIAS	P	RMSE	SDR	BIAS
Tmp	0.98	75.77	1.81	1.19	0.89	32.62	3.20	1.58
SHF	0.94	47.75	73.76	37.88	0.94	45.63	43.92	-4.26
LHF	0.69	16.16	40.90	-23.23	0.11	1.83	50.95	-31.85
GFX	0.94	45.45	43.60	15.03	0.94	45.59	47.22	16.90
u10	0.42	7.59	2.15	1.18	-0.26	-4.54	3.45	0.82
v10	0.23	3.87	2.94	-0.92	-0.30	0.17	0.66	0.06

(tmp), sensible heat flux (SHF), latent heat flux (LHF), ground heat flux (GFX), and the horizontal wind components at 10 meters (u10 and v10).

The metrics used include the Pearson correlation coefficient (P), the root mean square error (RMSE), the standard deviation ratio (SDR) relative to observations, and the bias (B).

The results show that for 2-meter temperature, NARR achieves a higher correlation ($P = 0.98$) compared to ERA5 ($P = 0.89$). However, NARR also presents a lower SDR and smaller bias, suggesting a slightly better match to observations in this variable. Although, the RMSE has a better performance in ERA5 than NARR, with 32.63 versus 75.77. For sensible heat flux, both datasets perform similarly well, with ERA5 slightly outperforming NARR in terms of lower bias (-4.25 W m^{-2} for ERA5 versus 37.88 W m^{-2} for NARR) and also lower SDR (43.92 W m^{-2} for ERA5 versus 73.76 W m^{-2} for NARR).

The consistent overprediction by NARR and the slightly muted response in ERA5 highlight differences in how each reanalysis models land surface energy dynamics, particularly under semi-arid urban climate conditions. SHF is a key component of the surface energy balance and has strong implications for urban climate modeling, especially under heat stress and pollution episodes. This comparison emphasizes the importance of evaluating

reanalysis datasets before their use in WRF simulations or other mesoscale atmospheric models within high-performance computing frameworks. While ERA5 provides a more reliable match with observations in Mexicali's hot and dry environment, its underestimation of daytime peaks suggests a need for urban-specific parameter tuning when used for detailed urban climate studies.

Figure 7a presents the temporal evolution of the latent heat flux (LHF) at the surface, comparing observations (red solid line) with WRF model outputs driven by NCEP-NARR (blue dashed line) and ERA5 (black dashed line) reanalysis datasets, for the period from June 15 to June 24, 2003 (local time, LT). The observations show a pronounced variability, with maximum values exceeding 80 W m^{-2} and minimum values near -30 W m^{-2} , reflecting strong day-to-day fluctuations associated with surface moisture availability and turbulent mixing processes. In particular, in the first 90 simulation hours, the LHF shows values higher than the maximum average in the day (39.2 W m^{-2}). This may be associated with external irrigation processes in the agricultural Mexicali region. The model simulations (both NARR and ERA5) consistently underestimate the amplitude of LHF.

Specifically, the NARR driven simulation mean peaks at approximately 20 W m^{-2} , while the ERA5

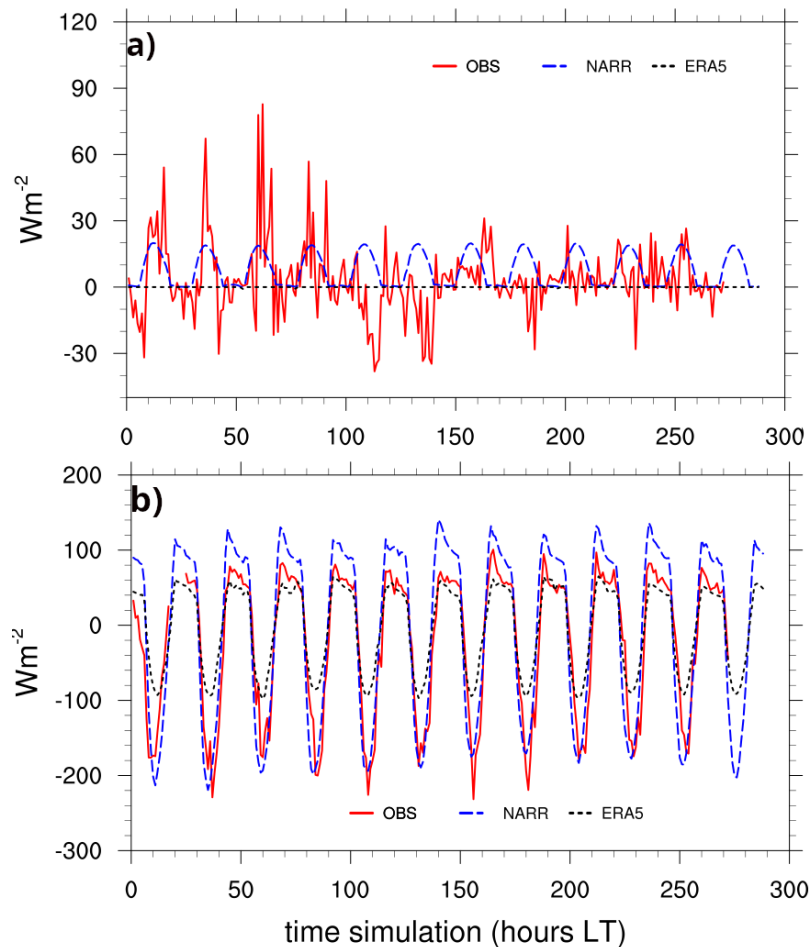


Fig. 7. Data series are presented for a) latent heat flux and b) ground heat flux. The red, blue, and black curves represent the observations, WRF model outputs using NCEP-NARR, and WRF model outputs using ERA5, respectively. The observational data correspond to the period from June 15 to June 24, 2003

driven simulation remains even lower, with values generally near to zero $W m^{-2}$.

Moreover, both simulations display a smoother diurnal cycle compared to observations, with less variability and limited occurrence of negative LHF values, indicating a reduced capacity to represent nighttime cooling and moisture flux reversals.

The results of the latent heat flux reveal significant challenges for both datasets, with notably low correlations ($P = 0.69$ for NARR and 0.11 for ERA5), large SDR (greater than $40 W m^{-2}$) and negative biases (B lower than $-23 W m^{-2}$). ERA5 tends to underestimate LHF

more strongly than NARR, reflecting the inherent difficulty of modeling moisture exchanges in arid urban environments.

These results emphasize the difficulties in accurately simulating surface moisture exchanges in arid and semi-arid urban environments, particularly under synoptically stable, dry conditions.

The Figure 7b is the same as Figure 7a but for ground heat storage (GFX). The observations and simulations initialized using NARR and ERA5 are represented by red, blue and black line, respectively.

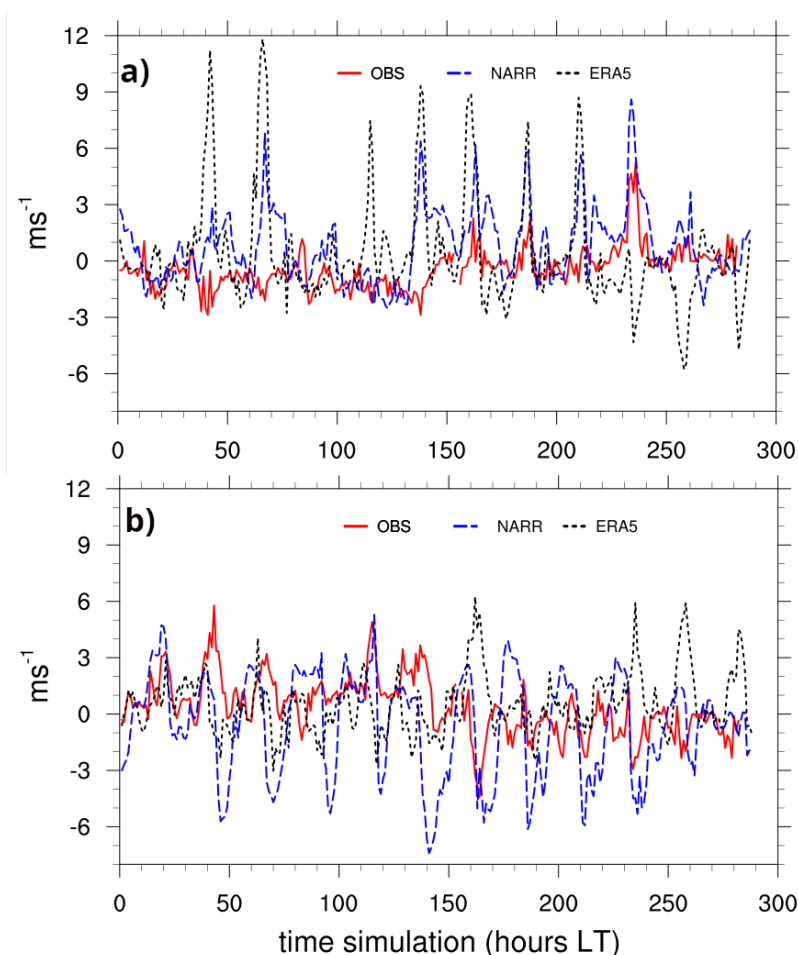


Fig. 8. Data series are presented for a) u-wind component and b) v-wind component. The red, blue, and black curves represent the observations, WRF model outputs using NCEP-NARR, and WRF model outputs using ERA5, respectively. The observational data correspond to the period from June 15 to June 24, 2003

The diurnal cycle of ground heat flux is clearly observed, with positive values during the daytime (net energy transfer into the ground) and negative values at night (release of stored energy back to the surface).

Observed ground fluxes (OBS) range approximately between 100 W m^{-2} and -240 W m^{-2} , showing typical desert surface thermal behavior with strong radiative heating during the day and rapid cooling at night.

NARR systematically overestimates both the daytime maxima and nighttime minima, with peak

values exceeding 140 W m^{-2} and dropping below -220 W m^{-2} .

This suggests a higher thermal conductivity or heat capacity assigned to the surface in the NARR model or a misrepresentation of the surface energy partitioning. ERA5 performs closer to the maxima of the observations, although it still shows a slightly muted amplitude, particularly in capturing extreme negative nighttime fluxes with values near to -100 W m^{-2} .

This indicates more conservative soil heat flux parameterization in ERA5, possibly influenced by its land surface model settings.

Regarding ground heat flux, both datasets show high correlation coefficients ($P \approx 0.94$) and similar RMSE near to 45 W m^{-2} , although ERA5 shows a slightly larger SDR and bias (Table 4).

Both reanalysis datasets capture the timing and shape of the flux cycles, but differ significantly in magnitude, particularly at night when radiative cooling dominates.

Ground heat flux plays a central role in the surface energy balance, affecting boundary layer development, surface temperatures, and nocturnal stability, especially in semi-arid regions like Mexicali. The overestimation by NARR may influence model simulations by enhancing nighttime heat retention, potentially reducing cooling rates and altering urban heat island intensity. In contrast, ERA5's more moderate fluxes suggest a better representation of the soil-atmosphere coupling during the day, making it more suitable for initializing or evaluating mesoscale models (e.g., WRF) in urban heat stress studies deployed on high-performance computing platforms.

Figures 8a and b present the temporal evolution of the u and v wind components at 10 meters above surface, comparing observations (red solid line) with WRF model outputs driven by NARR (blue dashed line) and ERA5 (black dashed line) reanalysis datasets, for the period from June 15 to June 24, 2003 (local time, LT).

The observational data (OBS) exhibit low variability, with component values u10 generally between 3 m s^{-1} and 3 m s^{-1} , suggesting moderate and stable zonal wind conditions at the surface during the study period. Specifically in the first 150 hours simulation, after that period, there is an intensification keeping positive values.

In contrast, both reanalyses show greater variability: NARR shows fluctuations from approximately 3 m s^{-1} to 9 m s^{-1} , frequently overestimating zonal wind intensity compared to observations. ERA5 presents even higher variability, with peaks exceeding 11 m s^{-1} and negative excursions down to 5 m s^{-1} , indicating strong short-term zonal wind events not reflected in the in-situ data. The large variability in the reanalysis products may be attributed to the influence of their coarser horizontal resolution or

differences in the parameterizations of the surface roughness, which can affect the representation of the wind near the surface. Both datasets capture the general timing of wind fluctuations, but tend to amplify the magnitude of variability compared to observations.

For the v10 wind component (Figure 8 b), the observational series shows higher variability than u10, with meridional wind values typically oscillating between 4 m s^{-1} and 5 m s^{-1} , suggesting strong and sectional north wind in the first 150 hours of simulation, with a change direction to south wind flow near the surface in the remaining block of simulation hours. Both NARR and ERA5 present larger amplitude fluctuations, occasionally exceeding $\pm 6 \text{ m s}^{-1}$, suggesting a tendency to overestimate short-term wind variability in the meridional component: NARR shows more frequent strong southward (negative) excursions, possibly reflecting differences in how topography and thermal gradients are resolved.

However, ERA5 tends to produce more pronounced northward spikes, especially during certain diurnal cycles. Both reanalyses reproduce the overall variability pattern, but often exceed the observed wind magnitudes, particularly during nighttime hours. An accurate representation of the wind components is essential in mesoscale simulations for atmospheric transport, boundary layer evolution, and surface convergence zone development. In urban and valley environments such as Mexicali, small errors in the meridional wind can significantly affect the simulation of local circulation features such as mountain-valley wind systems and urban breezes. The tendency of both reanalysis datasets to amplify meridional wind variability suggests a need for caution when using them as initial or boundary conditions in high-resolution simulations (e.g., with WRF) over complex or urban terrain.

Wind component analysis indicates that both datasets struggle to accurately reproduce near-surface winds. The correlations for u10 and v10 are notably lower than for other variables (with coefficient values lower than 0.5). ERA5 generally shows even lower correlations than NARR. This highlights a known difficulty of both

reanalyses in capturing fine-scale surface wind patterns in complex urban terrain such as Mexicali.

In general, Table 4 emphasizes the strengths and weaknesses of each reanalysis dataset, supporting the conclusion that while ERA5 is generally better for surface temperature and energy fluxes, neither dataset provides optimal performance for near-surface wind fields without further calibration.

4 Discussion

The comparative evaluation of WRF simulations initialized with ERA5 and NARR reanalysis datasets reveals important insights into model performance and its implications for applications in arid urban environments such as Mexicali.

ERA5 exhibited superior performance in simulating 2-meter temperature compared to NARR, with lower bias and stronger correlation with observations. These results are consistent with findings from other studies that have identified the same reanalysis product as providing the best performance for simulating temperature [26, 25].

Accurate representation of near-surface temperature is crucial for studies related to the urban heat island effect, thermal comfort, and public health during extreme heat events. Nevertheless, a slight warm bias was observed in daytime temperatures simulated with ERA5, suggesting that further refinement of urban surface characteristics may enhance model realism in semi-arid regions.

Both reanalysis-driven simulations captured the general diurnal cycle of sensible heat flux. However, NARR consistently overestimated daytime SHF values, while ERA5 provided values closer to observations, although with a slight underestimation of peak fluxes. Overestimation of SHF can lead to unrealistic boundary layer development, which would significantly affect pollutant dispersion modeling and surface energy balance studies. This result underscores the necessity of validating energy fluxes when applying regional climate models to desert environments.

Large discrepancies were observed in the simulation of latent heat flux. Both ERA5 and NARR underestimated the amplitude and

variability of LHF, highlighting a major limitation in modeling moisture exchanges in hyper-arid urban regions. As latent heat flux is closely linked to evapotranspiration and surface energy partitioning, its misrepresentation can lead to errors in simulating boundary layer humidity and temperature, ultimately impacting forecasts of heat stress and drought risk.

Both simulations captured the expected behavior of ground heat flux, including daytime storage and nighttime release of energy. However, NARR overestimated both daytime and nighttime fluxes compared to observations, while ERA5 showed better agreement in magnitude. Given the importance of GHF in regulating surface temperatures and nighttime cooling, particularly in urbanized desert areas, accurate modeling of this flux is essential for studies targeting thermal comfort and energy consumption in cities.

The simulation of 10-meter wind components revealed significant deficiencies. Both reanalyses overestimated wind variability, with ERA5 exhibiting larger fluctuations than NARR. Since surface wind plays a critical role in urban breeze formation, pollution transport, and thermal dispersion, inaccuracies in wind fields highlight the need for improved representation of local circulations, particularly in environments influenced by valley–desert interactions such as Mexicali.

The results demonstrate that while ERA5 offers notable improvements over NARR in capturing surface temperature and energy fluxes, significant challenges remain in simulating latent heat flux and near-surface winds in arid urban environments. These findings reinforce the importance of conducting localized validation of reanalysis products before their operational use in high-resolution mesoscale modeling.

For applications such as urban climate analysis, air quality management, and thermal vulnerability assessment, selecting appropriate initial and boundary conditions is essential. Moreover, improving land surface models and incorporating tailored urban canopy parameterizations for semi-arid cities should be a priority in future modeling efforts. Extending validation efforts across different seasons and testing ensemble modeling approaches could further enhance the

robustness and predictive capabilities of regional atmospheric simulations in rapidly evolving desert urban regions.

5 Conclusion and Future Work

This study provides a comparative evaluation of WRF simulations initialized with ERA5 and NARR–NCEP reanalysis datasets for an arid, urbanized region—Mexicali, Baja California. By focusing on a dry, synoptically stable period, the analysis offers insights into the ability of reanalysis-driven simulations to capture key surface and boundary layer processes under extreme heat conditions.

The results demonstrate that ERA5 outperforms NARR in the simulation of 2-meter temperature, sensible heat flux, and ground heat flux, exhibiting higher correlation and lower bias relative to surface observations. These improvements make ERA5 a more reliable choice for applications related to urban heat island studies, thermal comfort assessments, and energy balance modeling in semi-arid cities.

However, significant challenges remain, particularly in the representation of latent heat flux and near-surface wind components. Both reanalysis datasets underestimate latent heat flux and overestimate wind variability, highlighting persistent limitations in simulating moisture exchanges and local circulations over arid urban surfaces.

The findings emphasize the need for localized validation of reanalysis datasets prior to their operational use in high-resolution mesoscale modeling. They also underline the critical importance of selecting appropriate model physics, especially when studying surface–atmosphere interactions in complex, rapidly urbanizing environments. In future research, we proposed: As first work, extend the evaluation across different seasons to assess the robustness of model performance under varying atmospheric conditions (e.g., during wet or transitional periods).

Implement ensemble modeling approaches using multiple reanalysis products and different physical parameterizations to better quantify uncertainties.

By addressing these aspects, future studies can enhance the realism and applicability of high-resolution atmospheric simulations, contributing to better decision-making in urban planning, air quality management, and climate resilience efforts for arid regions experiencing rapid environmental and societal changes.

Finally, it is important to mention that running WRF numerical experiments on high-performance computing platforms provides critical advantages for model development in the arid region of Mexicali. The enhanced computational capacity enables higher spatial and temporal resolution, facilitating a more accurate representation of surface processes and boundary layer dynamics. This is particularly valuable for analyzing near-surface temperature (2m), energy fluxes, and wind components, which are highly sensitive to land–atmosphere interactions in arid environments. Ultimately, high-performance computing support strengthens model calibration and validation efforts, leading to improved simulation fidelity and more reliable assessments of local atmospheric conditions.

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