EFFECTS OF AEROSOLS FEEDBACKS IN MODELING METEOROLOGY AND AIR QUALITY IN THE ANDEAN REGION OF SOUTHERN ECUADOR

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ABSTRACT

Feedbacks are essential in atmospheric modeling. In this arena, aerosols promote direct and indirect effects. Direct effects are related to the scattering and absorption of solar radiation. Indirect effects correspond to cloud formation and cloud properties, which change the vertical temperature profile, relative humidity, and atmospheric stability. Modeling with direct and indirect effects should improve numerical performance based on a more detailed description of interactions. Benefits for air quality modeling were identified in the city Cuenca (Andean region of Southern Ecuador, 2,500 masl) when working with direct effects, compared to modeling without aerosols feedbacks. These benefits created expectations about the potential improvement when including direct and indirect effects. Therefore, we used the Weather Research and Forecasting with Chemistry Version 3.2 (WRF-Chem 3.2) model to assess aerosols feedbacks in modeling the meteorology and transport of air pollutants in Cuenca during September 2014. We considered the following scenarios: (1) No aerosols interaction (NI), (2) direct effects (DE), and (3) direct and indirect effects (DIE). Records were considered positive modeled if the maximum deviation between observed and modeled values agreed with prescribed accuracies (100% means all the records were captured by modeling). The NI scenario captured 82.7, 74.8, and 75.6% of short-term air quality, long-term air quality, and meteorological records. The DE scenario kept the performance for short-term (82.7%) and long-term (74.8%) air quality and increased to 76.2% for meteorological records. However, the DIE scenario decreased to 75.3% for short-term air quality, although it increased to 76.8% for meteorology. The inclusion of indirect feedbacks decreased the $PM_{2.5}$ modeling performance. WRF-Chem allows selecting numerous physics and scheme options that need to be assessed to identify a suitable combination for each region. Results can be notably affected by the selected parameters. Other aerosols schemes, alternatives for generating initial and boundary conditions, data assimilation, and updated emission inventories need to be assessed as components directly involved in modeling performance.
Keywords: WRF-Chem, Cuenca, modeling performance, direct effects, indirect effects.

1 INTRODUCTION

Air pollution is the result of complex interactions between atmospheric emissions and meteorology. Feedbacks are essential in atmospheric modeling. Recent research has shown that meteorology and chemistry feedbacks are essential for numerical weather and air quality forecasting [1]. In this arena, aerosols promote direct and indirect effects. Direct effects are related to the scattering and absorption of solar radiation [2]. Indirect effects correspond to cloud formation and cloud properties, which change the vertical temperature profile, relative humidity, and atmospheric stability. Therefore and based on detailed interactions, it is expected that including direct and indirect effects will improve atmospheric modeling performance.

Modeling both meteorology and air quality is challenging, especially in regions with complex topography, as the Andean region of South America. Based on the Eulerian Weather Research and Forecasting with Chemistry model (WRF-Chem), promising results were obtained for Cuenca [3], [4], a high (2,500 masl) Andean city of Southern Ecuador (Fig. 1). WRF-Chem is an online chemical transport model that includes treating the

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aerosols direct and indirect effects [5] with numerous options and parameters. WRF-Chem was used to assess the influence of planetary boundary layer schemes when modeling meteorology and air quality [3] and assessing the influence on air quality due to the shift from diesel to electric buses in Cuenca [4].

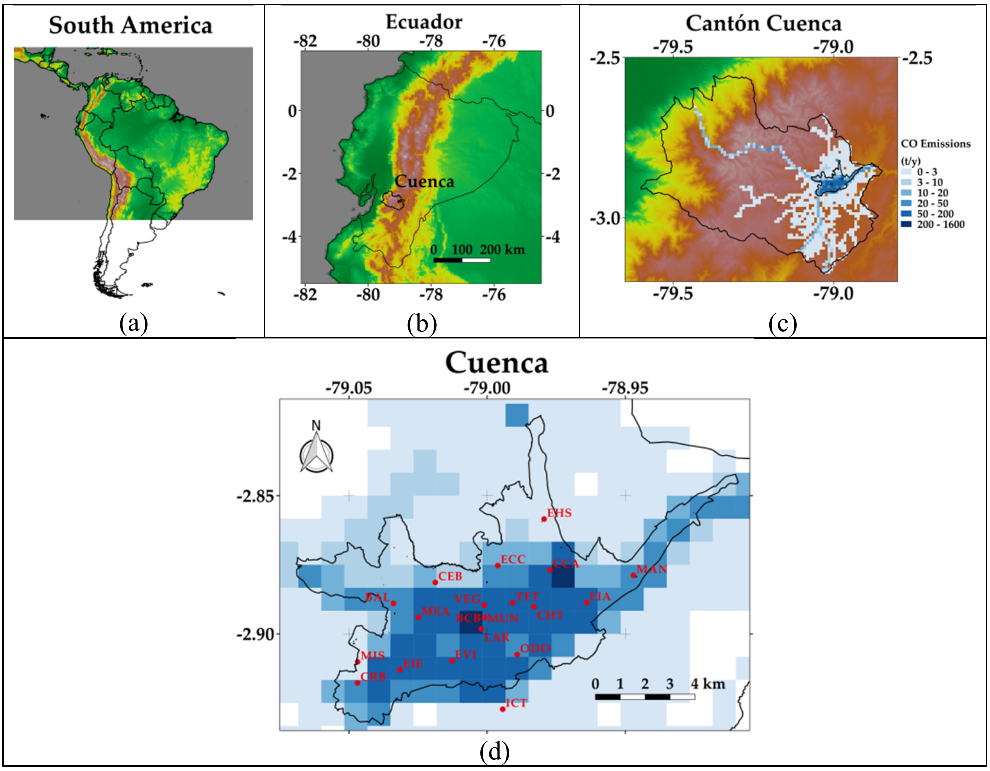

Figure 1: Location of: (a) Ecuador; (b) Cuenca; (c) CO emissions (t^{y-1}); (d) Urban area of Cuenca and the air quality stations (red dots). MUN station (2,500 masl) provides short-term air quality levels and meteorology. The others are passive stations for monitoring monthly-mean air quality levels.

Benefits for air quality modeling were identified in Cuenca when working with direct effects, compared to modeling without aerosols feedbacks [3]. These benefits created expectations about the potential improvement of a complete description of aerosols feedbacks through direct and indirect effects. Therefore, the main objective of this contribution focused on a preliminary assessment of the effects of a complete inclusion of aerosols feedbacks in modeling meteorology and air quality in this city.

2 METHOD

2.1 Emission inventory of Cuenca

The last emission inventory of Cuenca was made for the year 2014 [6], including the contribution from on-road traffic, vegetation, industries, a power facility, use of solvents, service stations, domestic GLP consumption, air traffic, landfills, handcrafted production of bricks, dust erosion, and mining. On-road traffic was the main source of most of the pollutants (94.9% of carbon monoxide (CO); 71.2% of nitrogen oxides (NO_x), 42.4% of fine particulate matter ($PM_{2.5}$), 39.6% of non-methane volatile organic compounds (NMVOC). Industries were the most important source (60.1%) of sulfur dioxide (SO_2). The power facility located at the NE of the urban area was also a significant source of SO_2 (35.1%) and NO_x (18.5%). About 600 artisanal producers of bricks located at the NW of the city were significant contributors of $PM_{2.5}$ (38.5%). Fig. 1 depicts the spatial distribution (1 km × 1 km of resolution) of CO emissions during 2014.

From this emission inventory, we generated hourly speciated emissions data for this contribution.

2.2 Modeling approach

We used the WRF-Chem Version 3.2 for modeling meteorology and air quality in Cuenca during September of 2014 for the following three scenarios: (1) No aerosols interaction (NI), (2) direct effects (DE), and (3) direct and indirect effects (DIE). September was selected because emissions from on-road traffic and other sources are representative for other months. Additionally, O_3 levels can be higher during this month than the World Health Organization guideline (100 µg m^{-3}, maximum 8 h mean). Meteorological simulations were carried through a master domain of 70 × 70 cells (27 × 27 km each) and three nested sub-domains. The third (100 × 82 cells of 1 km each and 35 vertical levels) covered the region of Cuenca (Fig. 1). Initial and boundary conditions were generated from the final NCEP FNL Operational Global Analysis data [7]. For the inner sub-domain, the chemistry option of WRF-Chem was activated, using the CBMZ [8] for gaseous pollutants and the MOSAIC [9] for aerosols. Table 1 indicates the schemes and options used for modeling.

Table 1: Schemes and options for modeling meteorology and the air quality in Cuenca (WRF-Chem V3.2) [10].

Component	Modeling approach			Scheme/model
	NI	DE	DIE	
Microphysics	2	2	2	Lin et al. [11]
Longwave radiation	1	1	1	RRTM [12]
Shortwave radiation	2	2	2	2 Goddard [13]
Surface layer	1	1	1	MM5 similarity [14]
Land surface	2	2	2	Unified Noah land surface [15]
Planetary boundary layer	1	1	1	Yonsei University [16]
Cumulus parameterization	5	5	5	Grell 3D Ensemble [17]
Chem_opt	7*	7*	9**	
Wet scavenging	Off	Off	On	
Cloud chemistry	Off	Off	On	
Aerosols to radiation feedback	Off	On	On	

*CBMZ chemical mechanism and MOSAIC using 4 sectional aerosol bins. **CBMZ chemical mechanism using 4 sectional aerosols bins including aqueous reactions.

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2.3 The air quality network of Cuenca

Since 2012, the city has one automatic station in the historic center (MUN station, Fig. 1), monitoring meteorology and short-term air quality. There are also about 20 stations with passive sensors for measuring monthly-mean air quality levels of NO_2 and O_3. Monitoring is based on methods established in the Ecuadorian air quality regulation, under the responsibility of the local government.

Meteorological and air quality records were considered positive modeled if the maximum deviation between observed and modeled values agreed with the accuracies (100% means all the records were captured by modeling) of Table 2. Also, modeled meteorological and short-term air quality values were assessed through the indicators of Table 2, corresponding to the following expressions:

$$GE = \frac{1}{N}\sum_{i=1}^{N}|Pi - Oi|,\ BIAS = Pm - Om,\ RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(Pi - Oi)^2},$$

where GE = gross error; RMSE = root mean square error; N = number of values; Pm = mean modeled value; Om = mean observed value; Pi = modeled value; and Oi = observed value.

Table 2: Accuracy and indicators for meteorological and air quality modelling [18].

Parameter	Accuracy	Indicator	Benchmark	Ideal value
Meteorology:				
Hourly surface temperature	±2°C	GE	< 2 K	
		BIAS	< ± 0.5 K	
Hourly wind speed at 10 m above the surface	$\pm$ 1 m s^{-1}	RMSE	< 2 m s^{-1}	
		BIAS	< ± 0.5 m s^{-1}	
Short-term air quality:				
Maximum 8 h CO mean	± 50% mg m^{-3}	RMSE		0
Maximum 8 h O_3 and 24 h $PM_{2.5}$ means	± 50% µg m^{-3}	RMSE		0
Long-term air quality:				
Monthly NO_2 and O_3 means	± 30% µg m^{-3}			

3 RESULTS AND DISCUSSION

Fig. 2 compares the observed and modeled temperatures. The NI and DE scenarios reached performances of 75.9 and 76.2%, respectively (Table 3). The DIE scenario increased the performance to 77.0%. Both GE and BIAS were in the benchmark range for temperature (Table 4). The observed wind rose indicated wind coming mainly from the east–northeast (ENE) direction (Fig. 3). However, modeled results indicated the east (E) as the main direction of the coming wind. The NI scenario captured 75.3% of observed wind speed values, The DE and DIE scenarios increased to 76.1 and 76.6%, respectively. GE and BIAS were in the benchmark range for wind speed (Table 4).

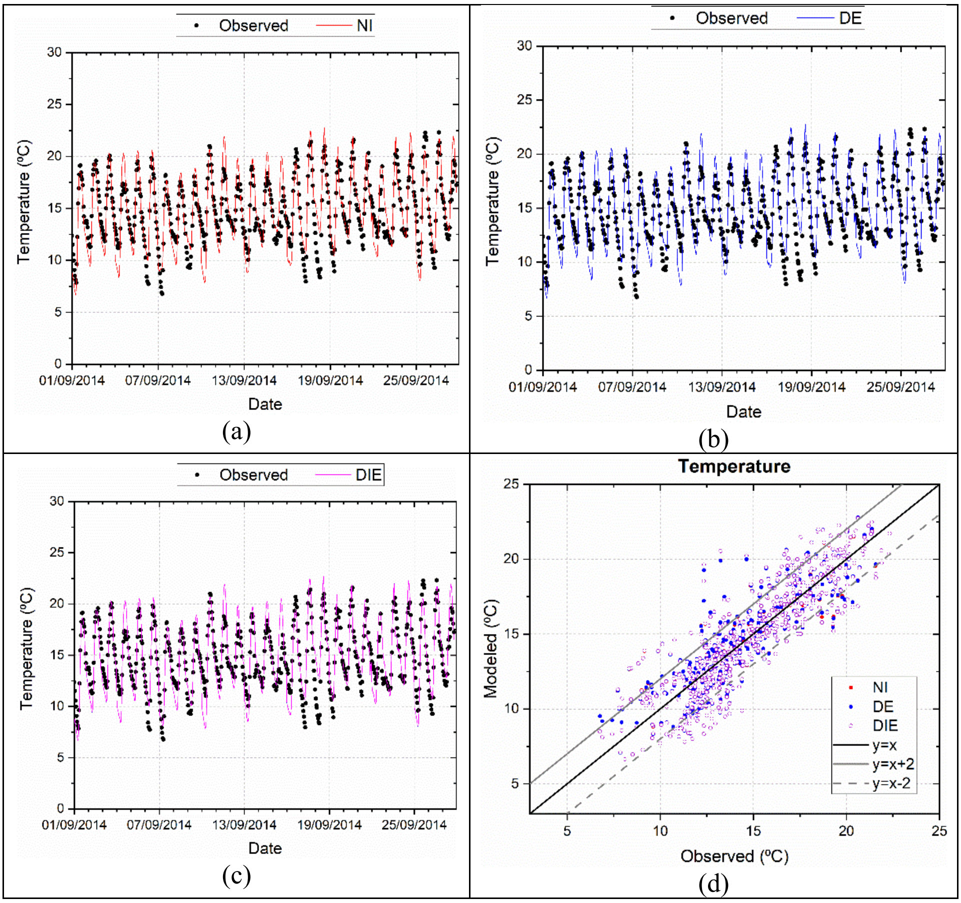

Figure 2: Observed and modeled temperature. (a) No aerosol interactions (NI); (b) Direct effects (DE); (c) Direct and indirect effects (DIE); and (d) Observed vs. modeled temperatures.

The DE mean daily profile for temperature was similar to NI (not showed). The DIE hourly mean values showed variations between –0.1 to 0.2°C compared to NI. The mean daily modeled profiles of global solar radiation and wind speed overestimated the observed values during daylight hours (Fig. 4). The DE mean profile for solar radiation showed reductions up to –4 W m^{-2} than NI. On contrary, the DIE increased hourly mean values up to 56 W m^{-2}. The DE mean profile for wind speed was similar to NI (Fig. 4), although the DIE showed variations between –0.1 to 0.1 m s^{-1} compared to NI. The average performances for modeling temperature and wind speed for the NI, DE, and DIE scenarios were 75.6, 76.2, and 76.8%, respectively.

Due to the numerous interactions involved, it is challenging the interpretations of results when modeling with aerosols feedbacks [19]. Direct effects can reduce surface temperature due to the reflection of solar radiation. However, the corresponding layer of the atmosphere can be warmed simultaneously due to the absorption of solar radiation by black carbon. The

Table 3: Percentage of records positively captured in modeling meteorology and air quality.

	Modeling approach		
Meteorology:	NI	DE	DIE
Surface temperature	75.9	76.2	77.0
Wind speed at 10 m	75.3	76.1	76.6
Average performance	75.6	76.2	76.8
Short-term air quality:			
CO, daily maximum 8 h mean	100.0	100.0	100.0
$PM_{2.5}$, daily 24 h mean	63.0	63.0	40.7
O_3, daily maximum 8 h mean	85.2	85.2	85.2
Average performance	82.7	82.7	75.3
Long-term air quality:			
NO_2, monthly mean	93.3	93.3	93.3
O_3, monthly mean	56.3	56.3	56.3
Average performance	74.8	74.8	74.8
Global performance	77.7	77.9	75.6

Table 4: Indicators for modeling meteorology and air quality.

	Modeling approach								
	NI			DE			DIE		
	GE	BIAS	RMSE	GE	BIAS	RMSE	GE	BIAS	RMSE
Meteorology:									
Surface temperature	1.3	0.1	–	1.3	0.1	–	1.3	0.0	–
Wind speed at 10 m	–	0.3	1.0	–	0.3	1.0	–	0.3	1.0
Short-term air quality:									
CO, daily maximum 8 h mean	–	–	0.19	–	–	0.19	–	–	0.18
$PM_{2.5}$, daily 24 h mean	–	–	3.05	–	–	3.04	–	–	5.19
O_3, daily maximum 8 h mean	–	–	19.1	–	–	19.1	–	–	19.4

increased solar radiation values provided by the DIE approach can be attributed to the increased light scattering in partly cloudy conditions.

Modeling performances and RMSE values for short-term air quality were equals or similar for CO (Table 3, Table 4, Fig. 5(a)) and O_3 (Fig. 5(c)).

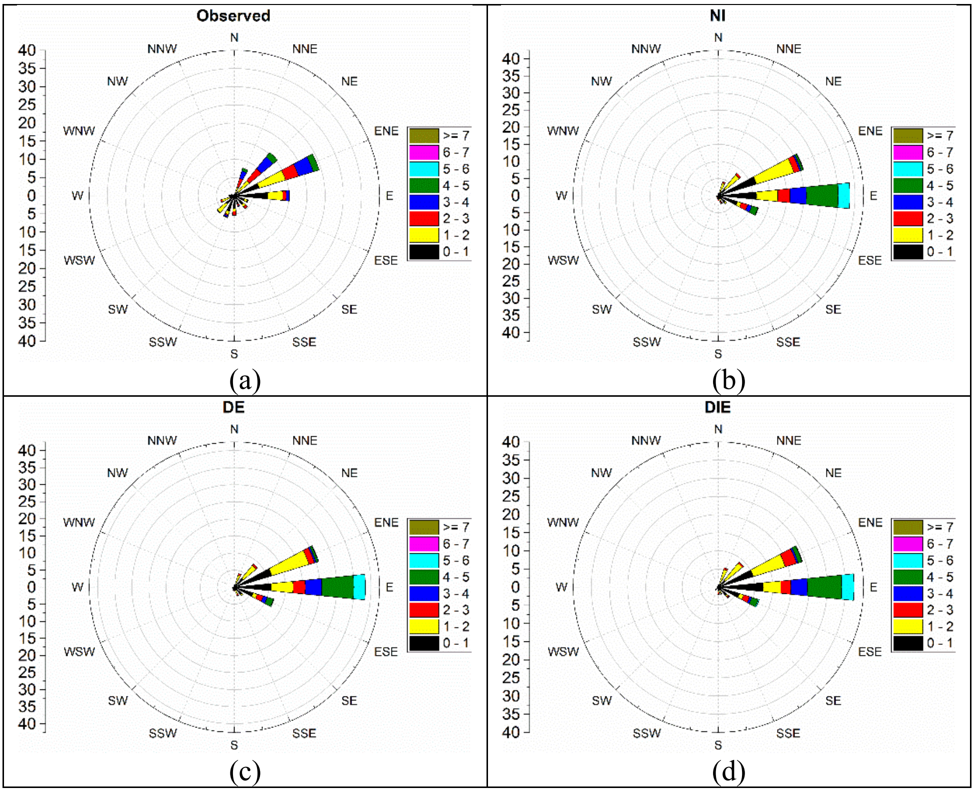

Figure 3: Wind roses. (a) Observed; (b) No aerosol interactions (NI); (c) Direct effects (DE); and (d) Direct and indirect effects (DIE).

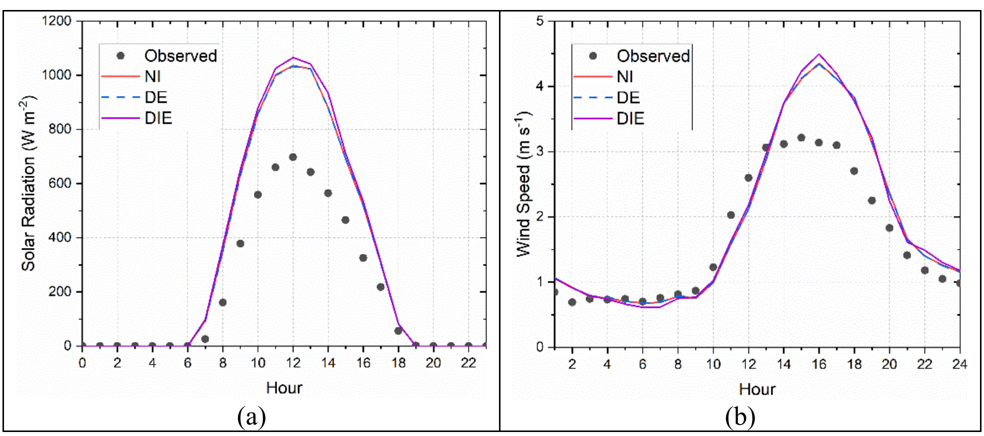

Figure 4: Mean daily profiles. (a) Global solar radiation; and (b) Wind speed.

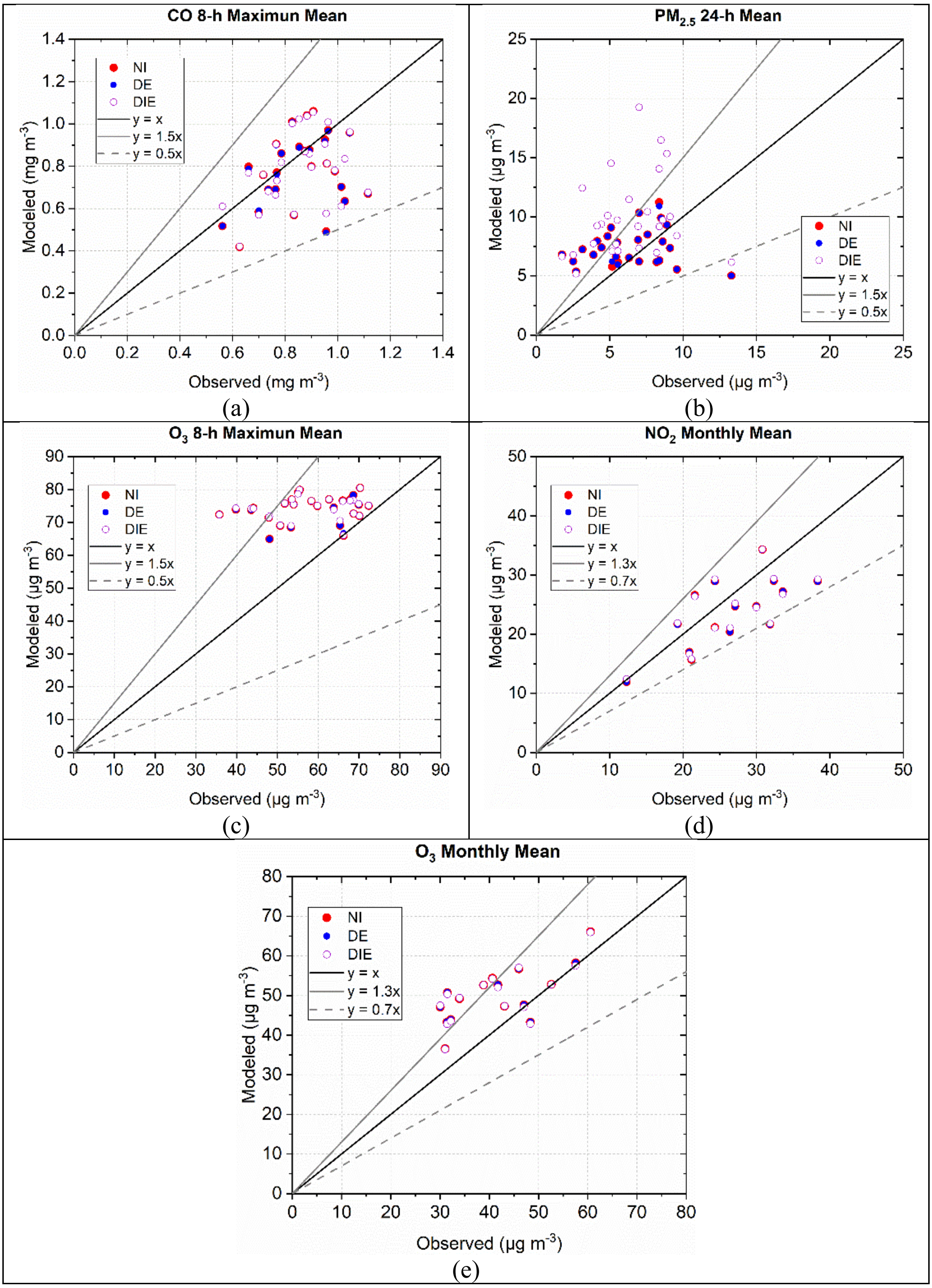

Figure 5: Observed vs. modeled concentrations. (a) CO 8 h maximum mean; (b) $PM_{2.5}$ 24 h mean; (c) O_3 8 h maximum mean; (d) NO_2 monthly mean; and (e) O_3 monthly mean.

For $PM_{2.5}$, the NI and DE reached modeling performances of 63.3%. However, it decreased to 40.7% when using the DIE approach (Fig. 5(b)). The RMSE parameter was similar for NI and DE (3 $\mu g\ m^{-3}$, Table 4), but increased to 5.2 for DIE.

NI and DE captured 82.7% of records for short-term air quality, which was decreased to 75.3% by DIE. For all the approaches, the performances for long-term air quality were the same (74.8%)(Table 3, Fig. 5(d) and 5(e)).

Results indicated a minute improvement performance when modeling with direct effects than without aerosols interactions. An additional improvement was obtained for meteorology using direct and indirect effects, although this approach increased the $PM_{2.5}$ concentrations. This increase resulted in higher modeled values than $PM_{2.5}$ records, decreasing the modeling performance as a consequence.

This result is consistent with the decrease of performance reported by Makar et al. [20] when modeling particulate matter using direct and indirect effects over domains in North America and Europe (Table 5). In Cuenca, on average, $PM_{2.5}$ mean daily concentrations were increased up to 2.5 $\mu g\ m^{-3}$ when considering indirect effects. For example, Fig. 6 shows the modeled $PM_{2.5}$ concentrations by the NI and DIE approaches on 21 September 2014, which depicts higher values for DIE in the historic center. This increase is consistent with the increase between 1 to 10 $\mu g\ m^{-3}$ for monthly PM_{10}, reported by Forkel et al. [21] for July 2006 over large parts of Continental Europe. In the same way, Tucella et al. [22] reported an overestimation of particle number concentration when modeling an event over Europe with direct and indirect feedbacks. However, Liu et al. [23] reported good performance for most meteorological fields and chemical concentrations when modeling over East Asia (Table 5).

The increase in $PM_{2.5}$ concentrations, when including indirect effects poises whether $PM_{2.5}$ emissions were overestimated or if this increase was excessive due to inadequate modeling of the aerosols indirect effects.

The treatment of indirect effects is one of the critical uncertainties. A better representation of aerosol processes and feedbacks, their interactions with clouds and radiation; currently, components need to be improved [24], especially for regions of complex topography as the Andean zone.

WRF-Chem allows selecting numerous physics and scheme options that need to be assessed to identify a suitable combination for the region. Results can be notably affected by the selected parameters. Land surface models and schemes of cumulus parameterizations deserve a special effort as components affecting atmospheric modeling.

Updated aerosols schemes, initial and boundary conditions, data assimilation, fusion with machine learning and artificial intelligence approach, and even the emission inventory need to be assessed as components directly involved in modeling performance.

4 CONCLUSIONS

To our knowledge, we made the first exercise of modeling meteorology and air quality in Cuenca, considering direct and indirect aerosols interactions.

Although being a preliminary assessment, our results suggested that modeling meteorology and air quality for the Andean region of Ecuador can be improved using direct aerosols effects. The parameterizations used for indirect feedbacks did not improve or even decreased the $PM_{2.5}$ modeling performance, which poises whether $PM_{2.5}$ emissions were overestimated or if this increase was excessive due to inadequate modeling of the aerosols indirect effects.

Table 5: Comparison with other studies on the influence of aerosols feedbacks modeling.

	Case or reference				
	This assessment	Makar et al. [20]	Forkel et al. [21]	Tucella et al. [22]	Liu et al. [23]
Region	Cuenca, Ecuador	North America and Europe	Europe	Europe	East Asia
Period	September 2014	2006 and 2010 for North America 2010 for Europe	June and July 2006	15 May 2008	January, April, July, and October 2008
Parameters assessed	Meteorology and air quality	Meteorology and air quality	Meteorology and air quality	Aerosols and cloud droplets number concentrations (CNDC)	Meteorology and air quality
Models	WRF-Chem 3.2	GEM-MACH, WRF-Chem 3.4.1 and WRF-CMAQ	WRF-Chem 3.3	WRF-Chem 3.4	WRF-Chem and MADRID
Spatial resolution	1 km	0.25° (≈27.8 km)	22.5 km	30 km	36 km
Summary of results reported about modeling performance	Higher values of $PM_{2.5}$. Higher values of solar radiation at surface. Modeling performance can be improved using direct aerosols effects. Using direct and indirect effects did not improve or even degraded modeling performance.	Summertime model performance for O_3 and other gases improved, although the particulate matter performance was degraded. Aerosol indirect effect dominated feedbacks compared to the direct effect. Direct and indirect effects competed.	Higher mean PM_{10} near the ground was simulated for significant parts of continental Europe. Significantly higher values of solar radiation at the surface for a large part of the model domain.	Overestimation of particle number concentration by a factor of 2 to 2.5 CDNC was overestimated by a factor of 5. Probably there was an excessive nucleation rate.	The model reproduced reasonably well the spatial and seasonal variations of most meteorological fields and chemical concentrations. Limitations by uncertainties in emissions and/or imperfectness in modeling aerosol processes.

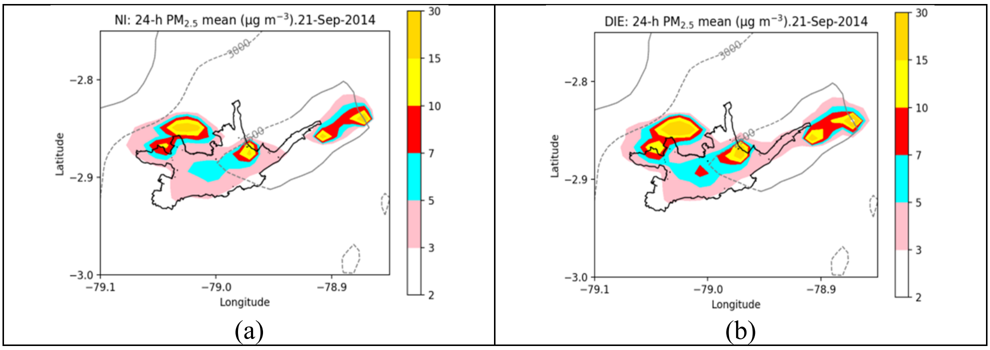

Figure 6: Modeled 24 h $PM_{2.5}$ mean at 21 September 2014: (a) No interaction (NI), (b) Direct and Indirect Effects (DIE).

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