



Using WRF-Chem for Simulating and Evaluating the Dust Three Emission Schemes during Severe Dust Storm 27 to 30 March 2018 over Sudan

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Abstract: The severe dust storm that invaded Sudan in late March was simulated using WRF-Chem model. The study objectives were to evaluate the model performance over Sudan for the three dust emission schemes the GOCART, AFWA, and UoC. Secondly, using the better scheme to discuss some meteorological aspects of dust emission and transport, such as changes in the quantities of winds, temperature, pressure, and relative humidity. Thirdly, demonstrating the meteorological mechanism by which dust moves farther distances. WRF-Chem was set for default and ran from 00:00 UTC 27 March to 18:00 UTC 30 March 2018 using NCEP final model data. Generally, all schemes of the model reproduced dust emission very well compared to MODIS and MERRA-2 satellite. The GOCART scheme has chosen to be the better scheme. In addition to emission part, the GOCART scheme (dust option = 1) simulated the meteorological variables very well compared to NCEP/NCAR and ERA5. WRF-Chem performed well and can be used for dust forecast over the Sahara regions, including Sudan.

Keywords: Sudan; Dust Emission Schemes; WRF-Chem; MODIS; MERRA-2; Meteorological Variables; NRMSE; R^2 ; NMB.

1. Introduction

Dust storms are defined as massive quantities of dust raised into the air by surface winds and reduced visibility to less than 1000 m (Middleton and Kang 2017). Dust storm occurs in arid and deserts areas in the world (Knippertz and Fink 2006; S. Wang et al. 2005; Yang et al. 2007). The dust storms distribution depends on the surface characteristics such as vegetation cover, composition and the wet content of the soil, in addition to surface wind speed (Eghbali, Mirrokni, and Memarian 2016). These storms are dangerous for transport means, and they can bring some light chemicals from one place to another. Also, the dusty air causes negative impacts on the human respiratory and cardiovascular systems (Achudume and Oladipo 2009; Khaniabadi et al. 2017; Zhang et al. 2016). Dust aerosol can impact the radiation balance of the earth system and atmosphere (Artaxo et al. 2013; Lindstrom 2018). Can affect the Earth's radiation budget through the scattering and absorbing of short wave radiation. Alters the radiative balance of the Earth's atmosphere, which is called the direct radiative effect (Gemma Shepherd et al. 2016; P. Ginoux et al. 2004). Through indirect effect, dust aerosol can impact the cloud physics by acting as cloud condensation nuclei and ice nuclei (Qi, Ge, and Huang 2013). In meteorology, dust storms occur due to changes in meteorological variables during frontal system passage and thunderstorms dissipation in spring, winter, and early summer (Cowie, Knippertz, and Marsham 2014; Die, Lei, and Hongbin 2014; Fountoukis et al. 2016; P. Ginoux et al. 2004; Holton et al. 2019; Kang et al. 2019; Knippertz 2015; Knippertz and Fink 2006; Parolari et al. 2016; Rizza et al. 2017; Shao, Jung, and Leslie 2002; Touré, Konaré, and Silué 2012; S. Wang et al. 2005; Yang et al. 2007). During the event, significant differences in meteorological variables usually occur and are markedly correlated to the dust storm (Knippertz 2015; Li et al. 2017; Tuccella et al. 2012). The reasonable method to study dust mechanisms is to plot the typical synoptic meteorological conditions on the surface and upper levels (Morales 1980), and of course, the proper use of meteorological boundary conditions is crucial (Parajuli et al. 2019).

The numerical simulation systems simulate dust emission and transport in a very interactive way with meteorological variables (Eghbali, Majid MirRokni, and Hossein Memarian 2016; LeGrand et al. 2019; Nguyen et al. 2019; Song et al. 2019; Ukhov et al. 2020). Comparing and Evaluating of WRF-Chem dust emission schemes the Goddard Chemistry Aerosol Radiation and Transport (GOCART), Air Force Weather Agency (AFWA), and the University of Cologne (UoC) are a newly studying issue in the numerical simulation community (Ma et al. 2019; Nikfal et al. 2018; Saidou Chaibou et al. 2019). The models usually underestimate Aerosol Optical Depth (AOD) (Feng et al. 2016; Govardhan et al. 2015; Palacios-Peña et al. 2020) for some reasons.

By comparing the aerosol scattering and absorption coefficients, the first reason was that the absorption coefficient shows better agreement with observations than the scattering coefficient. Meaning that the problem is due to underestimating the aerosol scattering coefficient (J. Wang et al. 1955). The second reason may be relative humidity bias (Feng et al. 2016), while the third reason could be the improper setting of boundary layer parameterization and emission schemes inventory (Govardhan et al. 2015). In terms of model verification and assessment, remote sensing techniques have been using to check the model performance for meteorological and dust emission variables (Karagulian et al. 2019; Luo et al. 2017; Mohamad 2015; Mokhtari et al. 2015; Nguyen et al. 2019; Rostkier-edelstein et al. 2019; Saidou Chaibou et al. 2019; Touré, Konaré, and Silué 2012). Moderate Resolution Imaging Spectro-radiometer (MODIS) products are widely used besides the numerical models for the fields of dust and aerosol emissions as a trial to generate results that are supposed to be near to reality. These trials usually give good results and reflected the model performance, too (Eghbali, Mirrokni, and Memarian 2016; Eltahan, Shokr, and Sherif 2018; Karagulian et al. 2019). Modern-Era Retrospective analysis for Research and Applications (MERRA-2) satellite version 2, in turn, has been using and gave good results for both large scale and regional (Aldabash, Balcik, and Glantz 2020; Bosilovich, Lucchesi, and Suarez 2016; He et al. 2019; Hersbach et al. 2020; Ostrenga Dana 2020). Many studies have been conducted temporally and spatially on dust storms over North Africa and the Sahara Desert areas (Cowie, Knippertz, and Marsham 2014; P. Ginoux et al. 2004; Knippertz and Fink 2006; Parajuli et al. 2019; Rostkier-edelstein et al. 2019; Saidou Chaibou et al. 2019). Sudan represents the southeastern extension of this Sahara Desert and usually is a dust storm receiver (Hereher 2011). Some studies stated that Sudan is the dustiest area in the Sahara area and north Africa with a very high frequency of dust emission and transport (Cowie, Knippertz, and Marsham 2014). Moreover, the satellite and ground-based stations have shown that most of the dust transportation over the Middle East and Arabian Peninsula comes from the eastern Sahara Desert areas (Sudan, Libya, and Egypt) during spring, summer, and autumn (Touré, Konaré, and Silué 2012). The study objectives were to evaluate the model performance over Sudan for the three dust emission schemes the GOCART, AFWA, and UoC. Secondly, using the better scheme to discuss some meteorological aspects of dust emission and transport, such as changes in the quantities of winds, temperature, pressure, and relative humidity. Thirdly, demonstrating the meteorological mechanism by which dust moves farther distances.

2. Materials and Methods

2.1. Model description and set-up

WRF-Chem model version 4 coupled with the GOCART aerosol module (LeGrand et al. 2019) (chem_opt=300) demonstrates the methodology used as the numerical simulation system for this study. The data used as boundary conditions are NCEP final (fnl) data of 1°×1° resolution. The numerical simulation domain designed over the study area was 50 Km resolution with a single nesting domain representing the mother domain's thirds. The three dust emission schemes set in the simulation name-list as dust options 1 for GOCART, 3 for AFWA, and 4 for UoC (for instance, dust_opt=1).

WRF-Chem is a fully coupled online community model for the prediction/forecast and simulation of weather, dispersion, air quality, dust, black carbon, etc. (Grell et al. 2005; LeGrand et al. 2019; Rizza et al. 2017; Ukhov et al. 2020). WRF-Chem can interactively simulate trace gases and particles and allow for feedback between the meteorology and radiative activity of the different atmospheric matters (Grell et al. 2005; Mues et al. 2018).

In this study, the model's dust emission schemes are set for default with ignoring radiative feedback (direct and indirect radiation feedback). Dust emission calculation process founded by Ginoux et al. (2001)(Paul Ginoux et al. 2001) is:

$$S = \left(\frac{Z_{maximum} - Z_i}{Z_{maximum} - Z_{minimum}} \right) \quad (1)$$

For the altitude Z_i , S represents the probability value of accumulated sediments for the i numbers of the grid cell, while $Z_{maximum}$ and $Z_{minimum}$; are the lowest and highest elevation for the grid i in the surrounding of 10×10 degrees, respectively (LeGrand et al. 2019; Nikfal et al. 2018; Saidou Chaibou et al. 2019).

2.1.1 GOCART

Can simulate and retrieve most of the aerosol materials into the boundary layer, including sulfate, dust, carbon compounds such as black carbon. The GOCART dust emission scheme is one of the most common aerosol schemes used in WRF-Chem (Ukhov et al. 2020). By aiding Gillette and Passi (1988) equation, the GOCART scheme generates dust flux (F_p) as follows:

$$F_p = \begin{cases} C S_{sp} u^2 (u_{10m} - u_t), & \text{if } u_{10m} > u_t \\ 0, & \text{otherwise,} \end{cases} \quad (2)$$

Where:

C of unit $\mu\text{g s}^2 \text{m}^{-5}$ implies the spatially constant factor that controls the dust emission flux magnitude. S stands for the source function Ginoux et al. (2001) (Paul Ginoux et al. 2001) that related to the spatial distribution of dust emissions process; u_{10m} stand

for the horizontal wind speed at 10 m. u_t implies the threshold velocity, s_p is the mass fraction that emitted into dustbin p.

The threshold velocity of dust generation is the most important parameter of the equation because it depends on some topographical features Gillette and Passi (1988). GOCART scheme set for (dust option=1) in the model name-list of simulation process (Ukhov et al. 2020) (Saidou Chaibou et al. 2019).

2.1.2 AFWA

Represents the second option of the dust emission schemes (that is implemented as dust option=3) in the model simulation name-list depending on Marticorena and Bergametti (1995) (Marticorena and Bergametti 1995) formula and is designed with three main components including the saltation flux, bulk vertical dust flux, and threshold Friction Velocity that given by Iversen and White (1982) as follows:

$$u_t(D_p) = 0.129 \frac{\left[\frac{\rho_p D_p}{\rho_a}\right]^{0.5} \left[1 + \frac{0.006}{\rho_p g D_p^{2.5}}\right]^{0.5}}{[1.928(aD_p^x + b)^{0.092} - 1]^{0.5}}; u_t = u_t(D_p) \frac{f(\text{moisture})}{f(\text{moisture})} \quad (3)$$

where g is the acceleration due to gravity, D_p is particle diameter; ρ_a is air density; $aD_p^x + b$ is the friction Reynolds number, the dust flux estimated through Saltation Flux over Bare Soil by Kawamura (1951) given as follows:

$$H(D_p) = C \frac{\rho_a}{g} u^3 \left(1 + \frac{u_t}{u}\right) \left(1 - \frac{u_t^2}{u^2}\right) \quad (4)$$

where C is an empirical constant, ρ_a is the density of air parcel, while u is the friction velocity and u_t is the threshold friction velocity. Bulk Vertical Dust Flux by Gillett, 1979 explained by the following formula.

$$F_{\text{bulk}} = H \propto S \quad \alpha = 10^{0.134(\% \text{clay}) - 6} \quad (5)$$

Where α stands for the sandblasting efficiency factor, S represents the dust erodibility, and %clay is the soil clay mass fraction by Ginoux et al. (2001) (Paul Ginoux et al. 2001).

2.1.3 University of Cologne (UoC)

UoC provided the third scheme of dust retrieval to work on WRF-Chem (that implemented as dust option=4 in the simulation name-list) based on Shao (2001, 2004) (Shao 2001, 2004), and Shao et al. (2011) (Shao et al. 2011) so, the dust emission generated by:

$$F(d_i, d_s = C_\gamma \eta_{fi}) [(1 - \gamma) + \gamma \sigma_p] (1 + \sigma_m \frac{gQ}{u_*^2}) \quad (6)$$

$F(d_i, d_s)$ stands for rate of dust emission for the i numbers of particle group of size d_i generated by the particles affected by the saltation of size d_s . C_γ is dimensionless factor or coefficient, and γ is a function that describes how simply aggregated dust can be liberating, described as, Q is the streamwise saltation flux of d_s , g is the acceleration due to gravity and u_* is friction velocity; u_{*t} is the threshold friction velocity; σ_m is the ratio between the mass of impacting particle (m) and mass ejected by bombardment m_Ω :

$$\sigma_m = \frac{m_\Omega}{m} \quad (7)$$

which can be explained as bombardment efficiency; so the ratio between the free dust and aggregated dust given by,

$$\sigma_p = \frac{\eta_{mi}}{\eta_{fi}} = \frac{P_m(d_i)}{P_f(d_i)} \quad (8)$$

Aerosol Optical Depth (AOD) retrieval formula simply is given by,

$$AOD_{550} = AOD_{440} \times \left(\frac{440}{550} \right)^{\frac{AE_{440}}{550}} \quad (9)$$

Where $AE_{440/550}$ is the Ångström Exponent represented for 0.44 and 0.550 micron wavelengths (Eltahan, Shokr, and Sherif 2018; LeGrand et al. 2019; Nikfal et al. 2018; Saidou Chaibou et al. 2019).

Table 1 The schemes used for simulation in WRF-Chrm's name-list

Simulation scheme on WRF-Chem	The chosen options
GOCART Simple Aerosol Scheme	300
Dust Emission Option (GOCART)	1
Dust Emission Option (AFWA)	3
Dust Emission Option (UoC)	4
Unified Noah Land Surface Scheme	2
Cumulus Scheme option	5
Microphysics Scheme option	3

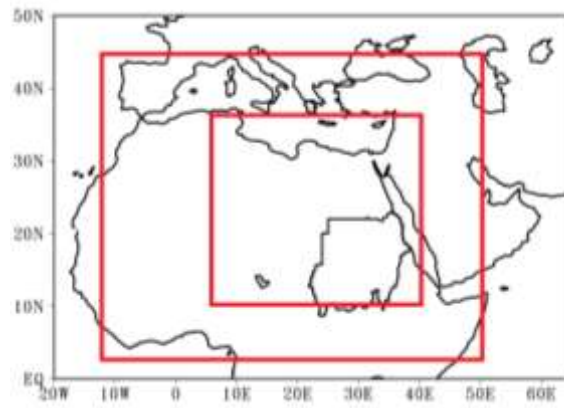


Figure 1 Simulation domain on the model

3. Results

The spatial and temporal distribution of AOD and dust concentration from the three schemes were compared with MODIS and MERRA-2 satellites, respectively. These time series are taken from the area average box over Sudan (21E-35E, 14N-23N). Simultaneously, the spatial distribution of AOD taken for the whole mother domain shows the area of dust emission and transport. Both distribution for the time from 27 March until 30 March 2018.

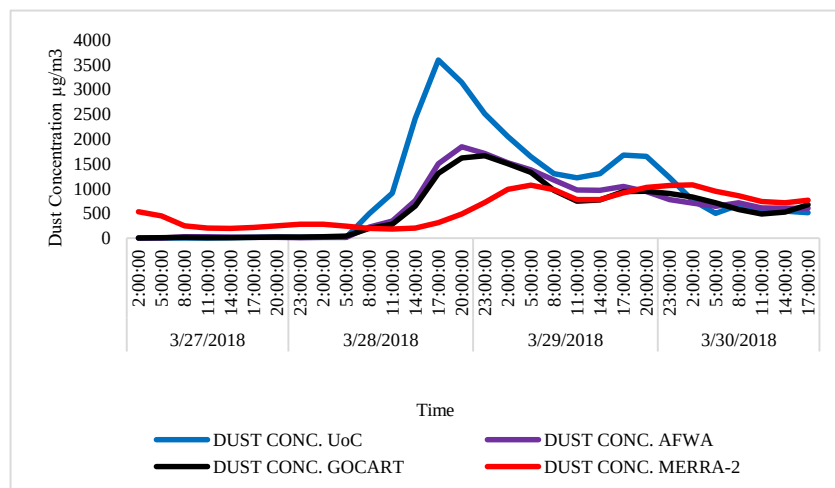


Figure 2 These are the three dust schemes compared to MERRA-2, where the solid red line is MERRA-2, the solid black line is GOCART, the solid violet line is AFWA, and the solid blue line is UoC.

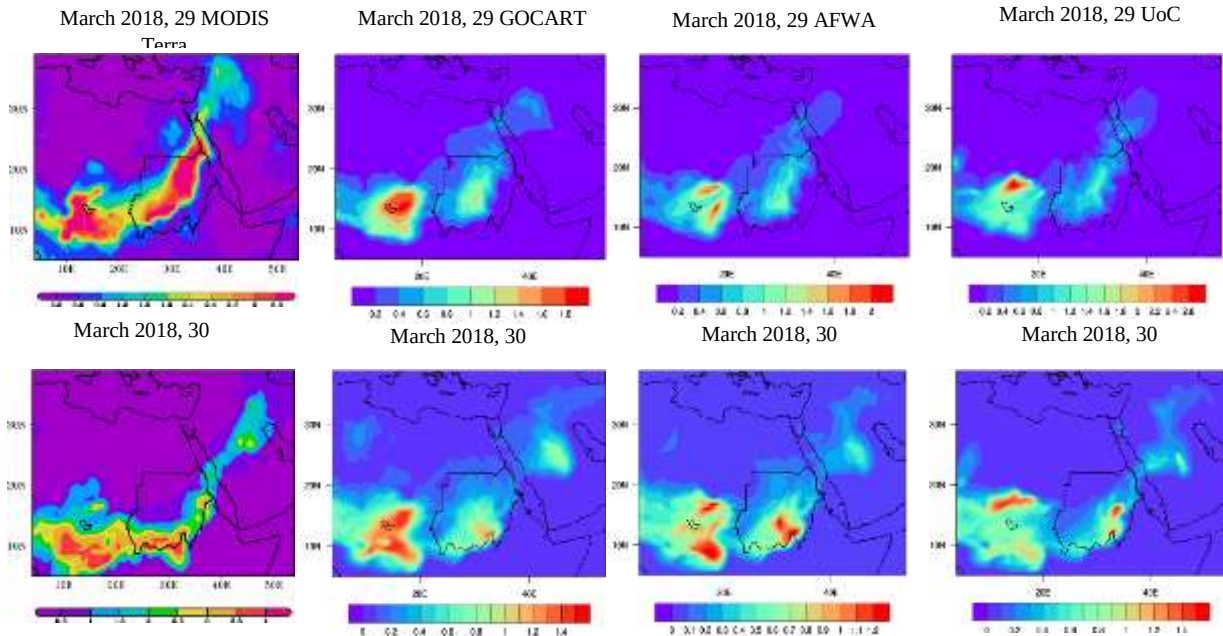


Figure 3 Spatial distribution of Aerosol Optical Depth (AOD) 0.55 micron from MODIS compared to the model three schemes, plotted for a daily mean during 29 to 30 March, the days when the dust invaded Sudan severely.

3.1 Model performance statistics

To check for the model performance, some statistical tests are used. Here it is essential to mention that for the simulation process in this study, the radiation feedback was ignored, which means there was not any consideration of the direct or indirect radiation feedback, so the meteorological variables were being the same for the three dust emission options (GOCART, AFWA, and UoC). To extract the time series of different variables, a box into the study area (longitude 21E-33E, latitude 10N-16N) was taken as a data field of meteorological variables and dust concentration.

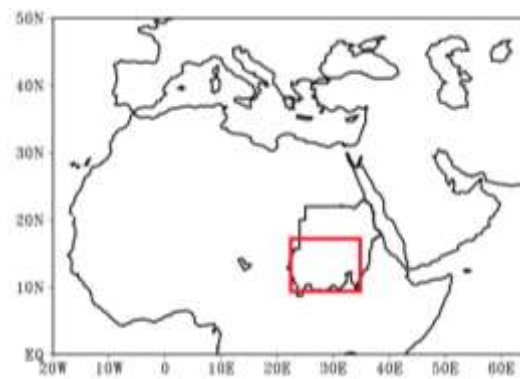


Figure 4 Area average that taken for time series for dust concentration, temperature, wind speed, and relative humidity

3.1.1. The bias (Normalized Mean Bias)

Normalized Mean Bias (NMB) is a statistical formula used to show how the model output records underestimation or overestimation compared to reanalysis data (Ma et al. 2019) (Kang et al. 2019)(Song et al. 2019). The bias enables evaluating whether predictions are accurate and whether the model tends to overestimate or underestimate the variable of interest's values. The computation is as follows:

$$\text{Normalized Mean Bias} = \frac{\sum_1^n (M-O)}{\sum_1^n (O)} = \frac{\sum (MODEL-ERA5)}{\sum (ERA5)}$$

Where O is ECMWF-ERA5 reanalysis data, and M represents the MODEL (WRF-Chem) or simulation output, so The more minor the bias (closer to 0), the better the model performance (Gustafson and Yu 2012).

3.1.2. Normalized Root Mean Square Error (NRMSE)

NRMSE defined as RMSE divided by the standard deviation of the observation. Where the smaller the value, the better model performance (Pelosi et al. 2020; Zhao et al. 2020).

$$\text{NRMSE} = \frac{\text{RMSE}}{\bar{o}} ; \text{ where } \bar{o} \text{ is the standard deviation of the observation, and}$$

$$\text{RMSE} = \sqrt{\sum_{i=1}^n \frac{(M-O)^2}{n}}$$

3.1.3 Coefficient of Determination (R²)

R² is the square of the correlation coefficient that describes the relationship between the variables from the Model and Observation. In statistics called the coefficient of determination, where the values closer to 1, the better the performance of the model (Zhao et al. 2020) (Holton et al. 2019)(Chang, Hu, and Liu 2014)(Rubinstein and Ben-hur 2020). The closer value to one, the better model performance (Aldabash, Balcik, and Glantz 2020; Schober and Schwarte 2018).

Table 2 Statistical reflections of the model performance

Variables from model versus MERRA-2					NRMSE	R ²	NMB
Dust	Concentration	Kg/m3	GOCART	vs	2.0	0.8	0.9
MERRA-2							
Dust	Concentration	Kg/m3	AFWA	vs	3.0	0.6	1.1
MERRA-2							
Dust	Concentration	Kg/m3	UoC	vs MERRA-2	5.9	0.2	2.1

How dust storm does emit and transport?

The synoptic situation maps at which the dust storm occurred should be designed to show the meteorological variables' role before and during the event (Morales 1980). In this study, general weather circulation of pressure, temperature, winds, and relative humidity, besides streamlines, were adopted. These maps were placed together side-by-side with their counterparts generated by the model to show the synoptic situation. Moreover, to show the model performance compared to the reanalysis data.

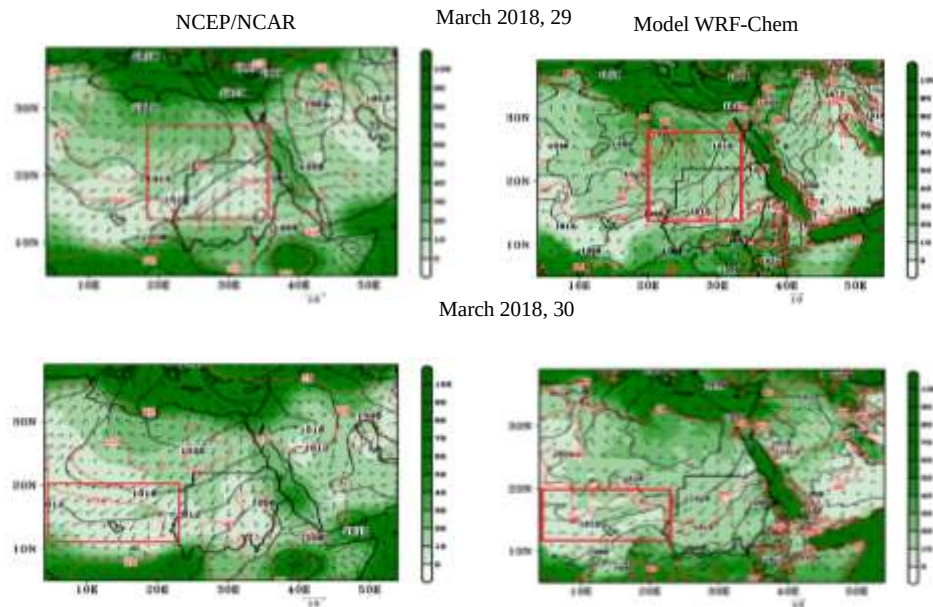


Figure 5 MSLP, RH, T2M, and WS describing the meteorological conditions from 29 to 30 March 2018 that contributing for the dust storm emission and transport from the Sahara Desert to Sudan and west countries of Sudan.

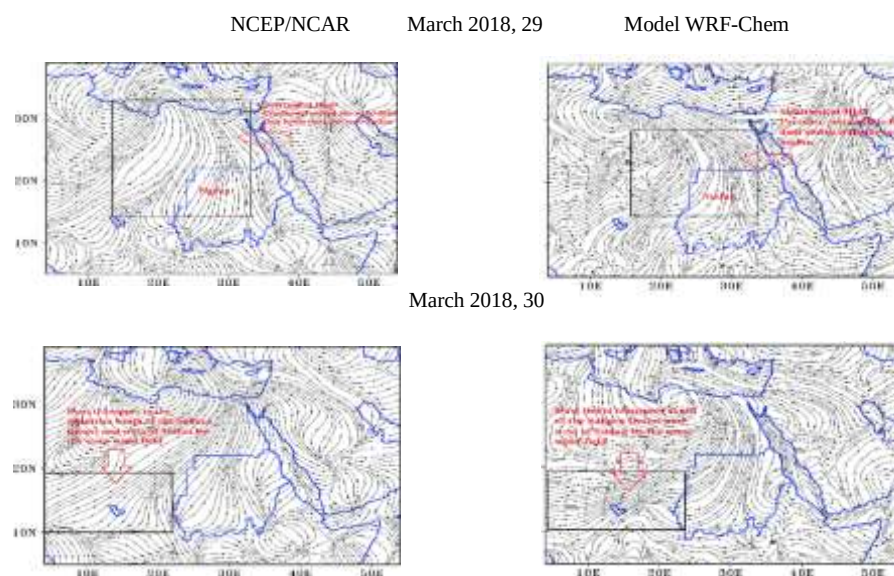


Figure 6 Streamlines describing the wind field from 29 to 30 March 2018 transferring the dust storm from the Sahara Desert to Sudan and west countries of Sudan.



Figure 7 MODIS image describing the dust storm coming from the Sahara Desert in late March 2018 (29-30)

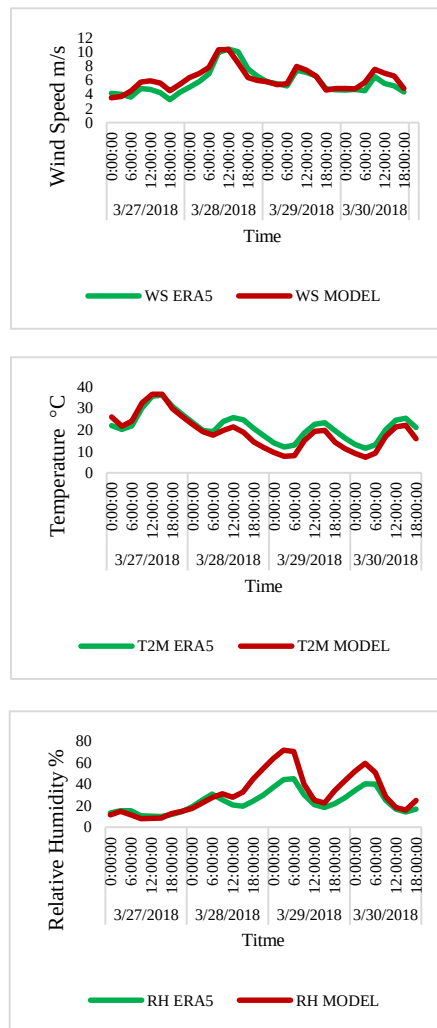


Figure 8 Meteorological variables interaction from ERA5 compared to WRF-Chem during the dust storm event intering Sudan from 27 to 30 March 2018.

Table 3 Statistical reflections of the model performance

Variables	from	model	versus	ERA5	NRMSE	R ²	NMB
reanalysis Data							
Relative Humidity %					0.1	0.8	0.3
Temperature °C					0.1	0.9	-0.1
Wind speed m/s					0.4	0.8	0.1

4. Discussion

Figure 2 shows the temporal distribution of dust concentration of the WRF-Chem three emission schemes compared to MERRA-2. The GOCART and AFWA schemes seem nearer to MERRA-2 satellite reanalysis data, while the UoC scheme was highly different. The three main dust emission schemes in the WRF-Chem model and their physical mechanism are different. The GOCART scheme focuses on the large-scale macro characteristics of the dust storm, such as the 10m horizontal wind speed in the circulation and the drivability of dust accumulation height in the sand source area. AFWA pays more attention to the friction speed, that is, the wind speed that directly drives the dust near the ground, and the types of sand, gravel, cobble, or other components in the sand source area. While, UoC scheme discusses the micro-dynamic process of dust, such as the dispersion and agglomeration of dust, the impact of dust, the effect of dust breaking and re-transmission. Figure 3 representing the spatial distribution of aerosol optical depth (AOD) 0.55 micron compared to MODIS Terra. The purpose of using AOD in this study is to compare the spatial distribution only without discussing the physics of the model contributing to dust reproduction. Table 2 demonstrating the statistical test that used for model performance regard. These tests used Normalized Mean Bias to determine how the model overestimates or underestimates the referenced data (satellite data or ground-based station data). The tests also used Normalized Root Mean Square Error (NRMSE) and the coefficient of determination (R²) to confirm each other for model performance. NMB, NRMSE, and R² reflected that the model performance was generally good, and the GOCART scheme was the best compared to AFWA and UoC. Therefore, the GOCART scheme used for the second part of the paper describing the meteorological conditions at which dust storms occurred.

Figures 5 and 6 represent the general circulation of the meteorological variables describing the conditions when the dust is emitted and transported. Figure 5 shows the situation dominated by subtropical anticyclones covering the Sahara Desert and the

Mediterranean Sea (the source of humidity). This system rotated over the Mediterranean Sea, pushing humid air over the Sahara Desert and contributing to the strengthening of this subtropical high. These dynamics made this high-pressure extend over the hot area over the desert towards the hottest area (Sudan Thermal Low), generating more gradients in pressure and temperature (the crowded lines of isobars and isotherms across short distances (Holton and Hakim 2012)). In these meteorological conditions mentioned, dust storms occurred because some studies stated that the pressure and temperature gradients are the leading causes of dust emission (Knippertz 2014; Knippertz and Fink 2006). In figure 6, the streamlines are defined as lines in parallelism with the local velocity vector (Illari and Marshall 2010) and represent the wind direction (Holton and Hakim 2012). Streamlines above ground level represented the wind flow's speed and direction that represented the air movement from an emission area. Streamlines also can determine the dust endpoint. Figures 5 and 6 showed that the meteorological system described both the dust emission and transport mechanisms; furthermore, showing how the model succeeded in the simulation of the meteorological conditions compared to NCEP/NCAR. Figure 7, the image from MODIS satellite confirming the dust transporting from the Sahara Desert southward to Sudan and west of Sudan. Figure 8 indicates the model simulation compared to ERA5 reanalysis data to assess meteorological variables' temporal distribution during dust events. The temporal distribution series are taken from the area average box shown in figure 4. This series was shown that the temperature dropped while relative humidity and the wind speed increased, meaning that the air mass was cold and wet. The series also showing the good performance of the model compared to ECMWF's well-prepared ERA5 reanalysis data. Some studies concluded that dust concentration directly proportional to the relative humidity. These studies suggested that dust storm forecasting models may be improved by adopting atmospheric humidity and wind speed as significant drivers for dust reproduction and transport (Csavina et al., 2014). This study found that the increment in dust concentration was associated with wind speed and relative humidity. Table 3 shows the statistical tests conducted on the model performance of the part related to the meteorological variables. NMB, NRMSE, and R^2 gave good results proving that the WRF-Chem model can simulate both dust materials and meteorological variables.

5. Conclusion:

The GOCART was a better scheme to stimulate dust materials (dust concentration and AOD) and meteorological variables over the Sahara Desert and Sudan. The pressure and temperature gradients generated by the subtropical high-pressure were responsible

for dust emission and transport. The streamlines techniques can describe the wind field by which dust moves and determine the dust storm endpoint. The statistical test (NMB, NRMSE, and R^2) conducted for both parts (dust emission and meteorological variables) proved that WRF-Chem was performed well and can be used for dust forecast and early warning for Sudan.

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