Development and evaluation of
desert dust emission model

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June 12, 2021
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Abstract

Laboratory of Atmospheric Physics

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Doctor of Physics

Development and evaluation of desert dust emission model

by Serafim Kontos

The PhD Thesis aims on the development and the update of the dust module within the Natural Emissions MOdel (NEMO) for applications on arid and semi-arid areas. The new dust module incorporates all the recent, state-of-art parameterizations, related to the physical mechanisms of wind-blown dust emissions. The updated dust module of NEMO enable the investigation of the differences originated from these parameterizations, in terms of dust emissions, as well the possibility to evaluate them and distinguish the best performing combination(s).

This study focuses on: a) the investigation of the variations produced from the three main components of the dust emissions mechanism, namely the horizontal mass flux, the drag partition efficiency and the sandblasting efficiency and b) the evaluation of all possible combinations with these parameterizations. The above are implemented at the Central Middle East area (CME), a region where these parameterizations are less studied, with significant dust sources and with available for evaluation data. The studied period selected is from April to June of 2015, where the dust events are more frequent. A total of 16
configurations with all possible combinations is utilized in order to investigate concretely the variations resulting from these parameterizations themselves.

The first part focuses on the differences among the 16 simulations for each parameterization of interest is done, in terms of emissions fluxes with absolute and relative values. Maps that emphasize their spatial differences in CME are also utilized. The total emissions’ budget is also calculated for all configurations. The final goal of this procedure is the quantification of their relative importance in terms of emissions, and their prioritization, creating a benchmark for future studies.

The second part focuses on the evaluation of these 16 configurations and the distinction of the best performing configuration(s). Their assessment is realized qualitatively with the aid of the MODIS Aerosol Optical Depths at 550 nm and quantitatively on-site measurements of PM10 concentrations for the days with significant dust events. For the quantitative assessment, two methods are applied in order to find concretely the best performing configuration(s): the application of a 50% acceptable level of uncertainty, utilizing all the common statistics and b) the FAIRMODE method, which enables, apart from the quantitative assessment, the determination of the origins of the uncertainties.
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List of Abbreviations

- **NEMO**: Natural Emissions MOdel
- **AOD**: Aerosol Optical Depth
- **CME**: Central Middle East
- **WRF**: Weather Research and Forecast Model
- **PM**: Particulate Matter
- **RMSE**: Root Mean Square Error
- **MB**: Mean Bias
- **MAE**: Mean Absolute Error
- **NMSE**: Normalized Mean Square Error
- **R**: Pearson Correlation Coefficient
- **Fac2**: Factor of 2
- **Fb**: Fractional bias
- **Fs**: Fractional standard deviation
- **CRMSE**: Centralized Root Mean Square Error
- **MQI**: Modeling Quality Index
- **MQI2_bias**: Squared Modeling Quality Index related to bias
- **MQI2_std**: Squared Modeling Quality Index related to standard deviation
- **MQI2_corr**: Squared Modeling Quality Index related to correlation
- **RMS_u**: Root Mean Square of measurements
Chapter 1

Introduction

Particulate matter (PM) is considered one of the major contributors to air pollution, posing adverse health effects (WHO, 2016) according to studies that have linked PM10 (particles with aerodynamic diameter of less than 10 µm) with cardiovascular and respiratory diseases (Brook et al., 2010; Heal, Kumar, and Harrison, 2012; Chen and Lippmann, 2009). PM originate from primary sources, typically distinguished to natural and anthropogenic, or secondary chemical transformations, and they can influence the air quality of areas far from their origin (Seinfeld and Pandis, 2016). Natural sources include aeolian erosion, sea salt from the oceans and biogenic material from the vegetation (Liora et al., 2016). The anthropogenic sources include all PM related to human activities e.g. transportation, energy production, industry, construction, and agriculture (Kim, Kabir, and Kabir, 2015).

Natural sources have the most important contribution to particulate matter (PM) emissions in the atmosphere, on a global scale (Viana et al., 2014). Among their different sources contributing to PM loads, mineral dust originated from arid and semi-arid areas, is considered to be the dominant, with an estimate of around 1500 Tg/year of dust (PM10) on a global basis (Zender, Bian, and Newman, 2003). Dust aerosols influence climate through different pathways, such as the radiative balance (Kumar et al., 2014), the cloud formation (Yin et al., 2002) and the chemistry of the atmosphere (Sokolik, 2003) while it has been shown that they have a negative impact on human health (Draxler et al., 2001;
Griffin and Kellogg, 2004). Thus, the accurate estimation of dust emissions is essential for the description of the physical and chemical mechanisms in the atmosphere, as well for the estimation of both its direct and indirect effects. In the next subsection the physical mechanisms of dust emissions and the current modeling approaches are briefly described.

1.1 Desert dust cycle in the atmosphere

The impact of the desert dust in the atmosphere is estimated with modeling systems that incorporate both meteorological and chemical transport, from global to regional scale (Kukkonen et al., 2012; Schaap et al., 2015; Lelieveld et al., 2015; Bey et al., 2001). During the last two decades, considerable effort has been made to simulate accurately the dust cycle on global and regional scale, with the aim of global circulation models (GCMs) and mesoscale models (Kok et al., 2014; Tanaka and Chiba, 2006; Zender, Bian, and Newman, 2003). The modeling systems utilized usually report dust emission fluxes, total emissions and concentrations. Despite the fact that these models can attribute the major sources, large uncertainties still remain on the dust emissions estimations. Concerning the total dust emissions globally for example the annual estimate can vary from 400 Tg (Huneeus et al., 2011) to 4500 Tg (Evan et al., 2014).

In terms of dust emission fluxes the diversity is even greater, and the reported values scarce. Global models focus on seasonal and/or annual temporal resolution and with a horizontal spatial resolution of $\sim 2^\circ$. For example, annual values of up to 500 $g/m^2 yr$ for the most intense dust sources were reported by Ginoux et al. (2001), $\sim 50$ $g/m^2 yr$ by Kok et al. (2014), 5-500 $g/m^2 yr$ by Luo, Mahowald, and Del Corral (2003), depending on the source definition and more than 100 $g/m^2 yr$ by Tanaka and Chiba (2006). Zender, Bian, and Newman (2003) reports the annual mean of dust fluxes of 0.1-5 $\mu g/m^2 s$, which is mostly related to the instant emissions.
1.1. Desert dust cycle in the atmosphere

On the other hand, the dust emission fluxes at regional scale focus on specific areas of interest, depending mainly on the available information for evaluation. Kang et al. (2011) applied WRF-Chem over East Asia with a resolution of 30 km during a dust event with three dust emission schemes. They found that the spatially averaged maximum dust emission fluxes ranged between 282 and 1488 $\mu g/m^2s$, and the instant fluxes reaching up to $10^4\mu g/m^2s$, as a result of the different parameterizations. For a similar area and spatial resolution in Asia, Liu et al. (2003) found maximum PM10 fluxes between 5 and 24 x$10^3\mu g/m^2s$ for a 10 days period and (Song et al., 2019) a mean up to 20 $\mu g/m^2s$ and a maximum of 325 $\mu g/m^2s$. In Middle East Area (MEA), the major dust sources emit 400-8000 $g/m^2yr$ annually (Shi et al., 2016), Fountoukis et al. (2016) reported monthly mean rates of 5-10 $\mu g/m^2s$, while Menut et al. (2013) found instant emission rates for both N.Africa and MEA of 50-20000 $\mu g/m^2s$. It can been seen that in general the range of annual total emission fluxes range between 5 and 500 $g/m^2yr$ and the instant mean fluxes between 10 and $10^4\mu g/m^2s$.

From the above, it can been seen that there isn’t any common approach to report emission rates, but their differences fall into 4 categories: a) spatial resolution (10-200km), b) temporal resolution of the reported values, c) dust emission schemes and d) input fields, either land use/soil texture either meteorological. Concerning the reported temporal resolution, one can distinguish two types of rates, periods’ mean fluxes and total period fluxes. Also it must be noticed that most of them have spatial resolution of 10 km or more, which is expected to have significant influence as we approach the local scale of the phenomenon.

The dust concentrations are usually estimated on a regional scale, with most of the studies of desert dust focusing in North Africa and the Sahel the transport of dust in South America and Mediterranean. These two regions produce the largest amounts of dust globally (Ginoux et al., 2001; Laurent et al., 2008; Laurent et al., 2010; Marticorena et al., 1997) and they can define the
background levels of particulate matter in remote areas (Katragkou et al., 2009; Mardi et al., 2018). Moreover, several studies have estimated the dust potential in Central and East Asia (Laurent et al., 2006; Shao, Jung, and Leslie, 2002; Sun et al., 2006) but little attention has been given to the Middle East Area (MEA).

MEA just recently started drawing attention because of its rapid growth in the sectors of energy and industry, while intense urbanization and construction emerge as a potent air pollution contributor (Hassan et al., 2017; Hassan, Kumar, and Kakosimos, 2016). Severe dust storms also affect the air quality in the region, as a result of frequent synoptic pressure gradients over the arid areas of Middle East (Yu et al., 2016; Walters Sr and Sjoberg, 1990; Namdari et al., 2018). The special synoptic patterns triggering these dust events originate from the convergence of two system. The first system is the Indian Monsoon depression, which begins to develop towards the Arabic Peninsula during the spring change-over period (Shalaby, Rappenglueck, and Eltahir, 2015). The second system is an anticyclone located over the eastern Mediterranean with a ridge extending southeast toward the northeast Persian Gulf (Al Senafi and Anis, 2015; Namdari et al., 2018). The aforementioned wind patterns are called Shamal winds or Shamal events (hereafter called Shamals). Shamals can trigger dust episodes, like the persistent event of July 3-8 of 2009 (Hamidi, Kavianpour, and Shao, 2014), leading to hundreds of emergency hospital admissions with respiratory ailments (Yu et al., 2016). Such dust events can be so intense that increase significantly even the indoor PM levels (Argyropoulos et al., 2016; Saraga et al., 2017).

The majority of the existing studies for the MEA focus on the impact of desert dust on air quality and human health (Abal et al., 2010; Al-Dawood, 2000; Draxler et al., 2001; Engelbrecht et al., 2008; Entisar, Fadi, and Muthanna, 2012). It has been also identified that PM levels in MEA vary from tenths to
thousands of $\mu g/m^3$ (Tsiouri, Kakosimos, and Kumar, 2015), with high fractions of mineral dust (Engelbrecht et al., 2009). Only few studies in this region focus on the contribution of the natural dust, (Prakash et al., 2015; Kalenderski, Stenchikov, and Zhao, 2013; Fountoukis et al., 2016), with a considerable variability among the modeling configurations. For example, Fountoukis et al. (2016) compared two dust emission schemes employing WRF-Chem over the Arabian Peninsula, and found significant differences on the amount and the spatial distribution of the dust emission fluxes. Similar results were reported by Kalenderski, Stenchikov, and Zhao (2013) and Prakash et al. (2015) when WRF-Chem upper level atmospheric estimates were compared with ground based and satellite measurements for two isolated dust storm events between 14-18 January 2009 and 18-20 March 2012 respectively.

In essence, there is a consensus on the criticality and the uncertainty of the dust emissions’ estimates and the consequent impact on PM10 estimations. More and longer modeling studies with validation against ground PM level concentrations are necessary to assess the impact of dust emissions on air quality in MEA and the neighboring regions (South-Eastern Europe, North Africa, and West Asia). In parallel, assessment of the modeling uncertainty and continuous improvement of dust modeling will improve progressively the confidence on the results.

1.2 Physics of wind blown dust

Every soil contains a number of particles in a wide range of diameters, with the erodible part ranging from few microns up to 600 $\mu m$. Most of the particles contained in the soil form aggregates of more than 40$\mu m$ because of the binding energies among the smaller particles, although a small mass fraction of them might be in free state (Chatenet et al., 1996).
The emission of dust particles is initiated when the wind stress is strong enough to mobilize them. The loose small particles (less than 20 $\mu$m in diameter) with weak bonds can be released directly to the atmosphere. This mechanism is usually assumed of minor significance, because of its’ small duration (\(\sim 120\) s) (Loosmore and Hunt, 2000).

The most important mechanism of dust emissions is the blasting of the large aggregates (i.e. sandblasting) on the surface, releasing indirectly the smaller particles, either from the soil or the aggregates themselves (Shao, 2008). These processes start when the friction velocity, i.e. the magnitude of wind speed’s turbulent fluctuations which defines the turbulent kinetic energy, exceeds a certain threshold, called threshold friction velocity. This threshold is determined from the balance of three forces, the wind’s drag, gravity and the attractive force binding the particle, and depends on Reynolds number and the particle’s diameter and density (Iversen and White, 1982).

Once the threshold is exceed the large aggregates are injected into the atmosphere, but because of their weight they return to the surface, following ballistic trajectories. This process is called saltation, the particles saltators and their vertically integrated horizontal flux in terms of mass as horizontal mass flux. When the saltators hit the soil, their momentum gained by wind is consumed, breaking the bonds of the smaller particles, leading eventually to suspension of small dust particles in the atmosphere. The release of dust particles from the soil is referred as saltation bombardment, while the breaking of saltators themselves as aggregate disintegration (Shao et al., 2011).

There are two factors that can reduce the turbulent momentum kinetic energy reaching the surface: a) roughness elements, which absorb part of this momentum and b) soil moisture, through the tensile strength applied on particles. Within the dust algorithms, these are included through factors that increase the threshold friction velocity, namely the drag partition scheme (ratio of covered surface threshold to uncovered threshold) and moisture tension factor (ratio
of the wet to dry erosion thresholds) for the roughness elements and moisture
effects respectively.

Although several wind tunnel measurements had been realized up to 1990,
mainly for the investigation of the horizontal mass flux (White, 1979; Owen,
1964), the first significant attempts to quantify the dust emissions started in the
early 90s. Shao, Raupach, and Findlater (1993) recognized the saltation bom-
bardment as the main constant mechanism for continuous, sustained emissions,
while Shao and Leslie (1997) used win tunnel measurements to calibrate the
first semi-empirical energy-based sandblasting parameterization. Marticorena
and Bergametti (1995) found an empirical equation for the sandblasting effi-
ciency, dependent only on soil’s clay content, while Marticorena et al. (1997)
developed the first drag partition scheme based on roughness length. Concern-
ing the latter, a new parameterization from (Raupach, Gillette, and Leys, 1993)
was also developed few years before, using the drag of each individual roughness
element.

The major improvements on dust emissions’ parameterization developed in
the next decade. Alfaro and Gomes (2001) derived a sandblasting parameteri-
zation, based on equivalent binding energies and the kinetic energy of the salta-
tors. Lu and Shao (1999) and later (Shao, Jung, and Leslie, 2002) deveoped the
mechanical concept of sandblasting efficiency, based on the volume scavenged
by each saltator, while (Shao, 2004) added the aggregate disintegration mecha-
nism. During the same year MacKinnon et al. (2004) updated Marticorena and
Bergametti (1995) drag partition scheme in order to include roughness lengths
up to 10 cm. The above sandblasting algorithms, together with the two drag
partition schemes (MacKinnon, Raupach) and the horizontal mass flux (White,
Owen) are considered as the most state-of-art modeling approaches, because
they incorporate all the micrometeorologically related variables, such as soil
particle distributions, friction velocity, soil plastic pressure etc.
1.3 Knowledge gaps on dust modeling

As shown in Section 1.1, information about the dust emissions estimations in MEA are limited in literature. Some studies have tried to identify the dust sources and attribute their contribution in MEA (Akbari, 2011; Alharbi, Maghrabi, and Tapper, 2013; Fountoukis et al., 2016; Gherboudj et al., 2015). Prakash et al. (2015) studied a dust storm during a 3-day period of March 2012 over Arabian Peninsula and they identified the major dust sources in the area while a modeling of a winter-time dust event was performed by Kalederski, Stenchikov, and Zhao (2013). Fountoukis et al. (2016) simulated dust emissions over Arabian Peninsula for July 2015 using two different emission schemes. Hassan, Kumar, and Kakosimos (2016) conducted measurements at specific locations in Qatar and estimated new emission factors for loose soil, based on carbonates. Most of the studies are focused on specific regions, like Middle East areas, and/or short time periods and may not represent adequately the dust sources in their most active timeframe. This lack of information is especially useful for policy-makers and governments, concerning the mitigation actions and measures needed to improve air quality in MEA. The above make MEA a special region for further investigation.

Another issue on dust emission modeling is the large range of the results produced and reported. The origins of the differences found on dust emissions can be divided into two categories: 1) uncertainties related to input data and 2) variations due to the dust parameterizations themselves. Shao et al. (2011) for example demonstrated that the coefficient of the horizontal mass flux can differ greatly, and might be soil texture dependent. The authors also pointed out the importance of the soil particle size distribution. Concerning the parameterizations, the combination of the three specific key-components of the dust modules, namely the horizontal mass flux of saltators, the drag partition scheme and the sandblasting efficiency can produce different results. Few studies have tried to
quantify the relative differences of the parameterizations, but not always with the state-of-art approaches (see Section 1.2). Kang et al. (2011) found significant variations between Marticorena and Bergametti (1995), Lu and Shao (1999) and Shao (2004), although the first is not the most comprehensive configuration, while the second is a subtractions of Shao (2004), Fountoukis et al. (2016) compared Marticorena and Bergametti (1995) and Shao et al. (2011), where the latter is the simplified version of Shao (2004) and Darmenova et al. (2009) compared Marticorena and Bergametti (1995) with Shao’s energy based schemes (Shao, Raupach, and Findlater, 1993; Shao and Leslie, 1997).

Although the input data can have a significant impact on dust emissions, the first step should be the distinction of the best performing combination of the components, and then to assess the uncertainties originated by the input fields. In order to do this, a concrete quantification of their differences of state-of-art parameterizations is need, aiming also on the prioritization of the components having the largest impact on dust emissions.

The above dictate the need for development of dust emission modeling system which will incorporate all the state-of-art dust schemes. Such emission models will enable the investigation of the differences between the existing parameterizations and their ability to simulate the desert dust in different areas.

An efficient and flexible emission model has created at the Aristotle University of Thessaloniki, called Natural Emissions MOdel (NEMO). NEMO has been utilized successfully in Europe for the study of sea salt, biogenic and the dust particles (Liora et al., 2015). Although the model contains a dust module, it isn’t optimizated for dust emissions from desert areas, like the Middle East. An extensive development of NEMO’s dust module would make it a valuable tool for studying the dust emissions.
1.4 Aim of the thesis

The PhD Thesis aims on the development of the desert dust module within the Natural Emissions MOdel (NEMO) for its application on arid and semi-arid areas. The new dust module incorporates all the recent, state-of-art parameterizations, related to the physical mechanisms of wind-blown dust emissions. The updated dust module of NEMO will enable the investigation of the differences originated from these parameterizations, in terms of dust emissions, as well the evaluation of them and the distinction of the best performing combination(s).
Chapter 2

Data and methodology

Based on the special synoptic conditions mentioned in Chapter 1, the potential for dust emissions (see also Fig. 2.2 and Prospero et al. (2002)), the scarcity of the scientific works in the area and the attention drawn by the World Health Organization (WHO, 2016), the central part of MEA is chosen (referred hereinafter as CME), for the estimation of the dust emissions differences among the possible combination of the state-of-the-art parameterizations; the horizontal mass flux, the drag partition and the sandblasting efficiency, as well for their indirect evaluation through in-situ and remote sensing measurements.

The next section describes the current state and the updates on NEMO, the modeling configurations, the data and methodology which is used for the sensitivity analysis of their dust emissions, as well for their evaluation.

2.1 The Natural Emissions MOdel

2.1.1 Dust emissions mechanisms and modeling

The dust production initiates after the mobilization of sand particles from the wind, when the friction velocity \( u_* \) exceeds a certain value, the so-called threshold friction velocity \( u_{*t} \). These sand particles, once they are released in the atmosphere, are accelerated from wind, but under their weight they return at
Chapter 2. Data and methodology

the surface, either scavenging the soil, a mechanism called saltation bombardment, either disintegrating, a process called saltation disintegration, releasing dust particles in the atmosphere. There is a third dust production mechanism, which is the direct suspension of dust particles in the atmosphere, namely aerodynamic entrainment. The latter is considered of minor significance (Loosmore and Hunt, 2000), because the binding energies of dust is usually much larger than the wind stress. The three production mechanisms are illustrated in Figure 2.1.

Figure 2.1: Dust production mechanisms: a) aerodynamic entrainment, b) saltation bombardment, c) aggregates disintegration (from Shao (2008))

The equation utilized in the dust modeling can be written in the general form:

\[ F(i, j, d_d) = S(i, j) \prod_{k=\text{veg, grav, snow, }} (1 - A_k(i, j)) \sum_{s} m_d(d_d) a(u_s, d_d, d_s) M_s(d_s) Q(d_s) \]

(2.1)

where \( i, j \) are the gridcell indices, \( S(i, j) \) is the soil erodibility factor, a calibration coefficient usually used as a weight factor of the dust source, the product of \( (1 - A_k(i, j)) \) is the erodible area fraction, including the vegetation, the gravel (non-erodible particles greater than 2mm diameter), snow etc., \( m_d \) is the emitted mass fraction of dust, \( a(u_s, d_d, d_s) \) is the sandblasting efficiency, \( M_s \) is the
mass fraction of the saltating dust particles, $Q(d_s)$ the horizontal mass flux for the saltating particles of diameter $d_s$, $F(i,j,d_d)$ is the emitted mass flux of the dust particles. $d_s$ and $d_d$ in the equation are the diameters of the saltating and emitted particles respectively.

Some factors that can inhibit the dust production are the soil moisture, the snow and the roughness elements, like rocks, vegetation etc. These effects reduce the available energy for the mobilization of the sand particle and are included in the above formalism through the increase of $u_{st}$, taking the general form

$$u_{st,eff} = f_{veg} \cdot f_{snow} \cdot \cdots \cdot f_{moist} u_{st}$$ (2.2)

where $f_{veg}, f_{snow}, f_{moist}, \ldots$ are the inhibiting factors for vegetation, snow, moisture etc., ranging between 0 and 1.

### 2.1.2 Current state of dust modeling in NEMO

The original version of the NEMO’s dust module (Liora et al., 2015) was mainly based on the methodology described in Schaap et al. (2009). The formulation of Iversen and White (1982) is utilized for the threshold friction velocity, as implemented by Marticorena and Bergametti (1995). Moreover, the effect of the soil moisture on the threshold friction velocity is included following Fécan, Marticorena, and Bergametti (1998), adopting the modification of Athanasopouloulou et al. (2010), which multiplies the soil moisture factor by 1.5. The drag partition scheme of Marticorena and Bergametti (1995) is used to modify the threshold due to the absorption of momentum from the roughness elements. The required roughness lengths for the drag partition take the constant values of $z_0 = 0.01cm$ and $z_{0s} = 0.0033cm$ for typical desert soils and smooth surfaces respectively. These roughness lengths are used for the calculation of the friction velocity.
The horizontal movement of the saltating particles (> 50µm) is calculated with the semi-empirical equation of White (1979). The soil size distribution adopted for the sand particles is based on Chatenet et al. (1996), reclassified according to Schaap et al. (2009). The energy-based dust emission scheme of Alfaro and Gomes (2001) is the physical dust mechanism in NEMO. This scheme has the advantage of producing by itself the mass size distribution for different meteorological conditions, avoiding the need to impose size distributions for the emitted particles. The calculated emitted dust is aggregated over the two bins used in CAMx, the first with particle diameters between 0.03µm and 2.5µm and the second between 2.5µm and 10µm.

### 2.1.3 Updates of dust modeling in NEMO

The revision of dust modeling in NEMO focuses on the three main components of the dust production formula, namely the horizontal mass flux, the drag partition and the sandblasting efficiency. Additional modifications on the input data, like the characterization of the roughness elements and of the soil texture, for the appropriate implementation of the three components.

#### 2.1.3.1 Horizontal Mass Flux

Few updates and additions on the horizontal mass flux parameterizations of sand particles are implemented within NEMO. A modification on the multiplication factor $c_b$ of the equation of White (1979) in 2.3

$$Q_h(d_s) = c_b \cdot u_*^3 \left( \frac{\rho_{\text{air}}}{g} \right) \left( 1 - \left( \frac{u_{*\text{eff}}}{u_*} \right)^2 \right) \left( 1 + \frac{u_{*\text{eff}}}{u_*} \right)$$

$c_b$ is set to 1 based on wind-tunnels measurements and re-evaluation of the formula (Laurent et al., 2006; Marticorena et al., 1997). The second most
The popular equation for the horizontal mass flux in state-of-the-art dust modules is that of Owen (1964), which is added to NEMO

\[
Q_h(d_s) = c_b \cdot u_s^3 \left( \frac{\rho_{\text{air}}}{g} \right) \left( 1 - \left( \frac{u_{*,\text{eff}}}{u_*} \right)^2 \right) \tag{2.4}
\]
equation 2.4 is a transport-limited equation, expressed by its multiplicative coefficient, where \( c_b \) takes the form

\[
c_b = 0.25 + \left( \frac{v_{\text{term}}}{3u_*} \right) \tag{2.5}
\]
with

\[
v_{\text{term}} = \left( \frac{4gd_sC_c\rho_s}{3Cd_{\text{air}}} \right) \tag{2.6}
\]
where \( v_{\text{term}} \) in 2.6 is the terminal velocity of the particle. Here, slip factor \( C_c \) is set equal to 1, while the drag coefficient \( C_d \) is the drag coefficient of the sand particles calculated based on Seinfeld and Pandis (2016), with \( d_s \) and \( \rho_s \) the sand particle’s diameter and density respectively. A comparison of White’s and Owen’s formalisms has already been done by Darmenova et al. (2009), assuming for both formalisms the coefficient \( c_b \) equal to 1. The authors have shown that these equations give similar results under bare soils. But even if Owen’s coefficient is expected to be close to 1 for the most common meteorological conditions, the transport-limited behavior of the equation, as expressed through the coefficient, is canceled. The Owen’s original equation is retained within NEMO with the variable coefficient, instead of a fixed one, maintaining this physical concept and equation’s consistency for all meteorological conditions. Their calculation is done for every diameter within the range 50-1000 \( \mu m \) for
every 5 µm, and only when the threshold friction velocity is exceeded. Also, the air density at the surface required by these equations is explicitly calculated based on the temperature, the surface pressure and the vapor mixing ratio of WRF model.

2.1.3.2 Drag Partition

Drag partition schemes take into account the absorption of the turbulent momentum by roughness elements, thus reducing the available energy for the mobilization of the sand particles. A major update is realized within NEMO by replacing the previous one (i.e. Marticorena and Bergametti (1995)) with the MacKinnon et al. (2004), because it enables the extension of drag partition to be utilized on roughness lengths up to 10 cm. MacKinnon’s equation uses the same physical considerations of the internal boundary layer between the roughness elements, as with Marticorena and Bergametti (1995) equation, but with recalculated wind’s fetch. The equation takes the form

\[
f_{\text{rough}} = \left(1 - \frac{\ln \left(\frac{z_o}{z_{os}}\right)}{\ln 0.7 \left(\frac{X}{z_{os}}\right)^{0.8}}\right)
\] (2.7)

where \(z_o\) is roughness length of the obstacles and \(z_{os}\) of the bare soil. \(X\) is the fetch length, equal to 12255 cm. The drag partition of Raupach, Gillette, and Leys (1993), with the recommended by Shao et al. (2011) parameters, has also been added in NEMO.

\[
f_{\text{rough}} = (1 - \sigma_v m_v \lambda_v) \left(1 + \beta_v m_v \lambda_v\right)^{0.5} \left(1 - \sigma_b m_b \frac{\lambda_b}{1 - A_v}\right)^{0.5} \left(1 + \beta_b m_b \frac{\lambda_b}{1 - A_v}\right)^{0.5}
\] (2.8)
\[ \sigma_b = 1; m_b = 0.5; \beta_b = 90 \quad \sigma_v = 1.45; m_v = 0.16; \beta_v = 202 \]

where \( \sigma, \lambda, \beta, m \) are the basal to frontal area ratio, the roughness density, the drag coefficients’ ratio of the roughness element to bare surface and the deviation factor from soil object approach for the vegetation (subscript \( v \)) and the bare soil (subscript \( b \)) respectively. This scheme utilizes the concept of the equivalent area and volume need to be set to zero to represent the absorption of the momentum by the roughness elements. In lack of detailed information concerning the types of the roughness elements in the studied area, the values from Darmenova et al. (2009) are adopted for the vegetation and the bare ground (i.e. \( \beta_v = 202, \sigma_v = 1.45, m = 0.16 \) and \( \beta_b = 90, \sigma_b = 1.0, m = 0.5 \) respectively). These values should be considered as mean properties of roughness elements’ types, in lack of additional information.

### 2.1.3.3 Sandblasting Efficiency

The last part of the dust module components that is modified is the sandblasting efficiency. It’s the most crucial part of the module since it defines the order of magnitude of the amount of dust. The current version utilizes the Alfaro and Gomes (2001), an energy based method. This method uses three dust logarithmic modes, assigning for each one a binding energy, namely \( e_1, e_2, e_3 \). The kinetic energy of the sand particle \( e_c \) is calculated, based on the diameter and the density of the particle and the friction velocity. Depending on the value of \( e_c \), the following energy fractions \( p_1, p_2, p_3 \) are calculated.
Chapter 2. Data and methodology

The scheme of Shao (2004) (SH04 hereinafter), which includes the full physics of sandblasting and commonly utilized on the recent models, is also added. Its physical context is based on the mechanical scavenging of the soil and the disintegration of the saltators themselves. For SH04 the sandblasting efficiency takes the form

\[ a(u_s, d_s, d_d) = \sigma_y g \frac{163p_iMMD_i^3}{6e_i} \sum_{i=1,2,3} \left( \rho_s \pi \frac{163p_iMMD_i^3}{e_i} \right) \]  \hspace{1cm} (2.13)

if \( e_c \leq e_3 \) then \( p_1, p_2, p_3 = 0 \)  \hspace{1cm} (2.9)

if \( e_3 \leq e_c \leq e_2 \) then \( p_1 = 0, p_2 = 0, p_3 = 1 \)  \hspace{1cm} (2.10)

if \( e_2 \leq e_c \leq e_1 \) then \( p_1 = 0, p_2 = \left( e_c - e_2 \right) \left( e_c - e_3 \right), p_3 = 1 - p_{23} \)  \hspace{1cm} (2.11)

if \( e_1 \leq e_c \) then \( p_1 = \left( e_c - e_1 \right), p_2 = (1 - p_1) \left( e_c - e_2 \right), p_3 = 1 - p_1 - p_2 \)  \hspace{1cm} (2.12)

the sandblasting efficiency for the specific \( d_s \) and the mass median diameter \( (MMD_i) \) is then calculated as:

\[ a(u_s, d_s, d_d) = \sigma_y g u_s^2 \left( (1 - \gamma) + \gamma \sigma_p \right) \]  \hspace{1cm} (2.14)

with
\[ \sigma_y = 12u^*_p \frac{\rho_{bulk}}{P} \left( 1 + \sqrt{\frac{\rho_{bulk}}{P}} \right) \] (2.15)

\[ \sigma_p = \frac{\eta_{mi}}{\eta_{fi}} \] (2.16)

\[ \gamma = \exp \left[ -k((u_s - u_{st})^3) \right] \] (2.17)

Here \( \eta_{fi} \) and \( \eta_{mi} \) are the mass fractions of the fully and minimally disturbed soils, \( \rho_{bulk} \) is the soil bulk density, \( P \) is the soil’s plastic pressure, defined as \( P = u^*_p \rho_{bulk} \) and \( k \) is a coefficient that defines the smoothness of the transition from coarser to finer particles. Following the recommendations of Shao et al. (2011), the coefficients \( k, c_y \) and \( u_{sp} \) are set to 0.5, 5.7e^{-5} and 4.5 respectively.

### 2.1.3.4 Soil and land cover properties

SH04 requires the particle size distributions under minimally and fully disturbed. The soil particle-size distributions from the WRF-Chem model are adopted (Fast et al., 2006; Grell et al., 2005), based on data collected by G.H. McTainsh and processed by Harry Butler and Martina Klose, following the assignment realized within the model. The addition of a second minimally dispersed distribution also enables us to investigate their indirect effect on dust emissions.

The Harmonized World Soil Data (HWSD) v1.2 is used to characterize the soil properties (available online at [http://webarchive.iiasa.ac.at/Research/LUC/External-World-soil-database/](http://webarchive.iiasa.ac.at/Research/LUC/External-World-soil-database/)). The soil database has 30 arc seconds spatial resolution and the percentages clay, silt, sand and gravel are imported.
in the emission model. In this way, all surface information are available and the dust erodibility factor $S$ is not necessary.

The Global Land Cover by National Mapping Organizations (GLCNMO) v.1 land use/land cover database is used (available online at http://www.iscgm.org/gm/glcnmo.html) for the land-use characterization. The database’s resolution is 30 arc seconds, created from MODIS data and comprise of 20 different classifications.

Three land use types that can act as potential dust sources: 1) sparse vegetation, 2) bare surface with consolidated material, like rocks and gravels and 3) bare soils with unconsolidated material as sandy areas. The middle type is assumed to be representative of gobi surfaces, which are flat, bare areas covered with gravel (Xian et al., 2002). Furthermore, in the current study, the roughness characterization is updated. The homogeneous value of $z_o$ (i.e. 0.01 cm) is replaced with a land use based field. Xian et al. (2002) took indirect measurements of the roughness lengths for gobi, and sand deserts in Asia. For gobi deserts they found that $z_o$ varies between 0.07-0.19 cm, depending on the dimensions and the density of the roughness elements. The authors mentioned that the lowest value (0.07 cm) may suffer from fetch issues. Ignoring this value, the average $z_o$ of the remaining measurements is adopted (i.e. 0.17 cm). The average value of 6.8 cm is assigned for the sparsely vegetated land use type, based on the Environmental (2006) and the fact that such areas can act as potential dust sources MacKinnon et al. (2004). A representative value of 0.01 cm for sandy areas is adopted, based on the average of Site 8 for the in-situ measurements of Marticorena et al. (2006), and the Environmental (2006). The selected roughness length for the gobi surfaces coincides with Marticorena et al. (2006) for Site 10, under neutral conditions over a surface of similar type in Tunisia, and consistent with the experimental values of Greeley et al. (1997) in the Death Valley. It is also comparable to the higher end of the satellite-based retrievals of Laurent et al. (2008) for hamadas surfaces (i.e. plateaux of bare rocks, stones
2.1. The Natural Emissions MOdel

and pebbles) of Sahara and similar to the weighted average over the Gobi desert in Asia (Laurent et al., 2005). The $z_o$ for the sandy areas is consistent with the respective satellite-derived values over the erg surfaces (sand dunes) of Sahara, although in some cases the roughness lengths can range between 0.001-0.01 cm (Laurent et al., 2008; Menut et al., 2013; Prigent, Jiménez, and Catherinot, 2012; Prigent et al., 2005). It should be mentioned that a similar range in the order of magnitude is found on the field measurements of Greeley et al. (1997) over the Namib sandy desert, indicating that the roughness length of sand dunes might depend strongly on the density and the arrangement of the dunes in the field.

Concerning the roughness densities, measurement data are limited in the literature. For the gobi and the sandy surfaces the values of 0.15, 0.002 cm are adopted, respectively, according to Darmenova et al. (2009). The sparse vegetation is treated with double drag partition method, assigning a roughness density of 0.018 (Darmenova et al., 2009). The above should be considered as representative values of gobi, sandy and vegetated surfaces.

2.1.4 Modeling set-up for the Central Middle East

CME chosen as the study area is mainly consisted by sparsely vegetated areas over the eastern part of Iraq and the southwestern Iran, with intermittent gobi surfaces. The rest of the domain consists of gobi and sandy surfaces. The land use cover utilized in CME are presented in Fig. 2.2.
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Figure 2.2: Global Land Cover by National Mapping Organizations database (GLCNMO, 2014). The assigned areas with a potential for dust production are indicated with yellow, light gray and dark gray for sparse vegetation, sandy and gobi surfaces respectively.

The dust emissions calculated with the Natural Emissions MOdel (NEMO) (Liora et al., 2015) are driven by the meteorological model WRF-ARW v3.7.1 (Grell et al., 2005). The model is applied over a 6 km horizontal resolution grid, covering CME (same area as in Fig. 2.2). The spring transition period and the early summer are selected as the simulated period, i.e. April, May, and June of 2015. For this 3-months’ time period the dust events over the Arabian Peninsula are considered to be frequent (Prakash et al., 2015), while in the middle of this period occurred one of the most severe dust storms (Saraga et al., 2017). All meteorological simulations were initialized at 1200 UTC every four days and the duration was set to 108h. The first 12 simulated hours were discarded as coinciding with the model’s spin-up period. For the initial and boundary conditions the analysis data of the European Center for Medium-range Weather Forecasts (ECMWF) are used, in 0.25º spatial resolution and 6h in temporal resolution. Microphysics processes are parameterized with the Thompson aerosol-aware scheme (Thompson and Eidhammer, 2014) for the inclusion of
their indirect effect on cloud formation. The surface layer is parameterized using the Revised MM5 scheme (Jiménez et al., 2012), while for the planetary boundary layer the ACM2 parameterization scheme (Pleim, 2007) was used. Land surface processes are coupled with the aim of Noah Land Surface Model (Tewari et al., 2004). Shortwave and longwave radiation processes are handled with the Dudhia shortwave scheme (Dudhia, 1989) and the RRTMG longwave parameterization (Iacono et al., 2008), respectively. The Kain-Fritsch scheme (Kain, 2004) is used for the cumulus convection in the domain. The above options on WRF were selected based on the assessment of Giannaros (2018). The evaluation of the meteorological fields in CME for the same period, which drive the dust emissions, has been implemented in the work of Kontos et al. (2018). Overall, it was concluded that the WRF model performs well on simulating the wind speed at 10-m, the most important driver of dust emissions. Also, the model replicates adequately the 2-m air temperature over the study area. Concerning the 2-m vapor pressure, the model seems to lack ability in simulating satisfactorily this variable.

2.1.5 Sensitivity analysis on dust emissions in CME

The variability of the following dust parameterizations on dust emissions is studied: a) the horizontal mass flux of the sand particles, b) drag partition scheme and c) sandblasting efficiency. The analysis is performed for PM10 dust emissions, implementing simulations with two horizontal mass fluxes formulas (White and Owen), drag partitions (MacKinnon and Raupach) and sandblasting efficiencies (AG01 and SH04). In order to implement SH04 scheme, the particle size distributions (PSD) of the sand particles adopted from WRF-Chem. This second PSD, together with Chatenet et al. (1996), give us the chance to provide an estimation of their indirect effect on each studied component, although this is not the main goal of the study. The study covers a three-month time
period, from 1st of April to 30th of June 2015, because of dust events that are frequent during this timeframe (Prakash et al., 2015) and the availability of high-quality ground level measurements for the subsequent evaluation in Doha, Qatar (Saraga et al., 2017).

In the following Chapter, the spatial distribution of the differences in the periods’ mean emission fluxes, the mean daily and the total emission fluxes over CME, as well their relative percentages. For the latter, the normalized relative differences (NRD) for each grid cell are calculated, as the sum of their emission fluxes differences divided by the sum of the averages of the two considered simulations over time (i.e. $NRD = \frac{2\sum_t (RJ - RI)}{\sum_t (RJ + RI)}$, where $RJ$ and $RI$ the considered simulated emissions). Domain-wide average, minimum and maximum values of the aforementioned statistics are also calculated and presented in tables. The configuration of each simulation is listed in Table 2.1.

<table>
<thead>
<tr>
<th>Sim. ID</th>
<th>Horizontal mass flux</th>
<th>Drag partition scheme</th>
<th>Sand Efficiency</th>
<th>Minimal PSD</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>White</td>
<td>MacKinnon</td>
<td>AG01</td>
<td>WRF-Chem</td>
</tr>
<tr>
<td>R2</td>
<td>White</td>
<td>MacKinnon</td>
<td>AG01</td>
<td>Chatenet</td>
</tr>
<tr>
<td>R3</td>
<td>White</td>
<td>MacKinnon</td>
<td>SH04</td>
<td>WRF-Chem</td>
</tr>
<tr>
<td>R4</td>
<td>White</td>
<td>MacKinnon</td>
<td>SH04</td>
<td>Chatenet</td>
</tr>
<tr>
<td>R5</td>
<td>White</td>
<td>Raupach</td>
<td>AG01</td>
<td>Chatenet</td>
</tr>
<tr>
<td>R6</td>
<td>White</td>
<td>Raupach</td>
<td>AG01</td>
<td>WRF-Chem</td>
</tr>
<tr>
<td>R7</td>
<td>White</td>
<td>Raupach</td>
<td>SH04</td>
<td>Chatenet</td>
</tr>
<tr>
<td>R8</td>
<td>White</td>
<td>Raupach</td>
<td>SH04</td>
<td>WRF-Chem</td>
</tr>
<tr>
<td>R9</td>
<td>Owen</td>
<td>MacKinnon</td>
<td>AG01</td>
<td>WRF-Chem</td>
</tr>
<tr>
<td>R10</td>
<td>Owen</td>
<td>MacKinnon</td>
<td>AG01</td>
<td>Chatenet</td>
</tr>
<tr>
<td>R11</td>
<td>Owen</td>
<td>MacKinnon</td>
<td>SH04</td>
<td>WRF-Chem</td>
</tr>
<tr>
<td>R12</td>
<td>Owen</td>
<td>MacKinnon</td>
<td>SH04</td>
<td>Chatenet</td>
</tr>
<tr>
<td>R13</td>
<td>Owen</td>
<td>Raupach</td>
<td>AG01</td>
<td>WRF-Chem</td>
</tr>
<tr>
<td>R14</td>
<td>Owen</td>
<td>Raupach</td>
<td>AG01</td>
<td>Chatenet</td>
</tr>
<tr>
<td>R15</td>
<td>Owen</td>
<td>Raupach</td>
<td>SH04</td>
<td>WRF-Chem</td>
</tr>
<tr>
<td>R16</td>
<td>Owen</td>
<td>Raupach</td>
<td>SH04</td>
<td>Chatenet</td>
</tr>
</tbody>
</table>

2.2 Evaluation of dust parameterizations

In an effort to narrow-down the list of the possible configurations and distinguish the most realistic parameterization(s) for the dust modeling, an extensive
evaluation of these 16 configurations is done, leading eventually to the identification of the best performing combination(s).

To achieve the above, we utilize the meteorological model WRF (Grell et al., 2005) and the chemistry transport model CAMx (Comprehensive Air Quality Model with Extensions, http://www.camx.com/) for the prediction of the PM10 concentrations in CME. The anthropogenic PM emissions are calculated with the aid of EDGAR v.4.3.1 database (Crippa et al., 2016), complementary to the application of the 16 configurations of NEMO, for the same 3-months period, as in the sensitivity analysis. The modeling system is evaluated against PM10 ground level concentration measurements (Saraga et al., 2017) and with the MODIS Aerosol Optical Depth satellite products (Lyapustin and Wang, 2018).

2.2.1 Modeling system WRF-NEMO-CAMx

The meteorological conditions of the study period were simulated using the WRF-ARW v3.7.1 model applied with a spatial resolution of 6 km to produce the meteorological fields on hourly basis. Further details on the configuration of the WRF model and its evaluation in the study area for the same period, can be found in Kontos et al. (2018).

In order to be consistent with the evaluation of the PM10 measurements and the satellite data, the anthropogenic sources have been added in the modeling system. The anthropogenic emissions were derived with the application of the Model for the Spatial and Temporal Distribution of Emissions (MOSESS) (Markakis et al., 2013) using data from the EDGAR v.4.3.1 emission database. The EDGAR v.4.3.1 database provides monthly emissions with a spatial resolution of 0.1°x0.1° (http://edgar.jrc.ec.europa.eu/pegasos/index.php) (Crippa et al., 2016). The emission data were analyzed chemically and spatially over the studied domain, on a weekly and hourly basis. The temporal profiles were applied taking into account the fact that the weekend in Middle East is
Friday to Saturday. Thus, the appropriate shift on the weekly profiles was made. The selected anthropogenic emissions include power generation, residential combustion, manufacturing industry, process emissions during production and application, fuel production/transmission, oil production and refining, road transport, non-road transport, transformation industry, and agriculture.

The chemical speciation of non-methane volatile organic carbons (NMVOC) and of the particulate matter (PM) was applied for each emission source following a successful methodology employed earlier for Europe by Liora et al. (2015) and Liora et al. (2016). The chemical profiles of PM were taken from the Netherlands Organization (TNO) for sulfates, elementary and organic carbon, and other minerals. NMVOCs were separated into 23 species, using averaged profiles over CME from the RETRO ratios and for the five HTAP v2 sectors (Power, Industry, Transport, Residential, Agriculture) (http://iek8wikis.iek.fzjuelich.de/HTAPWiki/). For the cases where no NMVOCs emissions existed in HTAP v2, the TNO chemical profiles were used.

The final step of the modeling system was the implementation of the chemical transport model CAMx (Comprehensive Air Quality Model with Extensions, www.camx.com) version 6.4. The horizontal extend and the spatial resolution was the same, as for the WRF model. The vertical spacing follows the WRF levels, aggregated to 17 layers. The vertical spacing varies from \( \sim 30m \) depth for a.g.l. up to 100\( m \), 120\( m \) up to 1000\( m \), 200\( m \) up to 2200\( m \) a.g.l. and above that height between 700 – 2000\( m \) depth. The initial and boundary conditions of the species were taken from the MACC III product of IFS (Inness et al., 2013). The PM concentrations were partitioned between coarse and fine CAMx species, where coarse and fine are defined as particles with diameters between 2.5 and 10 \( \mu m \) and between 0.03 and 2.5 \( \mu m \) respectively. For the studied period, a spin-up of 15 days was applied to ensure representative background concentrations. CAMx was configured with the Bott (1989) advection scheme,
the updated dry deposition of Zhang, Brook, and Vet (2003), and the wet depo-
sition of Seinfeld and Pandis (2016). The CB05 gas phase chemical mechanism
was used, with 51 species and 156 reactions (Yarwood et al., 2005), with the
EBI solver. The time step used in the implicit turbulent vertical mixing was
set to 30s, to ensure sufficient mixing from the bottom to the upper layers.

2.2.2 Data and methodology of evaluation

2.2.2.1 In-situ measurements

A monitoring campaign was performed from 1st March to 30th June 2015 at
Doha City, Qatar (UTM 39R 551180m E 2797980m N) which is located in the
center of the region of interest. PM number concentrations and meteorological
data were collected using an Environ Check 365#, based on laser light scat-
tering, and manufactured by Grimm Aerosol Technik GmbH & Co. KG, Ger-
many. PM mass concentrations were collected also using a reference gravimetric
method according to the EN 12341:2014 with a low volume sampler (LVS16 by
GRIMM Aerosol Technik GmbH & Co.). Values from both methods showed
very good agreement (Pearson correlation $r = 0.95$ with $p - value < 0.001$).
More details about the field campaign, employed gravimetric method, and pro-
tocols are provided by Saraga et al. (2017). In this study, the daily mean PM10
concentrations for the period April-June 2015 are used to evaluate quantita-
tively the performance of the aforementioned configurations (Table 2.1). For
the assessment of the natural dust emission parameterizations, only the days
with a PM10 daily mean concentration greater than $200 \mu g/m^3$ will be employed,
following the definition of significant dusty days by Draxler et al. (2001) to
minimize the influence of other local and underrepresented anthropogenic sources
(e.g. construction activities (Hassan et al., 2017; Hassan, Kumar, and Kakosi-
mos, 2016).
2.2.2.2 Satellite data

The Aerosol Optical Depth at 550 nm ($AOD_{550}$) of the Multi-Angle Implementation of the Atmospheric Correction Level-2 gridded (MCD19A2 L2G) product is used for the qualitative evaluation of the dust parameterizations (Lyapustin and Wang, 2018). It is derived from the combination of the Terra and Aqua MODIS L2 products, with a daily temporal resolution and 1 km pixel spatial size. The choice was based on the high resolution of the data and their availability for the specific time period (April-June 2015). The overpass times of MODIS $AOD_{550}$ for the studied region has been between 5 and 11 UTC.

The $AOD_{550}$ data from MODIS are compared with estimated $AOD_{550}$ values based on the CAMx results, after the former are reprojected on the CAMx grid (Lambert conformal conic projection), using the first order conservative method of the Climate Data Operator tool (Schulzweida, 2017). The estimation of the CAMx based $AOD_{550}$, follows the modified version of the IMPROVE algorithm (Malm and Hand, 2007; Pitchford et al., 2007), which takes into account the ammonium nitrate and sulfate salts, sea-salt, fine and coarse dust, particulate organic aerosols, and black carbon. The choice of this expression was done bearing in mind the extensive amount of the measured optical properties in the frame of IMPROVE campaign at regional scales, suitable for the extraction of the AOD from the fine and the coarse concentrations of CAMx. Specifically, the following equation was used to calculate the aerosols’ extinction efficiency at 550 nm:
\[
\sigma_{\text{ext}, 550} = 2.2 f_s(RH)[\text{small sulfate}] + 4.8 f_L(RH)[\text{large sulfate}]
+ 2.4 f_s(RH)[\text{small nitrate}] + 5.1 f_L(RH)[\text{large nitrate}]
+ 2.8 [\text{small organic mass}] + 6.1 [\text{large organic mass}]
+ 10 [\text{Black Carbon}] + 1 [\text{Fine dust}] + 0.6 [\text{Coarse dust}] + 1.7 f_{ss}(RH)[\text{sea salt}]
\]

(2.18)

where the coefficients represent the dry mass extinction efficiencies \((m^2/g)\), \(f(RH)\) are the enhancement factors as described in Pitchford et al. (2007), and the bracketed variables are the concentrations of each species \((\mu g/m^3)\). Here, only the sulfates, nitrates and sea salt are considered as hydrosopic. The large and small fractions of the species’ concentrations are calculated as:

\[
[\text{Large } X] = [\text{Total } X]^2/20, \text{ for } [\text{Total } X] < 20 \mu g/m^3
\]

(2.19)

\[
[\text{Large } X] = [\text{Total } X], \text{ for } [\text{Total } X] \geq 20 \mu g/m^3
\]

(2.20)

\[
[\text{Small } X] = [\text{Total } X] - [\text{Large } X]
\]

(2.21)

where \(X\) is the sulfates, nitrates, or organic mass concentrations. The ammonium sulfate and ammonium nitrate concentrations on this equation is assumed equal to 1.375 times the sulfate and 1.29 times the nitrate ions masses respectively. This implies that all sulfate and nitrate ions are neutralized by the ammonium cations. Finally, the calculated extinction efficiencies are integrated for the overpass time period of the satellites to produce the AOD\(_{550}\).

### 2.2.3 Statistical analysis

The statistical metrics that are used for the quantitative evaluation of the results are the Pearson’s correlation coefficient (R), the mean bias (MB), the normalized mean square error (NMSE), the factor of 2 (Fac2), the fractional bias (\(F_b\),
Chapter 2. Data and methodology

the fractional standard deviation ($F_s$), the Index of Agreement (IOA), which is indicative of the overall performance, and the centralized root mean square error (CRMSE). Unfortunately, there isn’t any unique, optimal and/or standardized method to define acceptance criteria for the configurations. For example, the EU Directives (EC, 2008) accept a 50% error level only for the annual PM10 and without an explicit definition of the error’s statistical metric. The U.S. E.P.A defines the absolute fractional bias of the 25 highest PM values as the statistical criterion with a less than 0.67 acceptance criteria (Cox, 1992). Kumar, Luo, and Bennett (1993) suggested as acceptance criteria a NMSE less or equal to 0.5, a $F_b$ between -0.5 and 0.5, and a Fac2 greater than 0.85. The Department for Environment, Food and Rural Affairs of UK (Defra) sets as criteria a Normalized Mean Bias (NMB) between -0.2 and -0.2 and a Fac2 equal or greater than 0.5 (Derwent et al., 2010). All the above converge towards a 50% acceptance level for metrics associated with the relative magnitude of the uncertainty, like NMSE, $F_b$ and $F_s$. Thus, for these three statistics the 0.5 upper limit is applied as an acceptance criterion on the evaluation of the configurations, while the accepted Fac2 lower limit is set to 0.5.

Complementary evaluation for the daily mean PM10 measurements in Doha is performed, using the Modeling Quality Indicator (MQI), constructed in the frame of the FAIRMODE project (Monteiro et al., 2018). This indicator is defined as the root mean-square error scaled with twice the estimated measurements’ uncertainty. The square of MQI can be broken into three components related to the bias, the correlation, and the standard deviation of the errors (referred hereinafter as $MQI^2_{bias}$, $MQI^2_{corr}$ and $MQI^2_{std}$ respectively). Using these components and the MQI it is possible to select, in addition to the other metrics, the best performing configuration(s), to rank them, and to identify which statistical components contribute mainly on the errors. An MQI less than 1 is adopted as acceptance criterion for good modeling performance, based to the definition of MQI. The calculation formulas for all statistical metrics are
2.2. Evaluation of dust parameterizations

presented in Appendix A.
Chapter 3

Simulations of dust emissions in
the Central Middle East area

3.1 Horizontal Mass Flux effect

The mean emission fluxes, mean daily and total emissions’ differences between simulations 9 and 1 (R9-R1) are illustrated in Figures 3.1a-3.1c, as well their NRD for the simulated period when different horizontal mass fluxes parameterizations are considered (Figure 3.1d). For the largest part of the domain, the magnitude of the mean emission fluxes differences over the simulated period don’t exceed the 10 $\mu g/m^2s$. Only few areas near Kuwait and the borders of Saudi Arabia show differences varying between 10 and 20 $\mu g/m^2s$. Owen’s formulation has a general tendency to increase the emission rates over the sandy areas and to decrease them over the sparsely vegetated ones.

Mean daily emission fluxes differences show a larger variation (Figure 3.1b). Despite the fact that their pattern remains almost the same with that of the mean emission fluxes, the accumulation of the latter differences, on a daily basis, results in variations of the order of 100 $mg/m^2day$. The domain-wide statistics in Table 3.1 for R9-R1 show that a choice of the White’s formula, will result in an overall increase of the emissions fluxes in CME. An inspection of the extremely negative values of the total emission fluxes differences (less than -1000 $g/m^2$) on maps (not shown here) are presented in two areas: 1)
near the borders of Kuwait and the north Saudi Arabia and 2) the coastline of Kuwait. In the former region, the clay content is less than 10%, indicating again the importance of soil texture when certain parameterizations are considered, while the latter is located in an area with higher $z_o$ and consequently with less potential to produce dust. The NRD of R9-R1 in CME (Figure 3.1d) range from $-68\%$ in the mountainous regions of Iran to $21\%$ over the sand dunes of Rub’Al Khali in Saudi Arabia.

In general, a reduction (promotion) of emission fluxes with Owen’s (White’s) formulation over all possible combinations is expected (Table 3.1). This behavior indicates that Owen’s equation is more sensitive, especially over the rough surfaces, leading to significantly lower emissions relative to White. The NRD spans a $31\%$ range (from $-15\%$ to $-44\%$), as a result of the other components. The chosen PSD contributes by $2 - 3\%$, with the exception of a $8\%$ difference when SH04 scheme is used (R11-R3 to R12-R4). With Chatenet’s PSD, there is a tendency for higher emissions, when White’s equation is used, over the sparsely vegetated areas of Iraq and Iran. Among the rest combinations, Raupach’s drag partition scheme has the higher indirect impact on NRD. A comparison of MacKinnon’s and Raupach’s related differences show a contribution of the latter by $18 - 20\%$ on the NRD reduction, when AG01 is used, and $11 - 22\%$ with SH04. This is a result of Raupach’s aggressiveness and Owen’s sensitivity, leading to substantial reduction of the emissions in the greater CME.
3.1. Horizontal Mass Flux effect

**Figure 3.1:** Mean emission fluxes (a), mean daily fluxes (b), total emission fluxes differences (c) and NRD (d) between R9 and R1.
Table 3.1: Domain-wide averages, minimum and maximum for mean emission fluxes differences (MEF), mean daily emission fluxes differences (MDE), total emission fluxes differences (TE) and relative differences (NRD), related to horizontal mass flux parameterizations. With bold the max/min of each statistic is highlighted.

<table>
<thead>
<tr>
<th>Sim. Differences (RJ-RI)</th>
<th>MEF ($\mu g/m^2s$)</th>
<th>Min. MEF ($\mu g/m^2s$)</th>
<th>Max. MEF ($\mu g/m^2s$)</th>
<th>MDE ($mg/m^2day$)</th>
<th>Min. MDE ($mg/m^2day$)</th>
<th>Max. MDE ($mg/m^2day$)</th>
<th>TE ($g/m^2$)</th>
<th>Min. TE ($g/m^2$)</th>
<th>Max. TE ($g/m^2$)</th>
<th>NRD (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R9-R1</td>
<td>-1.02</td>
<td>-298.54</td>
<td>2.23</td>
<td>-88.08</td>
<td>-25763.90</td>
<td>192.34</td>
<td>-8.02</td>
<td>-2347.25</td>
<td>17.50</td>
<td>-15.09</td>
</tr>
<tr>
<td>R11-R3</td>
<td>-1.87</td>
<td>-720.23</td>
<td>0.65</td>
<td>-161.50</td>
<td>-62227.46</td>
<td>56.14</td>
<td>-14.70</td>
<td>-5662.70</td>
<td>5.11</td>
<td>-22.35</td>
</tr>
<tr>
<td>R12-R4</td>
<td>-4.58</td>
<td><strong>2093.44</strong></td>
<td>1.51</td>
<td><strong>396.09</strong></td>
<td><strong>180872.84</strong></td>
<td>0.00</td>
<td>-36.04</td>
<td><strong>16459.43</strong></td>
<td>0.00</td>
<td>-30.80</td>
</tr>
<tr>
<td>R13-R5</td>
<td>-0.28</td>
<td>-249.37</td>
<td>3.41</td>
<td>-24.56</td>
<td>-21545.12</td>
<td>294.61</td>
<td>-2.24</td>
<td>-1960.61</td>
<td>26.81</td>
<td>-34.66</td>
</tr>
<tr>
<td>R14-R6</td>
<td>-1.16</td>
<td>-194.24</td>
<td>2.04</td>
<td>-99.84</td>
<td>-16782.12</td>
<td>176.50</td>
<td>-9.09</td>
<td>-1527.17</td>
<td>16.06</td>
<td>-36.09</td>
</tr>
<tr>
<td>R15-R7</td>
<td>-0.51</td>
<td>-485.69</td>
<td>1.93</td>
<td>-43.68</td>
<td>-41963.48</td>
<td>166.81</td>
<td>-3.98</td>
<td>-3818.68</td>
<td>15.18</td>
<td><strong>-44.21</strong></td>
</tr>
<tr>
<td>R16-R8</td>
<td>-1.27</td>
<td>-981.67</td>
<td><strong>14.93</strong></td>
<td>-109.83</td>
<td><strong>1289.65</strong></td>
<td>-10.00</td>
<td>-7718.30</td>
<td><strong>117.36</strong></td>
<td>-41.39</td>
<td></td>
</tr>
</tbody>
</table>
3.2 Drag Partition

Figure 3.2a illustrates the magnitude and the spatial distribution of the drag partition scheme differences between R5 and R1 (R5-R1). The mean emission fluxes differences between Raupach’s and MacKinnon’s formulations show slightly positive values over the sandy areas. The maximum positive difference reaches up to 14 $\mu g/m^2s$ in the domain. On the other hand, the regions of Kuwait and Iran are affected greatly from the drag partition. With MacKinnon’s scheme, increased mean emission fluxes of 5 $\mu g/m^2s$ are found in these areas. In terms of percentages, the respective mean increase expected with MacKinnon’s scheme is $\sim 97\%$. The cumulative effect of the mean daily and the total emissions is evident in Figures 3.2b-3.2c, amplifying the contrast and the spatial variability in the region. The Raupach scheme increases the mean daily emissions in southern Saudi Arabia and UAE by 50-200 $mg/m^2day$ over the regions with the lowest roughness lengths/densities. For the rest of the domain, the MacKinnon’s scheme influence dominates, with a mean daily difference of -433 $mg/m^2day$.

The spatial variability is also evident on the minimum/maximum of the domain-wide mean emission fluxes differences in Table 3.2. The greatest differences on these statistics are attributed to the SH04 scheme, which produces emission patterns with large spatial heterogeneity, increasing the range of the emission differences. Concerning the indirect effect of PSD on drag partition differences, there is a slight promotion with Chatenet PSD when the MacKinnon scheme is used. The NRD ranges from $-91\%$ to $-118\%$, indicating a doubling of the emissions with MacKinnon scheme relative to Rapauch’s, thus, making the choice of the appropriate drag partition scheme an important issue on dust modelling. Most of the 27% variance is attributable to sandblasting scheme (11 – 25%). When AG01 scheme (R5-R1, R6-R2, R13-R9, R14-R10) is used, the mean NRD is around $-98\%$, while SH04 (R7-R3, R8-R4, R15-R11
Chapter 3. Simulations of dust emissions in the Central Middle East area

Figure 3.2: Mean emission fluxes (a), mean daily fluxes (b), total emission fluxes differences (c) and NRD (d) between R5 and R1.

and R16-R12) leads to a value of $-115\%$. A significant part of the remaining NRD variance is caused from the horizontal mass flux parameterization ($3-8\%$) and a similar percent range from the utilized PSD ($0-9\%$).
Table 3.2: Domain-wide averages, minimum and maximum for mean emission fluxes differences (MEF), mean daily emission fluxes differences (MDE), total emission fluxes differences (TE) and relative differences (NRD), related to drag partition parameterizations. With bold the max/min of each statistic is highlighted.

<table>
<thead>
<tr>
<th>Sim. Differences (RJ-RI)</th>
<th>MEF (µg/m²s)</th>
<th>Min. MEF (µg/m²s)</th>
<th>Max. MEF (µg/m²s)</th>
<th>MDE (mg/m²day)</th>
<th>Min. MDE (mg/m²day)</th>
<th>Max. MDE (mg/m²day)</th>
<th>TE (g/m²)</th>
<th>Min. TE (g/m²)</th>
<th>Max. TE (g/m²)</th>
<th>NRD (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R5-R1</td>
<td>-5.02</td>
<td>-139.03</td>
<td>14.30</td>
<td>-433.80</td>
<td>-12011.77</td>
<td>1235.58</td>
<td>-39.48</td>
<td>-1093.07</td>
<td>112.44</td>
<td>-96.85</td>
</tr>
<tr>
<td>R6-R2</td>
<td>-7.57</td>
<td>-113.35</td>
<td>15.45</td>
<td>-654.32</td>
<td>-9793.45</td>
<td>1335.19</td>
<td>-59.54</td>
<td>-891.20</td>
<td>121.50</td>
<td>91.12</td>
</tr>
<tr>
<td>R7-R3</td>
<td>-6.24</td>
<td>-3184.91</td>
<td>71.31</td>
<td>-539.45</td>
<td>-275176.14</td>
<td>6160.99</td>
<td>-49.09</td>
<td>-25041.03</td>
<td>560.65</td>
<td>-115.55</td>
</tr>
<tr>
<td>R8-R4</td>
<td>-10.72</td>
<td>-4327.35</td>
<td>98.08</td>
<td>-926.57</td>
<td>-373883.31</td>
<td>8474.07</td>
<td>-84.32</td>
<td>-34023.38</td>
<td>771.14</td>
<td>-115.79</td>
</tr>
<tr>
<td>R13-R9</td>
<td>-4.29</td>
<td>-101.81</td>
<td>17.39</td>
<td>-370.28</td>
<td>-8796.76</td>
<td>1502.20</td>
<td>-33.70</td>
<td>-800.51</td>
<td>136.70</td>
<td>-103.96</td>
</tr>
<tr>
<td>R14-R10</td>
<td>-6.15</td>
<td>-127.99</td>
<td>18.01</td>
<td>-531.52</td>
<td>-11058.40</td>
<td>1555.70</td>
<td>-48.37</td>
<td>-1006.32</td>
<td>141.57</td>
<td>-98.70</td>
</tr>
<tr>
<td>R15-R11</td>
<td>-4.88</td>
<td>-2997.01</td>
<td>73.37</td>
<td>-421.63</td>
<td>-258941.74</td>
<td>6338.74</td>
<td>-38.37</td>
<td>-23563.70</td>
<td>576.83</td>
<td>-118.95</td>
</tr>
<tr>
<td>R16-R12</td>
<td>-7.41</td>
<td>-3138.75</td>
<td>94.93</td>
<td>-640.31</td>
<td>-271188.06</td>
<td>8201.87</td>
<td>-58.27</td>
<td>-24678.11</td>
<td>746.37</td>
<td>-109.70</td>
</tr>
</tbody>
</table>
3.3 Sandblasting Efficiency effect

Figure 3.3a shows the differences in the mean emission fluxes between SH04 and AG01 (R3-R1). AG01 parameterization dominates by 10 µg/m²s or more relative to SH04, delimiting a region from the northeastern Saudi Arabia and the borders with Iraq and Kuwait up to UAE. This part of CME is associated with low roughness elements (Fig. 3.4). A comparison between the clay content (Fig. 3.5) and these differences (Fig. 3.3d) highlights the influence of the former. Differences between -20 and -50 µg/m²s are associated with clay content of 11% or less. On the other hand, the SH04 formalism tends to produce higher emissions over the coastline of Oman and UAE in the Gulf of Oman, the west flank of Qatar, the Sistani province and the mainland of Iran. The majority of the above areas are associated with clay content between 20 – 30%, showing that SH04 has the tendency to produce much more dust relative to the AG01 in soils with large amounts of fine particles, while AG01 produces dust even over the sandy areas, where fine material is usually absent. Similar conclusion can be drawn for the mean daily and the total emission fluxes differences and NRDs (Figures 3.3b-3.3d). Even if AG01 has in general a much larger impact, the SH04 peaks are more pronounced and focused on the areas determined by the soil texture. Thus, the selected soil texture can change substantially the response of each scheme and the origins of the dust. A characteristic examples of the change in the dust source with the SH04 scheme and its sensitivity to soil texture is depicted in Figure 3.6a for the total emission fluxes of R4 configuration. A comparison with R2 in Fig. 3.6b emphasizes the change in the pattern of the dust sources over Kuwait and along the eastern flank of Saudi Arabia, when the SH04 is utilized.

The domain-average NRDs are the lowest among the three components, ranging from −118% to −158% (Table 3.3). Most of this variance in NRD (≈ 40%) is attributed to the drag partition schemes utilized, while PSDs contribute
only a few percent on NRDs (less than 2%). It is worth-mentioning that the lowest total emissions’ difference is found between R4 and R2 \((-0.28\, g/m^2)\), which can be considered as equivalent, in terms of emission fluxes in CME, among the 16 simulations performed in this study.
### Table 3.3: Domain-wide averages, minimum and maximum for mean emission fluxes differences (MEF), mean daily emission fluxes differences (MDE), total emission fluxes differences (TE) and relative differences (NRD), related to sandblasting efficiency parameterizations. With bold the max/min of each statistic is highlighted.

<table>
<thead>
<tr>
<th>Sim. Differences (RJ-RI)</th>
<th>MEF  ( (\mu g/m^2s) )</th>
<th>Min. MEF ( (\mu g/m^2s) )</th>
<th>Max. MEF ( (\mu g/m^2s) )</th>
<th>MDE  ( (mg/m^2day) )</th>
<th>Min. MDE ( (mg/m^2day) )</th>
<th>Max. MDE ( (mg/m^2day) )</th>
<th>TE  ( (g/m^2) )</th>
<th>Min. TE ( (g/m^2) )</th>
<th>Max. TE ( (g/m^2) )</th>
<th>NRD  ( (%) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>R3-R1</td>
<td>-2.82</td>
<td><strong>-589.48</strong></td>
<td>3692.11</td>
<td>-243.50</td>
<td><strong>-50930.98</strong></td>
<td>318998.54</td>
<td>-22.16</td>
<td><strong>-4634.72</strong></td>
<td>29028.87</td>
<td>-117.97</td>
</tr>
<tr>
<td>R4-R2</td>
<td>-0.04</td>
<td>-231.79</td>
<td>5747.36</td>
<td>-3.10</td>
<td>-20026.40</td>
<td>496572.27</td>
<td>-0.28</td>
<td>-1822.40</td>
<td><strong>45188.08</strong></td>
<td>-118.18</td>
</tr>
<tr>
<td>R7-R5</td>
<td>-4.04</td>
<td>-450.45</td>
<td>977.28</td>
<td>-349.15</td>
<td>-38919.26</td>
<td>84436.62</td>
<td>-31.77</td>
<td>-1303.73</td>
<td>12334.42</td>
<td>-155.35</td>
</tr>
<tr>
<td>R8-R6</td>
<td>-3.19</td>
<td>-165.82</td>
<td>1568.79</td>
<td>-275.35</td>
<td>-14326.69</td>
<td>135543.06</td>
<td>-25.06</td>
<td>-1303.73</td>
<td>12334.42</td>
<td>-155.35</td>
</tr>
<tr>
<td>R11-R9</td>
<td>-3.67</td>
<td>-290.94</td>
<td>3253.75</td>
<td>-316.92</td>
<td>-25137.19</td>
<td>281124.13</td>
<td>-28.84</td>
<td>-2287.48</td>
<td>25582.30</td>
<td>-121.60</td>
</tr>
<tr>
<td>R12-R10</td>
<td>-2.04</td>
<td>-159.87</td>
<td><strong>3800.49</strong></td>
<td>-176.55</td>
<td>-13812.31</td>
<td>328362.53</td>
<td>-16.07</td>
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<td>-17374.24</td>
<td>44063.08</td>
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<td>4009.74</td>
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<td>R16-R14</td>
<td>-3.30</td>
<td>-87.74</td>
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<td>69079.64</td>
<td>-25.97</td>
<td>-689.81</td>
<td>6286.25</td>
<td>-156.94</td>
</tr>
</tbody>
</table>
3.3. Sandblasting Efficiency effect

Figure 3.4: Roughness length (a) and density (b) utilized within NEMO for the drag partition schemes.

Figure 3.5: Clay content (in %) of the Harmonized World Soil Data.

Figure 3.6: Integrated emission fluxes of R4 (a) and R2 (b) over the period of April-June 2015.
3.4 Total dust emissions in CME

Similarly to the previous analysis, large differences in total emissions exist among the 16 simulations over the studied area, ranging from 21 to 139 Tg (Table 3.4). Two kinds of ranges can be recognized, based on the drag partition scheme utilized. When MacKinnon’s drag partition is used, total emissions range between 63-139 Tg (R1-4, R9-12), while with Raupach’s parameterization range between 21-67 Tg (R5-8, R13-16). A value of 65 Tg separates these two cases for the period of April to June. Thus, the choice of the drag partition scheme can restrict the range of the total emissions in MEA or, if the total emissions can be evaluated with a certain accuracy, to dictate which drag partition scheme is more appropriate. The differences resulting from the drag partition schemes range from 47-102 Tg. On the other hand, the transition from AG01 to SH04 corresponds to reductions of 20-41 Tg. In terms of total emissions, the drag partition effect is the most important. Horizontal mass flux effect on the total emissions ranges from 3 to 44 Tg, followed by the PSD effect with 7-26 Tg. In summary, the drag partition scheme is the most sensitive concerning the total emissions in CME, followed by sandblasting efficiency, horizontal mass flux and PSD.

On a monthly basis, all the simulations show increased emissions during April, the highest on June and the lowest on May, as a consequence of the wind speed intensity in CME. The same conclusions can be drawn for the monthly variations with respect to the different parameterizations. April emissions range from 9 to 52 Tg, for May are almost the half (4-32 Tg), while during June are slightly higher relative to April’s emissions (8-60 Tg).
Table 3.4: Monthly and total emissions of the period April–June 2015.

<table>
<thead>
<tr>
<th>Sim. ID</th>
<th>April (Tg)</th>
<th>May (Tg)</th>
<th>June (Tg)</th>
<th>Total (Tg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>35</td>
<td>25</td>
<td>47</td>
<td>107</td>
</tr>
<tr>
<td>R2</td>
<td>47</td>
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<td>81</td>
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<td>52</td>
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<td>139</td>
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<td>R10</td>
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<td>R11</td>
<td>25</td>
<td>13</td>
<td>26</td>
<td>63</td>
</tr>
<tr>
<td>R12</td>
<td>36</td>
<td>19</td>
<td>40</td>
<td>95</td>
</tr>
<tr>
<td>R13</td>
<td>18</td>
<td>13</td>
<td>26</td>
<td>57</td>
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<td>R14</td>
<td>19</td>
<td>12</td>
<td>25</td>
<td>56</td>
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<tr>
<td>R15</td>
<td>7</td>
<td>2</td>
<td>7</td>
<td>16</td>
</tr>
<tr>
<td>R16</td>
<td>10</td>
<td>5</td>
<td>10</td>
<td>25</td>
</tr>
</tbody>
</table>
Chapter 4

Evaluation of the dust modeling parameterizations in the Central Middle East

4.1 Qualitative evaluation

Figures 4.1 and 4.2 illustrate the mean of the $AOD_{550}$ from MODIS and each CAMx simulation of Table 2.1, respectively, for the whole study period. The spatial Pearson correlation, between the MODIS product in Fig. 4.1 and each simulation, is also given in Fig. 4.2, and altogether in Figure 4.3. Most of the simulations show an area of higher AODs on the eastern flank of Saudi Arabia and Rub’ Al Khali desert, consistent with the MODIS product. This is mainly a result of the wind pattern and the persistent emissions in the region, as it was discussed in Kontos et al. (2018). MODIS indicates urban and industrial areas as hot spots, like Doha in Qatar, which have not been reproduced by any of the CAMx simulations. This can be attributed to the lack of additional anthropogenic activities, the representativeness of the emission factors in these areas, and/or the resuspended dust in the urban fabric (Hassan et al., 2020), which is not included in the current version of the modeling system. Several differences appear among each simulation exclusively because of the
different dust modeling parameterizations. The parameterizations associated with the MacKinnon’s scheme (in configurations R1 to R4 and R9 to R12; Fig. 4.2a,4.2c,4.2e,4.2g,4.2i,4.2k,4.2m,4.2o) produce higher AODs in the CME with respect to MODIS. For R2-R4 and R10-R12 the highest $\text{AOD}_{550}$ are located near the Tigris and Euphrates and in the mountainous areas of Iran, which is not consistent with the MODIS pattern.

Differences can be also found on the patterns affected by the sandblasting efficiency scheme. The use of Shao’s scheme (SH04) in configurations R3, R4, R7, R8, R11, R12, R15, R16 (Fig. 4.2e,4.2f,4.2g,4.2h,4.2m,4.2n,4.2o,4.2p) leads to distinct hot spots of AODs, while the use of Alfaro and Gomes scheme (AG01) in configurations R1, R2, R5, R6, R9, R10, R13, R14 (Fig. 4.2a,4.2b,4.2c,4.2d and 4.2i,4.2j,4.2k,4.2l) to more widespread areas. The latter behavior but for the emissions patterns was also identified in Kontos et al. (2018), where SH04 proved more sensitive on the soil texture. An intercomparison between the spatial correlations of AG01 and SH04 configurations, as illustrated in Fig. 4.3 (e.g R1 with R3, R2 with R4 etc.) shows AG01 to perform always better than SH04. A similar intercomparison between White’s and Owen’s configurations (e.g. R1 with R9, R2 with R10 etc.) shown slightly better spatial correlations for the latter.

Overall, qualitatively, the best performance in the spatial pattern has been achieved with the R13 configuration, followed by the R5, R9, R14, and R1 ones (spatial Pearson correlation larger than 0.6). Moderate performance is found for configurations R6, R7, R10, R15 and R16 while most of the configurations with the MacKinnon’s (R2, R3, R4, R11, R12) have poor spatial correlation (less than 0.4).
4.1. Qualitative evaluation

Figure 4.1: AOD at 550 nm from the MODIS Terra and Aqua combined product for the period April-June 2015.
Chapter 4. Evaluation of the dust modeling parameterizations in the Central Middle East

Figure 4.2: AOD at 550 nm from CAMx for a) R1, b) R5, c) R2, d) R6, e) R3, f) R7, g) R4 and h) R8 configurations for the period April-June 2015. The spatial correlation with MODIS product is written on the lower right corner of each figure.
4.1. Qualitative evaluation

Figure 4.2: AOD at 550 nm from CAMx for i) R9, j) R13, k) R10, l) R14, m) R11, n) R15, o) R12 and p) R16 configurations for the period April-June 2015. The spatial correlation with MODIS product is written on the lower right corner of each figure.
Chapter 4. Evaluation of the dust modeling parameterizations in the Central Middle East

Figure 4.3: Spatial correlations between MODIS and the calculated from CAMx concentrations’ AOD at 550 nm for all configurations. The red and blue colors on the ID namings depict the configurations where MacKinnon’s and Raupach’s drag partition scheme is used respectively. The lime and yellow colors indicate the configurations where the AG01 and SH04 sandblasting schemes respectively, The shaded and non-shaded bars indicate the configurations where White’s and Owen’s horizontal mass flux equations are used. Lines with 0.6 and 0.4 spatial correlations define the thresholds for good and poor performance.

4.2 Quantitative evaluation

Table 4.1 presents the evaluation metrics of the simulation results against the on-site measurements in Doha, Qatar for the daily mean PM10 concentrations. The mean bias indicates a consistent overestimation on the PM10 concentrations when the MacKinnon’s drag partition scheme is utilized (configurations R1 to R4 and R9 to R12) and in contrast a respective underestimation for Raupach’s scheme (R5 to R8 and R13 to R16). As described in Kontos et al. (2018), the aerodynamic entrainment of dust was assumed negligible. This should have led to small underestimations of the concentration levels, even if the dust emission scheme for the other two considered processes (disaggregation and sandblasting) was “perfect”. Given these points and the similar issues for AOD, the MacKinnon’s formulation is assumed inappropriate for the drag partition simulation in this study and the corresponding simulations are excluded.
4.2. Quantitative evaluation

from any further analysis (i.e. configurations R1 to R4 and R9 to R12).

IOAs range from moderate (0.68, R13) to very good (0.81, R14), for the remaining configurations (i.e. R5 to R8 and R13 to R16). The upper limit of 50% set for NMSE, \( F_b \), and \( F_s \) holds simultaneously for the R5, R7, R13, R14, and R16 configurations. These five configurations are characterized by lower CRMSE, ranging from 81.45(R7) to 100.69 \( \mu g/m^3 \) (R16), which also indicates their ability to reproduce the variability during the dust events. Altogether, these five configurations are the candidates for the proposed dust emission configuration(s).

Following the FAIRMODE project evaluation methodology (Monteiro et al., 2018), Figure 4.4 consolidates the performance of all 16 configurations in a single target plot for completeness. From the 16 configurations, only eight pass the MQI criterion of less than one (green circle in Fig. 4.4). From these, one is located in the upper left quarter (R9) and the rest in the lower left quarter (R14, R5, R13, R7, R15, R16, R6), as a result of MB, confirming the previous conclusion about drag partition schemes.

For further analysis, Table 4.2 presents the components of the squared MQI that relay to the bias, standard deviation, and correlation, as well the \( RMS_u \), which is an estimation of the measurements’ uncertainty, as dictated by the FAIRMODE method. The two best performing configurations are the R14 and R5, followed by the R13, R7, R15, R16, and R6. The high values of \( MQI2_{corr} \) metric for R5, R6, R13 and R14 indicates that the AG01 performance is mainly affected by the correlation component (mostly worse than SH04), which can be attributed to the intrinsic nature of the AG01 formalism being independent of the soil’s particle distribution. In other words, AG01 results always to the same emitting distribution of PM, for the same meteorological conditions, regardless of the soil. On the other hand, SH04 (R7, R8, R15, R16) performance is affected mainly by the bias (\( MQI2_{bias} \)) component (mostly worse than AG01), which might originate from the improper parameters’ calibration and/or the missing
Chapter 4. Evaluation of the dust modeling parameterizations in the Central Middle East

aerodynamic entrainment mechanism. Summing up, SH04 or AG01 can be chosen for improved correlation or optimum bias, respectively, depending on the objectives of a dust modeling system’s goal in the region of interest.

As has been noted, the soil size distribution influences indirectly the performance of a modeling system. Such an influence is prominent, in Table 4.2, for the transition from WRF-Chem to Chatenet’s distributions (i.e. R5 to R6, R13 to R14 and R15 to R16) which leads always to the reduction of the \( MQI_{bias} \) but with a respective increase to \( MQI_{std} \) and \( MQI_{corr} \). This transition from bias to variance related errors due to the soil texture influences the evaluation and the aim of the modeling system, in a similar fashion to the sandblasting scheme discussed earlier. The transition from the White to Owen schemes for the horizontal mass flux does not show any consistent trend, thus these two can be used equally without expecting significant differences.

Table 4.1: Metrics for the evaluation of the modeling system configurations with the on-site daily mean measured PM10 surface concentrations. The statistics used are the Mean Bias (MB, in \( \mu g/m^3 \)), Normalized Mean Square Error (NMSE), Pearson correlation coefficient (R), the factor of 2 percentage (Fac2), the Fractional bias (\( F_b \)), the Fractional standard deviation (\( F_s \)), the Centralize Root Mean Square Error (CRMSE, in \( \mu g/m^3 \)) and the Index of Agreement. The optimum values are indicated with bold.

<table>
<thead>
<tr>
<th>Sim. ID</th>
<th>MB</th>
<th>NMSE</th>
<th>R</th>
<th>Fac2</th>
<th>( F_b )</th>
<th>( F_s )</th>
<th>CRMSE</th>
<th>IOA</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>61.70</td>
<td>0.34</td>
<td>0.61</td>
<td>0.80</td>
<td>0.21</td>
<td>0.64</td>
<td>163.12</td>
<td>0.66</td>
</tr>
<tr>
<td>R2</td>
<td>199.41</td>
<td>1.09</td>
<td>0.62</td>
<td>0.71</td>
<td>0.54</td>
<td>1.11</td>
<td>313.86</td>
<td>0.44</td>
</tr>
<tr>
<td>R3</td>
<td>54.268</td>
<td>0.92</td>
<td>0.78</td>
<td>0.63</td>
<td>0.18</td>
<td>1.08</td>
<td>278.76</td>
<td>0.60</td>
</tr>
<tr>
<td>R4</td>
<td>236.41</td>
<td>2.48</td>
<td>0.73</td>
<td>0.59</td>
<td>0.61</td>
<td>1.41</td>
<td>531.25</td>
<td>0.37</td>
</tr>
<tr>
<td>R5</td>
<td>-57.97</td>
<td>0.19</td>
<td>0.70</td>
<td>0.78</td>
<td>-0.24</td>
<td>0.08</td>
<td>84.76</td>
<td>0.77</td>
</tr>
<tr>
<td>R6</td>
<td>-3.33</td>
<td>0.30</td>
<td>0.73</td>
<td>0.78</td>
<td>-0.01</td>
<td>0.63</td>
<td>145.48</td>
<td>0.75</td>
</tr>
<tr>
<td>R7</td>
<td>-101.49</td>
<td>0.37</td>
<td>0.85</td>
<td>0.57</td>
<td>-0.46</td>
<td>0.35</td>
<td>81.45</td>
<td>0.77</td>
</tr>
<tr>
<td>R8</td>
<td>-41.47</td>
<td>0.61</td>
<td>0.78</td>
<td>0.61</td>
<td>-0.17</td>
<td>0.84</td>
<td>188.35</td>
<td>0.70</td>
</tr>
<tr>
<td>R9</td>
<td>27.85</td>
<td>0.22</td>
<td>0.62</td>
<td>0.82</td>
<td>0.10</td>
<td>0.43</td>
<td>128.92</td>
<td>0.73</td>
</tr>
<tr>
<td>R10</td>
<td>114.00</td>
<td>0.58</td>
<td>0.63</td>
<td>0.73</td>
<td>0.35</td>
<td>0.87</td>
<td>216.57</td>
<td>0.57</td>
</tr>
<tr>
<td>R11</td>
<td>1.66</td>
<td>0.56</td>
<td>0.79</td>
<td>0.67</td>
<td>0.11</td>
<td>0.98</td>
<td>201.82</td>
<td>0.70</td>
</tr>
<tr>
<td>R12</td>
<td>104.18</td>
<td>1.23</td>
<td>0.76</td>
<td>0.65</td>
<td>0.32</td>
<td>1.19</td>
<td>341.39</td>
<td>0.52</td>
</tr>
<tr>
<td>R13</td>
<td>-75.63</td>
<td>0.24</td>
<td>0.64</td>
<td>0.78</td>
<td>-0.33</td>
<td>-0.17</td>
<td>83.26</td>
<td>0.68</td>
</tr>
<tr>
<td>R14</td>
<td>-49.48</td>
<td>0.18</td>
<td>0.74</td>
<td>0.80</td>
<td>-0.20</td>
<td>0.24</td>
<td>89.89</td>
<td>0.81</td>
</tr>
<tr>
<td>R15</td>
<td>-119.67</td>
<td>0.44</td>
<td>0.86</td>
<td>0.55</td>
<td>-0.57</td>
<td>0.09</td>
<td>60.02</td>
<td>0.72</td>
</tr>
<tr>
<td>R16</td>
<td>-88.76</td>
<td>0.37</td>
<td>0.83</td>
<td>0.59</td>
<td>-0.39</td>
<td>0.46</td>
<td>100.69</td>
<td>0.77</td>
</tr>
</tbody>
</table>
4.2. Quantitative evaluation

Table 4.2: Performance metrics, as defined in the frame of FAIRMODE project, of the modeling system configurations with the on-site daily mean PM10 measured surface concentrations. The metrics used are the Modeling (MQI) its components i.e. the square of the bias (MQI2_bias), the square of the correlation (MQI2_corr) and the square of the standard deviation (MQI2_std), and additionally the Root Mean Square Error (RMSE, in $\mu g/m^3$) and the Root Mean Square uncertainty of the measurements (RMSu, in $\mu g/m^3$). The optimum values are indicated with bold.

<table>
<thead>
<tr>
<th>Sim. ID</th>
<th>MQI</th>
<th>MQI2_bias</th>
<th>MQI2_std</th>
<th>MQI2_corr</th>
<th>RMSE</th>
<th>RMSu</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>1.08</td>
<td>0.15</td>
<td>0.39</td>
<td>0.66</td>
<td>174.40</td>
<td>80.42</td>
</tr>
<tr>
<td>R2</td>
<td>2.31</td>
<td>1.54</td>
<td>2.74</td>
<td>1.15</td>
<td>371.85</td>
<td>80.42</td>
</tr>
<tr>
<td>R3</td>
<td>1.77</td>
<td>0.11</td>
<td>2.42</td>
<td>0.64</td>
<td>283.99</td>
<td>80.42</td>
</tr>
<tr>
<td>R4</td>
<td>3.62</td>
<td>2.16</td>
<td>9.75</td>
<td>1.38</td>
<td>581.48</td>
<td>80.42</td>
</tr>
<tr>
<td>R5</td>
<td><strong>0.64</strong></td>
<td>0.13</td>
<td><strong>0.003</strong></td>
<td>0.28</td>
<td>102.69</td>
<td>80.42</td>
</tr>
<tr>
<td>R6</td>
<td>0.91</td>
<td><strong>0.0004</strong></td>
<td>0.37</td>
<td>0.46</td>
<td>145.52</td>
<td>80.42</td>
</tr>
<tr>
<td>R7</td>
<td>0.81</td>
<td>0.40</td>
<td>0.08</td>
<td>0.18</td>
<td>130.14</td>
<td>80.42</td>
</tr>
<tr>
<td>R8</td>
<td>1.20</td>
<td>0.07</td>
<td>0.93</td>
<td>0.47</td>
<td>192.86</td>
<td>80.42</td>
</tr>
<tr>
<td>R9</td>
<td>0.82</td>
<td>0.03</td>
<td>0.13</td>
<td>0.52</td>
<td>131.90</td>
<td>80.42</td>
</tr>
<tr>
<td>R10</td>
<td>1.52</td>
<td>0.50</td>
<td>1.04</td>
<td>0.81</td>
<td>244.74</td>
<td>80.42</td>
</tr>
<tr>
<td>R11</td>
<td>1.26</td>
<td>0.00</td>
<td>1.12</td>
<td>0.48</td>
<td>201.82</td>
<td>80.42</td>
</tr>
<tr>
<td>R12</td>
<td>2.22</td>
<td>0.42</td>
<td>3.75</td>
<td>0.84</td>
<td>356.93</td>
<td>80.42</td>
</tr>
<tr>
<td>R13</td>
<td>0.70</td>
<td>0.22</td>
<td>0.01</td>
<td>0.26</td>
<td>112.48</td>
<td>80.42</td>
</tr>
<tr>
<td>R14</td>
<td><strong>0.64</strong></td>
<td>0.10</td>
<td>0.03</td>
<td>0.29</td>
<td><strong>102.61</strong></td>
<td>80.42</td>
</tr>
<tr>
<td>R15</td>
<td>0.83</td>
<td>0.55</td>
<td>0.004</td>
<td><strong>0.14</strong></td>
<td>133.88</td>
<td>80.42</td>
</tr>
<tr>
<td>R16</td>
<td>0.84</td>
<td>0.31</td>
<td>0.16</td>
<td>0.24</td>
<td>134.23</td>
<td>80.42</td>
</tr>
</tbody>
</table>

Figure 4.4: Target plot for the 16 modeling configurations, as defined in the frame of FAIRMODE project.
4.3 Discussion

Concerning the qualitative evaluation with the satellite data, R13 produced the best $AOD_{550}$ patterns in CME, followed by R5, R9, R14 and R1. The quantitative evaluation showed that R5, R7, R9, R13, R14 and R16 are performing within the 50% acceptance threshold (NMSE, $F_b$ and $F_s$). Although R9 shows a generally good statistical performance, its consistent overestimation of the concentration levels due to the MacKinnon’s parameterization, as explained in Section 3.2, led to its exclusion. Bearing in mind the above, the shortlisted configurations are R14, R5 and R13. The FAIRMODE project’s method enables the ranking of these three configurations. In particular, based on MQI index, R14 and R5 are the best performing, followed by R13. Taking into account also the IOA, the final ranking of the dust modelling configurations is: R14, R5, and R13 in this study. Thus, R14 is found to perform best.

Figure 4.5 illustrates the daily mean PM10 concentrations of the on-site observations, as well as those simulated using for the CAMx set-up the best three configurations discussed above. Generally the modeling system reproduces satisfactorily the major dust events associated with PM levels greater than 300 $\mu g/m^3$, like those at the 13th of April and at the 21st to 24th of June. On the other hand, the modeling system underestimates by $\sim 104 \mu g/m^3$ on average the events associated with less than 300 $\mu g/m^3$, but still higher than the applied threshold (200$\mu g/m^3$). Bearing in mind the good performance of the modeling system on the major dust events and on the simulation of wind speeds for the selected time period as in Kontos et al. (2018), the causes of the underestimation could be to local source. Indeed, a recent study by Hassan et al. (2020) suggests that more than 50% of the PM10, below the 200 $\mu g/m^3$ threshold, is apportioned to sources of local character i.e. resuspension, traffic, fuel oil combustion, and shipping. Furthermore, they estimated higher PM emission rates for both road dust resuspension and vehicles’ exhaust, and highlighted the presence of large
4.3. Discussion

patches of barren land (e.g. construction activities) within the urban area.

![Figure 4.5: Daily mean PM10 measurements at Doha station (UTM 39R 551180m E 2797980m N), as well the best performing configurations R14, R13 and R5. The red dashed line indicate the 200 $\mu g/m^3$ threshold applied for the distinction of the major dust event.](image)

The performance of the regional dust modeling, evaluated with the on-site measurements, might be affected by factors relevant with the modeling set-up. These are the initial conditions and boundary conditions (BCs), the latter representing the external sources (natural or anthropogenic), that might affect the evaluation with the measured data at the Doha station. In order to better understand the impact of these factors on the evaluation of the dust modelling, the R14 configuration was run with the option of source apportionment. Figure 4.6 illustrates the absolute contribution of the initial and boundary conditions on PM10 surface concentrations for the dusty days (i.e. 51 days with PM10 levels > 200$\mu g/m^3$). The initial conditions were found to have negligible contribution on the surface PM10 concentrations of Doha station, an expected result because of the 15 days spin-up period. The boundaries contribute by 84 $\mu g/m^3$ on average to the PM10 levels, having a standard deviation of 31 $\mu g/m^3$ and an average relative contribution of $\sim 45\%$. For the non-dusty days, the results were very similar, with 67 $\mu g/m^3$ average PM10 values, 24 $\mu g/m^3$ standard
deviation, and 47% average relative contribution respectively. This quasi consistent contribution of the BCs at the Doha station enhances the validity of the conclusions drown here, since any difference found on the evaluation of the applied configurations is mainly attributable on the emissions produced within the domain, rather than the BCs. Most of the relative contribution of the BCs on the daily mean PM10 concentrations at Doha site come from the western boundary (33%), followed by south (7%), east (4%) and north (3%). Out of the 33% of the western origin, 25% is dust in the fine mode, 5% in coarse mode and the rest being the other anthropogenic aerosols. Although the main conclusions about the configurations are not expected to change, the BCs can have a significant contribution on the background PM10 levels. Thus, the choice of the appropriate boundary conditions should be considered with care when such regional domains are desirable.

![Figure 4.6: Source apportionment of the R14 configuration for the dusty days (IC: Initial Conditions, BC: Boundary Conditions, CAMx: Modeling Results, and Obs: Observations).](image)

One factor that might affect the evaluation of CAMx outcomes is the dry deposition scheme, since this mechanism effectively removes dust from the atmosphere. In all simulations we used the most up-to-date Zhang, Brook, and
Vet (2003) scheme, while CAMx also provides the option of the Wesely (1989) deposition scheme, both based on the expressions of Slinn (1982) and Slinn and Slinn (1980) respectively. These two schemes are the most commonly utilized in the current air quality models. An evaluation analysis with the FAIRMODE’s method for the R14 with the Wesely’s dry deposition scheme was done. An MQI of 0.69, with $MQI_{bias}$ of 0.29, $MQI_{std}$ of 0.01 and $MQI_{corr}$ of 0.17 was found, showing a slightly worse performance relative to R14 in Table 4.2. Figure 4.7 presents the daily mean PM10 concentrations simulated with the two dry deposition schemes. The Wesely’s dry deposition scheme leads to excessive underestimation of the daily mean PM10 concentrations, especially for the dust events with levels greater than 300 $\mu g/m^3$. This result is reflected also on the MB, which is found to be -87 $\mu g/m^3$. Similarly to the previous analysis, assessment with MODIS AOD was also done for R14 with the two dry deposition schemes (Fig. 4.8). The patterns are similar, with a slightly better spatial correlation with the Wesely’s deposition scheme. Although a definite conclusion cannot be drawn, the Zhang’s dry deposition scheme was found to be the best choice for this particular modeling system.

**Figure 4.7:** Daily mean PM10 measurements at Doha station (UTM 39R 551180m E 2797980m N) and simulated values using the best performing configurations R14 with Zhang and Wesely’s dry deposition schemes.
Chapter 4. Evaluation of the dust modeling parameterizations in the Central Middle East

Figure 4.8: AOD at 550 nm from CAMx for R14 configuration with Zhang’s (a) and Wesely’s (b) dry deposition schemes for the period April-June 2015. The spatial correlation with MODIS product is written on the lower right corner of each figure.

In this study, the aerodynamic entrainment has been neglected based on the results of Loosmore and Hunt (2000) and Shao, Raupach, and Findlater (1993) for long-term fluxes. Although this is the usual practice in dust modeling, recent results from wind tunnels propose that the aerodynamic contribution has been underestimated. Wu et al. (2018) investigated aerodynamic entrainment and found rates of 800-5400 µg/m²s and 3-126 µg/m²s for the sand dunes and clay crusted surface respectively. Zhang et al. (2016) proposed the renewal of the surface material as a possible mechanism for the sustained aerodynamic entrainment, beyond the expected, and proposed rates of 30-700 µg/m²s for a 3 minutes duration and for $u_*$ between 0.34-0.44 m/s. The emission rates are comparable with these of saltation bombardment plus disaggregation applied in our dust modeling system during dust events, as in the case investigated by Kontos et al. (2018) between 18-26 of June 2015 for the same region. Also, Roney and White (2004) found that the average concentrations of the aerodynamic entrainment can be 5 – 30% of that at the threshold friction velocity during steady saltation. Based on their results, under the assumption of an average concentration of 222 µg/m³, which is the mean value of the PM10 measurements in this study and with the application of a mean of ∼ 20% from aerodynamic entrainment, an estimated contribution on the concentrations corresponds to
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\[ \sim 44 \mu g/m^3 \]. The latter result is close to the MB found for R14, R13 and R5 here. Thus, aerodynamic entrainment could be one possible mechanism to explain a part of the underestimation.
Chapter 5

Conclusions

A major update on the dust emission module of NEMO has been implemented, incorporating the state-of-art parameterizations related to the physics of the dust emissions. In order to investigate the differences among them, all the possible combinations were incorporated, resulting in 16 distinct configurations. As a region of interest for their application, the Central Middle East area has been chosen, bearing in mind the potential sources and the available information for subsequent evaluation.

PM10 dust emission fluxes, as well their total amount emitted, were estimated in the Central Middle East (CME) for April-June of 2015, utilizing the Natural Emissions Model and the meteorological model WRF. The sensitivity of the emissions in CME, resulting from the different parameterizations (horizontal mass flux, drag partition, sandblasting efficiency) was investigated.

The sensitivity analysis on the emission fluxes revealed that large differences can rise from each components. Concerning the horizontal mass flux parameterization, White’s equation tends to increase the emissions relative to Owen’s over rough surfaces by 68%, while the opposite is true for the sandy areas (21%). Drag partition schemes lead to large spatial variability on the fluxes, closely following the distribution of roughness lengths/densities. The domain-wide mean difference between the drag partition schemes was found to be 91 – 118% in favor of the MacKinnon’s. For the sandblasting efficiency schemes, AG01 leads to increased fluxes or more relative to SH04 over the areas of MEA with the
lowest roughness lengths. It was also found a correlation between the soil texture and the differences in regions with clay content between 20 – 30%. Thus, the response of each sandblasting scheme differs significantly with soil texture. For NRD, the differences range from $-118\%$ to $-158\%$ in favor of AG01. In terms of fluxes the sandblasting efficiency has the largest effect, followed by drag partition and horizontal mass flux.

The total dust emissions in the region, among the 16 simulations, were found to range between 21-139 Tg and the most important component appears to be the drag partition scheme, followed by the sandblasting efficiency and the horizontal mass flux.

An extensive evaluation of the 16 configurations has been implemented with MODIS satellite data as well with on-site measurements of PM10 for significant dust events. The evaluation process aims on the distinction the best performing configuration(s).

The qualitative evaluation with the MODIS data have shown that most of the simulations produce the pattern with the higher $AOD_{550}$ on the eastern flank of Saudi Arabia and Rub’ Al Khali desert. The main differences between the simulated and satellite $AOD_{550}$ levels were found for the drag partition schemes, with Raupach’s scheme producing comparable values with MODIS. Thus, Raupach’s drag partition scheme is recommended for high resolution simulations in CME. Between AG01 and SH04 sandblasting efficiency schemes, the former produces more widespread AOD patterns relative to SH04 and always better spatial correlation. The differences between the horizontal mass flux parameterizations were small, with Owen’s parameterization being the best performing.

Overall, five configurations have been distinguished from the qualitative assessment, with three out of five to be a combination of Raupach’s and Alfaro and Gomes (AG01) schemes. Although out of the scope of this study, the
modeling system could not reproduce the $AOD_{550}$ hot spots in urban and industrial areas, because of the lack of the representative anthropogenic activities. An update of the anthropogenic emissions will improve the performance of the modeling system in these areas. The evaluation with the on-site measurements in Doha show clearly an overestimation on the PM10 concentration levels, when the MacKinnon’s drag partition scheme is utilized. Although not conclusively, this drag partition scheme might need recalibration, in order to meet the PM10 levels.

Upon the 16 simulations, when the upper limit of 50% criterion is applied for NMSE, $F_b$, and $F_s$, only R5, R7, R13, R14, and R16 configurations fulfill it. These five configurations present also lower CRMSE, ranging from 81.45 (R7) to 100.69 $\mu g/m^3$ (R16), which also indicates their ability to reproduce the variability during the major dust events. The best performance is found for R14 with this evaluation method, presenting the highest IOA among them.

The FAIRMODE methodology confirmed also the conclusions about the drag partition schemes. It also revealed that the AG01 and SH04 sandblasting parameterization’ errors come mainly from correlation and bias, respectively. If an improved bias or correlation is desirable for a dust modeling system in the region of interest, AG01 or SH04 can be chosen respectively. In a similar way, the soil size distribution leads to increased bias or variance related errors, when the approach of WRF-Chem or Chatenet is utilized, respectively. The sources of these errors need further investigation, with measurements and modeling studies focusing on the sandblasting parameterizations and their indirect relation with the soil size distribution. No significant differences were found between White’s and Owen’s horizontal mass flux parameterizations.

The combination of the qualitative and the quantitative evaluation with both methods led to the distinction of three configurations, namely R14, R5 and R13, ordered from the best to the worst performance. These three configurations have in common the Raupach’s drag partition scheme and the Alfaro
Chapter 5. Conclusions

and Gomes sandblasting efficiency parameterization, indicating these two as the most appropriate for regional dust modeling. The best performing configuration in this study was found to be R14.

The analysis of the timeseries of R14, R5 and R13 shown a satisfactory performance of dust events with PM10 levels above 300 $\mu g/m^3$, but a systematic inability to reproduce the magnitude and the pattern of dust events below this value, with the most probable cause the local dust sources near Doha not represented by the modeling system. The boundary conditions found to have an average contribution of 45% and 47% for dusty and non-dusty days at Doha site, with $\sim 33\%$ resulting from the western boundary. Among the available dry deposition schemes in CAMx, Zhang, Brook, and Vet (2003) produces the best results for the specific regional modeling system. The aerodynamic entrainment neglected in this study could be a possible mechanism to explain part of the overall underestimation of the best three configurations (R14, R13 and R5).

Several aspects should be investigated in the future. Although a first indication of the best performing configurations has been found in this study, more evidence is needed, in terms of measurements and modeling effort, to justify the validity or not of each one and to conclude about the final best performing configuration. Future scientific effort could focus on soil properties, and specifically over areas with distinct soil texture and soil size distributions. Also variations could result from the definition of the roughness elements, and especially on the dust budget of the area of interest, which is mainly affected by the drag partition and consequently by roughness lengths/densities. The aerodynamic entrainment’s potential should be investigated also as a possible significant mechanism. In addition, the contribution of the local sources should be incorporated, since recent studies with focus on the local PM sources (e.g. fugitive fPM) revealed significantly higher emission rates for the road dust re-suspension and the presence of large patches of barren land (e.g. construction activities) within the urban area (Hassan et al., 2020).
Appendix A

The statistical metrics used to evaluate the parameterizations performances are defined as follow:

Mean Bias (MB):

\[ MB = \frac{\sum_{i=1}^{N} (M_i - O_i)}{N} \quad (A.1) \]

Factor of two criterion (Fac2):

\[ Fac2 = 2 \leq \frac{M_i - O_i}{O_i} \leq 2 \quad (A.2) \]

Normalized Mean Square Error (NMSE):

\[ NMSE = N \frac{\sum_{i=1}^{N} (M_i - O_i)^2}{\sum_{i=1}^{N} M_i \sum_{i=1}^{N} O_i} \quad (A.3) \]

Fractional Bias (\( F_b \)):

\[ F_b = \frac{\sum_{i=1}^{N} M_i - \sum_{i=1}^{N} O_i}{0.5(\sum_{i=1}^{N} M_i + \sum_{i=1}^{N} O_i)} \quad (A.4) \]

Fractional Standard Deviation (\( F_s \)):

\[ F_s = \frac{\sqrt{\sum_{i=1}^{N} (M_i - \overline{M})^2} - \sqrt{\sum_{i=1}^{N} (O_i - \overline{O})^2}}{0.5(\sqrt{\sum_{i=1}^{N} (M_i - \overline{M})^2} + \sqrt{\sum_{i=1}^{N} (O_i - \overline{O})^2})} \quad (A.5) \]
Pearson’s Correlation coefficient (R):

\[
R = \frac{\sum_{i=1}^{N} (M_i - \bar{M})(O_i - \bar{O})}{\sqrt{\sum_{i=1}^{N} (M_i - \bar{M})^2 \sqrt{\sum_{i=1}^{N} (O_i - \bar{O})^2}}} \tag{A.6}
\]

Index of Agreement (IOA):

\[
IOA = 1 - \frac{\sum_{i=1}^{N} (M_i - O_i)^2}{\sum_{i=1}^{N} (|M_i - \bar{O}| + |O_i - \bar{O}|)^2} \tag{A.7}
\]

where \( N \) the number of values/measurements, \( M_i \) the model values, \( O_i \) the observed values, \( \bar{M} \) the model’s mean and \( \bar{O} \) observation’s mean.

Modeling Quality Indicator (MQI):

\[
MQI = \frac{RMSE}{bRMS_u} \tag{A.8}
\]

where \( RMSE \) the root mean square error defined as:

\[
RMSE = \sqrt{\frac{\sum_{i=1}^{N} (M_i - O_i)^2}{N}} \tag{A.9}
\]

\( b = 2 \) and \( RMS_u \) the root mean square uncertainty of the measurements, as defined in Monteiro et al. (2018).

Bias related MQI component (\( MQI_{2bias} \)):

\[
MQI_{bias} = \left( \frac{MB}{bRMS_u} \right)^2 \tag{A.10}
\]

Standard deviation related MQI component (\( MQI_{2std} \)):

\[
MQI_{std} = \left( \frac{\sigma_M - \sigma_O}{bRMS_u} \right)^2 \tag{A.11}
\]

where \( \sigma_M \) and \( \sigma_O \) the standard deviations of the model and of the measurements respectively.

Correlation related MQI component (\( MQI_{2corr} \)):
\[ MQI^{2}_{\text{corr}} = \frac{2\sigma_{M}\sigma_{O}(1 - R)}{bRMS_{u}} \quad (A.12) \]
Bibliography


Argyropoulos, Christos D et al. (2016). “Modeling of PM10 and PM2.5 building infiltration during a dust event in Doha, Qatar”. In: 2nd International Conference on Atmospheric Dust, Castellaneta Marina, Italy.


Darmenova, Kremena et al. (2009). “Development of a physically based dust emission module within the Weather Research and Forecasting (WRF) model: Assessment of dust emission parameterizations and input parameters for


Bibliography


Kukkonen, J et al. (2012). “A review of operational, regional-scale, chemical weather forecasting models in Europe”. In: *Atmospheric Chemistry and Physics*.


Laurent, B et al. (2005). “Simulation of the mineral dust emission frequencies from desert areas of China and Mongolia using an aerodynamic roughness


Pitchford, Marc et al. (2007). “Revised algorithm for estimating light extinction from IMPROVE particle speciation data”. In: 57.11, pp. 1326–1336. ISSN: 1096-2247.


Saraga, Dikaia et al. (2017). “Chemical characterization of indoor and outdoor particulate matter (PM2.5, PM10) in Doha, Qatar”. In: Aerosol and Air Quality Research 17.5, pp. 1156–1168. issn: 1680-8584.


Shi, Mingjie et al. (2016). “Quantifying the impacts of landscape heterogeneity and model resolution on dust emissions in the Arabian Peninsula”. In: Environmental Modelling & Software 78, pp. 106–119.


Wu, Wei et al. (2018). “Wind tunnel experiments on dust emissions from different landform types”. In: 10.4, pp. 548–560. ISSN: 1674-6767.

Xian, Xue et al. (2002). “Field and wind-tunnel studies of aerodynamic roughness length”. In: Boundary-layer meteorology 104.1, pp. 151–163. ISSN: 0006-8314.


Zhang, Jie et al. (2016). “Surface renewal as a significant mechanism for dust emission”. In: 16.24, pp. 15517–15528. ISSN: 1680-7316.