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The Development of a Dust Mineralogy Map from Satellite Retrievals and Implementation in WRF-Chem †

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Abstract: Mineral dust particles are key ingredients of the atmosphere. They interact in atmospheric physics and chemistry and have important implications for human health. Therefore, it is important to examine the properties of these aerosols, including their ambient concentrations, size distributions, shape and mineral composition. In this work, we use satellite remote sensing from Sentinel 2A and EMIT missions to derive the mineralogical composition of surface areas, and we describe the development of a new module to represent the atmospheric life cycle of individual dust minerals in WRF-Chem. In the first step, the GMINER30 mineralogical database is implemented in WRF-Chem to describe the emission, transport, dry and wet deposition of different mineral types.

Keywords: desert dust; mineralogy; WRF-Chem

1. Introduction

A broad spectrum of environmental processes, such as radiation, cloud formation and ocean fertilization, and human health are affected by the presence of mineral dust. The transport of dust particles is dictated by the prevailing meteorological conditions, as well as the composition and physiochemical properties of the particles themselves. The latter factors are determined by the soil mineralogy in the source region. To develop a more refined mineralogical categorization that can significantly improve the dust transport estimations from numerical models and prepare for their implications on weather, biogeochemistry and health, we have worked to achieve two goals: (i) derive a finer mineralogical partition of the source regions through the utilization of high-resolution multi-spectral (Sentinel 2) [1] and hyperspectral (EMIT-NASA) EO datasets [2]; (ii) implement the existing GMINER30 mineralogical database [3] in the WRF-CHEM model and perform sensitivity tests.

2. Methodology and Results

2.1. Mineralogy from Multispectral (Sentinel 2A) and Hyperspectral (EMIT) Satellite Retrievals

The broader area of Lake Chad in Africa was our selected test-bed for the calculation of mineralogical abundances. Satellite estimates were derived for specific dates in Spring and Autumn in order to efficiently exclude areas of dense vegetation (NDVI > 0.3) and identify a number of minerals via spectral indices. The reference spectrum of minerals related to dust was derived from the USGS Spectral Library v7 [4] and analyzed for signature reflectivity characteristics in specific wavelengths, upon which a number of custom band ratios were created. From Sentinel 2 estimates, Alteration, Ferric Oxides and All Iron were calculated (as both Plagioclase and Orthoclase in the Feldspar group are featureless in the specific bands). As the number of bands in the Sentinel 2A estimates are limiting to identifying individual minerals, an approach of calculating mineralogical categories was preferred instead. Ferric Oxides includes minerals such as Hematite, Goethite and Jarosite, whereas All Iron includes both ferrous as well as ferric oxides of iron. The Alteration index defines areas that are rich in clay content. These three categories can be seen in Figure 1.

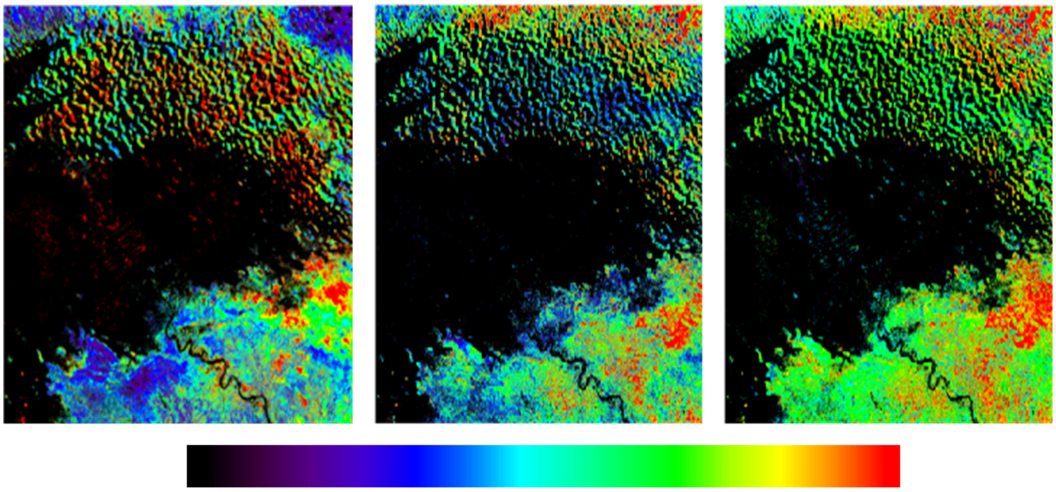

Figure 1. Alteration, Ferric Oxides and All Iron Oxides, as calculated using Sentinel data. Black color indicates no identification and red color indicates high identification of each mineral.

On the other hand, the 285 narrow spectral bands of EMIT reflectance products allow a significantly more refined partition in the identification of specific minerals, as presented in Figure 2. The Level 2a product that is currently available provides surface reflectance, which is derived by screening clouds and correcting for atmospheric effects. By utilising the L2A estimates and resorting to the aforementioned custom band ratios in Table 1, we identified a number of minerals that relate to the dust particle uptake. In 2023, the Level 2b product is expected to offer mineralogy data derived from fitting reflectance spectra after screening for non-mineralogical components, so we could input these categories into a global Numerical Weather Prediction (NWP) model.

2.2. Implementation of GMINER30 Database in WRF-Chem

To represent atmospheric transport as well as the dry and wet deposition mechanisms of the different mineral components of desert dust, we developed a dust mineralogy module in the framework of the WRF-Chem regional model [5], which we updated with the MODIS-NDVI active dust sources definition, as described in [6]. In order to achieve this, we implemented the global 30sec GMINER30 high-resolution mineralogical gridded database of dust-productive soils for atmospheric dust modeling [3]. This dataset includes a mean global distribution of the soil mineral composition and is appropriate for implementation in global and regional numerical studies. The distribution of the effective mineral content in soil in percentages is given for quartz, illite, kaolinite, smectite, feldspar, calcite, hematite and gypsum. The mineral fraction is weighted in terms of the clay and silt content in the soil. To derive the mass size distribution for each emitted mineral, we followed the process described in [7], where, for the normalized mass size distribution for each emitted mineral, we assumed that aggregates are homogeneous mixtures of minerals with similar fragmentation properties. The modeled surface mineralogical composition is shown in Figure 3, as obtained via the implementation of GMINER30 in WRF-Chem. Important spatial variability is evident for most minerals, such as kaolinite and quartz, throughout the Saharan and Arabian deserts, which is in accordance with earlier studies [3]. The developed module is able to handle various datasets with minimal tampering, and therefore, additional mineralogical databases from satellite missions (e.g., Sentinel 2 and EMIT) will be used as inputs in the model as soon as they become available. As an example, the partitioning of total dust to specific elements (in this case, quartz) is shown in Figure 4. As shown in this plot, the variability of quartz particles for a typical desert dust episode depends on both the atmospheric circulation and the surface mineralogy.

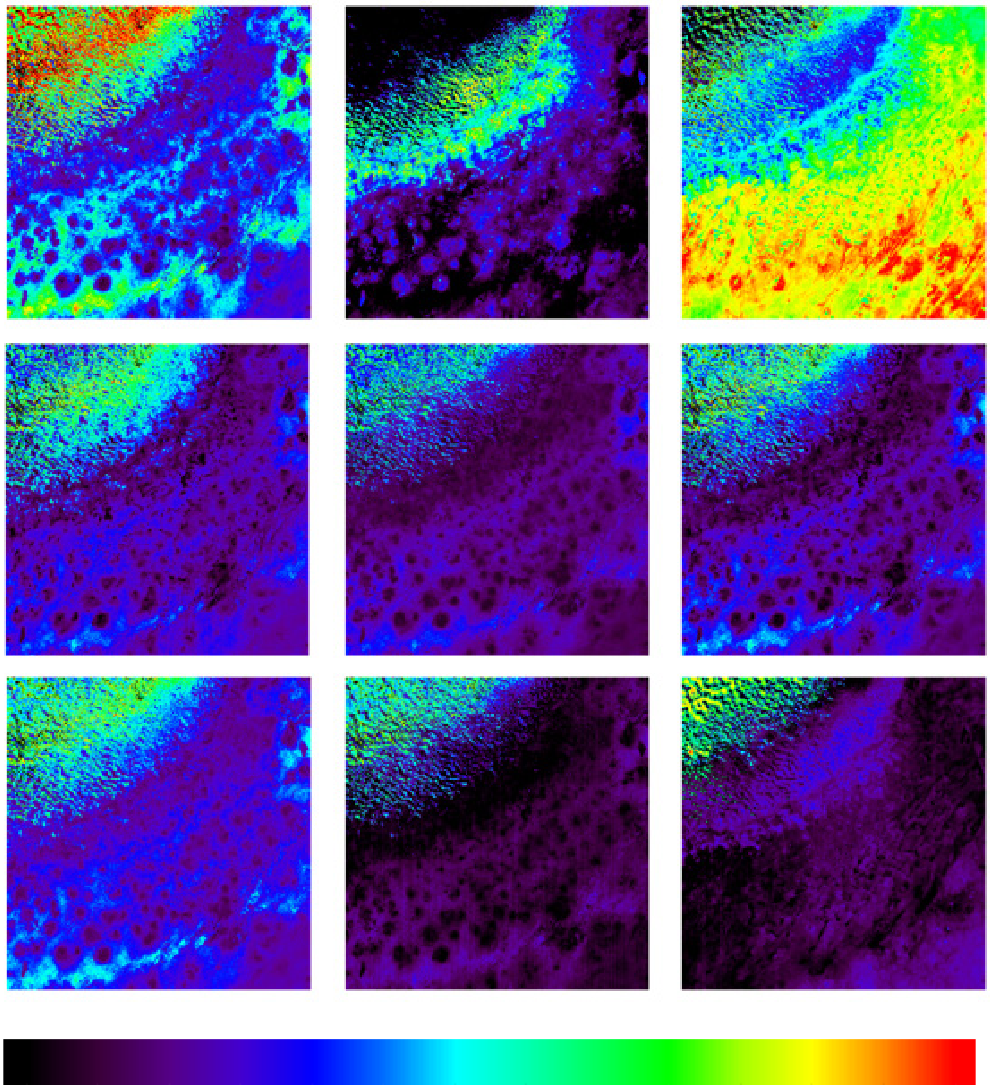

Figure 2. Calcite, Feldspar, Hematite, Clays, Smectite, Kaolinite, Ilite, Gypsum and Phosphorus, as identified from the custom band ratios from EMIT. Black color indicates no identification and red color indicates high identification of each mineral.

Table 1. Custom spectral indices for EMIT.

Name	Chemical Formula	Ratio in Wavelengths (nm)	Band Ratio
Feldspar (plagioclase anorthite-albite)	Albite ($NaAlSi_3O_8$)—anorthite $CaAl_2Si_2O_8$	1700/1300	178/124
Clays (illite, montmorillonite, kaolinite)	$Al_9FFeHK_3MgO_41Si1_{4+8}$, $Al_2H_2O_{12}Si_4$, Al_2Si_2O 5$(OH)_4$	1700/2200	178/245
Illite	$(K,H_3O)(Al,Mg,Fe)_2(Si,Al)_4O_{10}[(OH)_2,(H_2O)]$	1700/2300	178/259
Montmorillonite (smectite)	$(Na,Ca)0.33(Al,Mg)_2(Si_4O_{10})(OH)_2{\cdot}nH_2O$	1700/2056	178/226
Kaolinite	$Al_2Si_2O_5(OH)_4$, or in oxide notation: $Al_2O_3{\cdot}2SiO_2{\cdot}2H_2O$	1700/2160	178/240
Calcite	$CaCO_3$	1700/2330	178/263
Hematite	Fe_2O_3	745.37/530	50/21
Gypsum	$CaSO_4{\cdot}2H_2O$	1670/1751.8	174/185
Phosphorus (apatite)	$Ca_5(PO_4)_3(F,Cl,OH)$	768/797.89	53/57

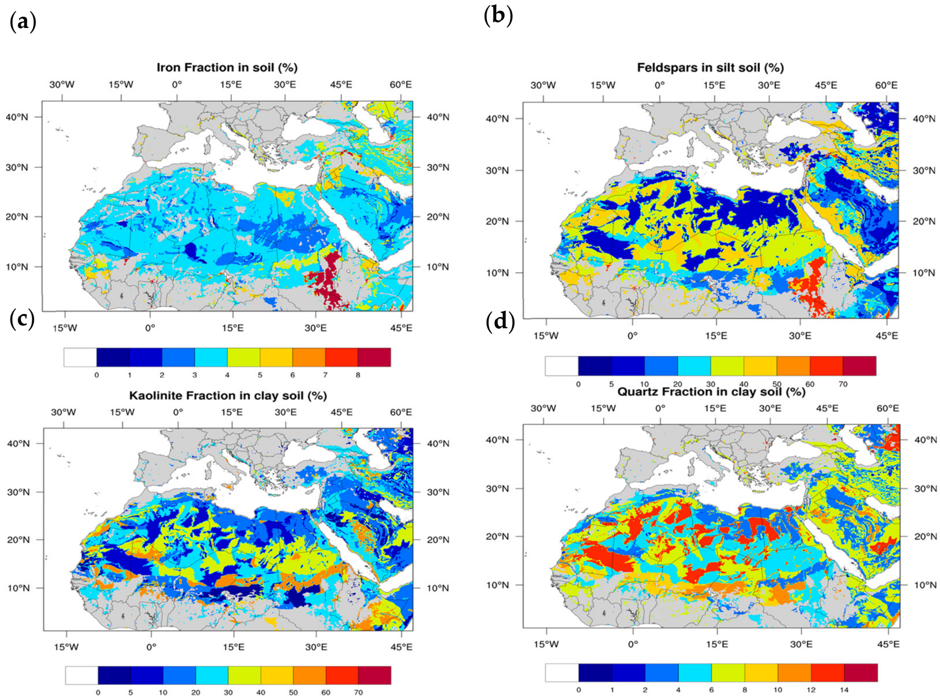

Figure 3. Percentage distribution of the effective mineral contents in soil for (**a**) iron, (**b**) feldspars, (**c**) kaolinite and (**d**) quartz.

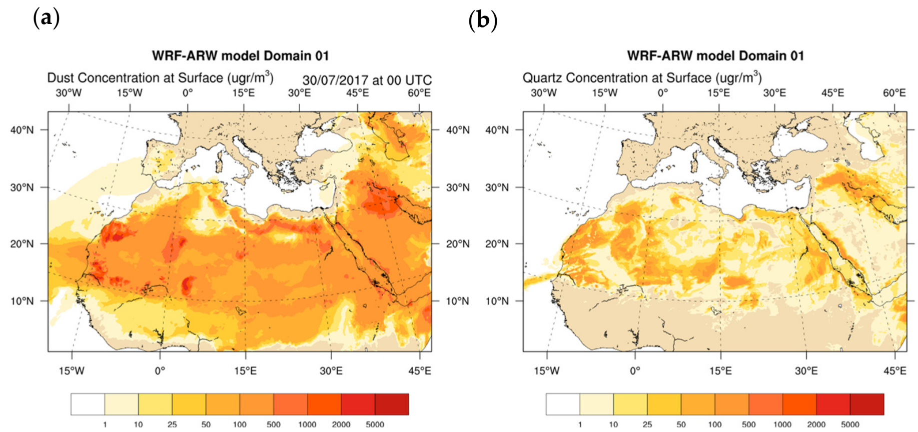

Figure 4. Desert dust concentration at the surface (**a**) and the corresponding quartz mineral concentration (**b**).

3. Conclusions and Future Plans

The more detailed mineralogical mapping of dust uptake areas can greatly benefit atmospheric dust transport estimates from NWP models. Multispectral estimates such as those form Sentinel 2 can provide broad mineralogical categories instead of individual minerals due to their limited bands, but offer global coverage and open data access. Hyperspectral estimates allow the fine identification of particular minerals to be made. Current products, such as EMIT from NASA, also offer a formerly missing strength, which is extensive coverage and data availability. The necessary developments to include detailed mineralogical databases in the atmospheric model have been completed and tested using existing mineralogical databases. The next steps include the performance of sensitivity tests and model–data intercomparisons with WRF-Chem to investigate the impacts of different minerals in atmospheric processes and human health. Additionally, spectral unmixing techniques will be used to derive the more refined identification of minerals from satellite retrievals.

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