From Sugar to Flowers: A Transition of Shallow Cumulus Organization During ATOMIC

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Abstract

The Atlantic Tradewind Ocean-Atmosphere Mesoscale Interaction Campaign (ATOMIC) took place in January-February 2020. It was designed to understand the relationship between shallow convection and the large-scale environment in the trade-wind regime. Lagrangian large eddy simulations, following the trajectory of a boundary-layer airmass, can reproduce a transition of trade cumulus organization from “sugar” to “flower” clouds with cold pools, observed on February 2-3. The simulations were driven with reanalysis large-scale meteorology and ATOMIC in-situ aerosol data. During the transition, large-scale upward motion deepens the cloud layer. The total water path and optical depth increase, especially in the moist regions where flowers aggregate. Mesoscale circulation leads to a net convergence of total water in the already moist and cloudy regions, strengthening the organization. Stronger large-scale upward motion reinforces the mesoscale circulation and accelerates the organization process by strengthening the cloud-layer mesoscale buoyant turbulence kinetic energy production.

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Key Points:

- Lagrangian LES can reproduce the transition of shallow cumulus organization from sugar to flowers observed on Feb 2-3, 2020 during ATOMIC
- While large-scale upward vertical wind deepens the cloud layer, mesoscale wind renders moist areas moister assisting cloud organization
- Stronger large-scale upward motion strengthens the mesoscale circulation and accelerates the sugar-to-flowers transition process

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Abstract

The Atlantic Tradewind Ocean-Atmosphere Mesoscale Interaction Campaign (ATOMIC) took place in January–February, 2020. It was designed to understand the relationship between shallow convection and the large-scale environment in the trade-wind regime. A Lagrangian large eddy simulation, following the trajectory of a boundary-layer airmass, can reproduce a transition of trade cumulus organization from "sugar" to "flower" clouds with cold pools, observed on February 2–3. The simulation is driven with reanalysis large-scale meteorology and ATOMIC in-situ aerosol data. During the transition, large-scale upward motion deepens the cloud layer. The total water path and optical depth increase, especially in the moist regions where flowers aggregate. This is due to mesoscale circulation that renders a net convergence of total water in the already moist and cloudy regions, strengthening the organization. An additional simulation shows that stronger large scale upward motion reinforces the mesoscale circulation and accelerates the organization process by strengthening the cloud-layer mesoscale buoyant turbulence kinetic energy production.

Plain Language Summary

Fair-weather shallow clouds have different sizes and cloud properties. A field study called the Atlantic Tradewind Ocean-Atmosphere Mesoscale Interaction Campaign (ATOMIC) and Elucidating the Role of Clouds-Circulation Coupling in Climate (EUREC^{4}A) was designed to further understand the properties of these clouds. On February 2–3, very small and shallow "sugar" clouds grow into wider and deeper "flower" cloud clusters, no more than 3 km high. The clear spaces between the clouds expand. This study finds that local air circulation is responsible for making the moist and cloudy areas moister, and dry and cloud-free areas drier, enabling a process responsible for this transition. The large-scale vertical winds modulate the rate and strength of this process which occurs locally at smaller scales.

1 Introduction

Low-level clouds forming in the warm marine boundary layer continue to be a leading source of uncertainty in global climate models (i.e. Bony & Dufresne, 2005; Boucher et al., 2013; Zelinka et al., 2016). Challenges associated with the study of these clouds include resolving the internal cloud processes at a fine scale while maintaining an accurate representation of the meteorology in which the clouds occur. The time scale and seasonality are also important, as summertime and wintertime shallow cumuli observed from the same oceanic regions may exhibit different characteristics (Nuijens et al., 2014; Lamer et al., 2015; Nuijens et al., 2015; Vogel et al., 2020).

Previous studies have used high-resolution simulations and satellite retrievals to help understand the relationships between shallow cumulus properties and the large-scale atmospheric and oceanic conditions. For example, the Barbados Oceanographic and Meteorological Experiment (BOMEX) examined the turbulent dynamics of summertime shallow cumuli in the Atlantic Ocean using different large eddy simulation (LES) models (Holland & Rasmusson, 1973; Siebesma et al., 2003). The Cloud Feedback Model Intercomparison Project—Global Atmospheric System Study Intercomparison of Large Eddy Models and Single Column Models (CGILS) investigated the mechanisms of cloud feedback of shallow cumulus and stratocumulus under idealized climate change perturbations based on summertime subtropical atmospheric conditions in the Pacific Ocean (Zhang et al., 2013; Bretherton et al., 2013; Blossey et al., 2013). Bretherton and Blossey (2017) (referred to as BB2017 for short) further explored a mechanism of shallow cumulus organization in different large-scale conditions, including those from BOMEX and one of the CGILS cases. Organization of precipitating shallow cumulus clouds in the presence of cold pools during the Rain in Cumulus over the Ocean (RICO) (Rauber et al., 2007) has been studied with LES by Seifert and Heus (2013), Zuidema et al. (2017), and the references therein. In addition, Mieslinger et al. (2019) examined how different meteorological conditions affect cloud properties across different oceanic basins using high-resolution satellite imagery.

Other studies have used LES models to explore cloud processes that require finer representation of shallow cumuli. For instance, Vial et al. (2019) found that the cloudiness of wintertime North Atlantic trade shallow cumuli is sensitive to the diurnal cycle, both for nonprecipitating and precipitating clouds. Vogel et al. (2020) found that trade cumuli with stratiform cloudiness forming downstream of the trade wind region are tightly controlled by the inversion strength, deepening of the cloud layer, and longwave radiative cooling. Narenpitak and Bretherton (2019) used LES with forcings derived from the trade wind region of an idealized aquaplanet cloud-resolving model to explore the response of shallow cumulus in a warmer climate, and found that radiative cooling and free-tropospheric humidity are keys to controlling the cloudiness in their simulations. The use of in-situ observations, high-resolution simulations and remote sensing tools over the years have enabled studies that lead to better understanding of shallow cumulus processes.

A field campaign designed to study shallow convection in the trade wind region occurred in January–February, 2020 in the Atlantic Ocean east of Barbados. The Atlantic Tradewind Ocean–Atmosphere Mesoscale Interaction Campaign (ATOMIC) and its European counterpart, the European field campaign called Elucidating the Role of Clouds-Circulation Coupling in Climate (EUREC^{4}A), formed a field campaign that used instruments on research aircrafts and ships to observe the properties of shallow cumulus clouds in order to better understand their relationship with the large-scale environment (Quinn et al., 2020; Pincus et al., 2021; Stevens et al., 2021). Recent studies (i.e. Stevens et al., 2020; Rasp et al., 2020; Bony et al., 2020) have categorized the mesoscale organization of shallow cumuli based on the Moderate Resolution Imaging Spectroradiometer (MODIS) imagery into four types: sugar, gravel, fish, and flowers. Different states of organization have different cloud properties including boundary layer depth, amount of precipitation, cloud fraction, and cloud radiative effect.

On February 2–3, 2020, a transition from small and shallow clouds called "sugar" to larger and deeper clouds called "flowers" occurred over the field campaign region (Fig. 1a; animation in Movie S1 in the Supporting Information (SI)). Backward trajectories following the airmass at 500 m altitude show that these flower clouds originated from a shallow sugar cloud layer northeast of National Oceanic and Atmospheric Administration's (NOAA) Research Vessel Ronald H. Brown (RHB). Larger flowers with cold pools were observed to the southwest, closer to Barbados. This study uses a Lagrangian LES, with the domain following a boundary-layer trajectory (red box and yellow dots in Fig. 1a), to simulate this organization event. To understand the relationship between the large-scale vertical velocity and the transition of the mesoscale organization, an additional LES with modified large-scale vertical velocity is included.

The structure of this paper is as follows. Section 2 describes the simulation configurations and the observations used to initialize the simulations. Sections 3 shows the transition from sugar to flowers represented by the LES. Section 4 discusses the mechanisms that are important for the organization. Section 5 identifies the role of large-scale vertical motion on the sugar-to-flowers transition and the circulation at the mesoscale.

Finally, conclusions are given in Section 6. Appendices A through D are found at the end of the manuscript. Movies S1-S3 are found in the SI.

2 Data and Simulations

The System for Atmospheric Modeling (SAM) (Khairoutdinov & Randall, 2003) is employed. The large-scale meteorology and forcings of the simulations are derived from the European Centre for Medium-Range Weather Forecasts (ECMWF) Reanalysis 5^{th} Generation (ERA5) (Hersbach et al., 2020), following the airmass at 500 m altitude through the location of the RHB (54.5°W and 13.9°N) at 17 UTC on February 2. The airmass trajectory was calculated by the Hybrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT) model (Stein et al., 2015; Rolph et al., 2017) in the ERA5 pressure-level data. The large-scale meteorology along the trajectory is, however, from the model-level data. This makes use of ERA5's full 137 vertical levels, especially for the vertical velocity forcings. The horizontal winds are nudged toward ERA5 with Newtonian relaxation, with a 30 min time scale. Since the trajectory moves approximately with the boundary layer, large-scale horizontal advection of the temperature and humidity is not included. Instead, to account for horizontal advection in the free troposphere, the temperature and humidity profiles of the simulation are nudged toward ERA5 with a 30 min relaxation time scale. The temperature and humidity nudging begins 100 m above the inversion, defined as the height of maximum vertical gradient of liquid water static energy in SAM (or of liquid water potential temperature in ERA5, whichever is higher). From this nudging base level, the nudging tendencies increase smoothly over a height interval of 500 m from a value of zero to a value corresponding to the nudging. The surface fluxes are calculated by SAM based on the horizontal wind speeds nudged toward ERA5, and the temperature and humidity profiles calculated by SAM in the boundary layer. Figure 1b-e shows that at the times when the trajectory is within 1-degree distance from the RHB, the outputs from SAM are consistent with the RHB radiosondes.

2.1 Simulations

The control simulation (CTL) is configured with 100 m horizontal grid spacing and a horizontal domain extent of 192×192 km^2. The vertical grid spacing is 50 m, increasing geometrically from 5 km to the domain top at 8 km (total of 120 levels). Above that, the atmospheric profiles from ERA5 are used up to the top of the atmosphere for the

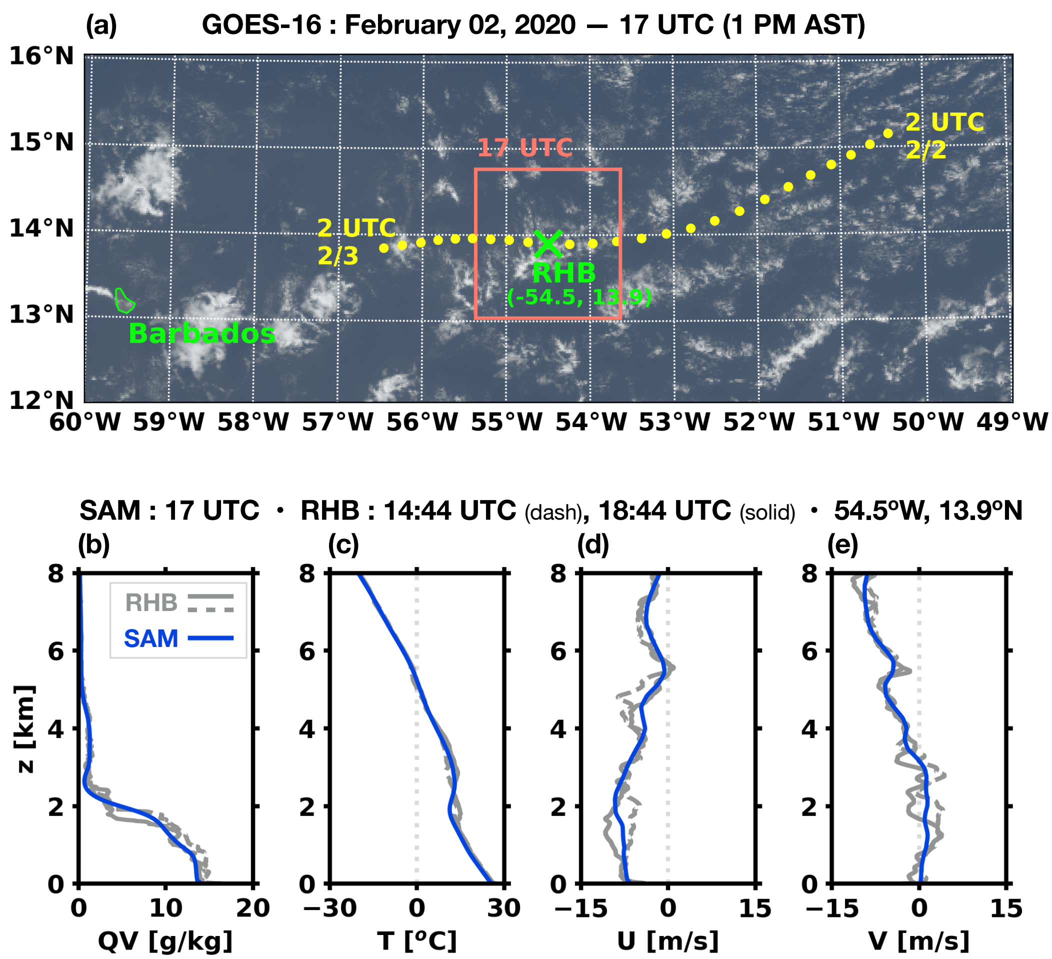

Figure 1. (a) A satellite image from the Geostationary Operational Environmental Satellite-16 (GOES-16) on February 2, 2020. The yellow dots represent hourly coordinates of the airmass-following trajectory on which the Lagrangian simulations are based. The red box indicates the simulation's 192×192 km^2 domain extent, centered on the Research Vessel Ronald H. Brown (RHB, green '×') at 17 UTC. (b-e) The comparisons between radiosondes from the RHB (grey) and domain-mean profiles from the System for Atmospheric Modeling (SAM) control simulation (blue) of the following variables: water vapor mixing ratio (QV), temperature (T), zonal wind (U) and meridional wind (V). The RHB radiosondes are taken at 14:44 UTC and 18:44 UTC, during which time the RHB is within SAM's domain.

radiation calculation. The simulation uses a bulk two-moment (bin-emulating) microphysics scheme (Feingold et al., 1998) and the Rapid Radiative Transfer Model for global climate model applications (RRTMG) (Mlawer et al., 1997) with time varying atmospheric profiles above the domain top and the diurnal cycle of solar radiation. The radiation is computed every 10 seconds. The model's time step is 2 seconds, and the duration of the simulation is 24 hours, from 2 UTC on February 2 to 2 UTC on February 3, 2020.

An additional simulation called WeakW is performed using the same model configuration as CTL, except with a modified vertical velocity (W) in the forcings. The W profiles for WeakW are 50% weaker than CTL during a period with strong upward motion, between 11 UTC and 19 UTC. Since SAM linearly extrapolates the hourly W forcing profiles to the model's time step, W in WeakW diverges from CTL at 10 UTC, and converges again at 20 UTC (Fig. 3b-c).

2.2 The Initialization of Aerosol

There are two types of aerosol in the simulations: sea salt and mineral dust. Sea salt is included as it is the dominant non-dust aerosol type during for particles with diameters smaller than 10μm, based on the shipboard measurement from the RHB (Quinn et al., 2020). Mineral dust was also present in the free troposphere east of Barbados during this time. The RHB radiometer measurements, together with the surface aerosol measurements, indicated the presence of scattering and absorbing aerosol in the free troposphere. (Quinn et al., 2020). Visual observation during flights of the ATOMIC field campaign confirmed the presence of such aerosol above the cloud tops. Therefore, sea salt and mineral dust are initialized at the beginning of the simulation and allowed to advect vertically by large-scale vertical velocity, and horizontally within the domain by trajectory-relative horizontal winds throughout the simulation. The sea-salt particles interact with the cloud microphysics scheme, while the mineral dust is coupled with the radiation scheme. See Appendix A for details on the initialization of the aerosol species.

3 Transition of Shallow Cumuli: From Sugar to Flowers

Simulation CTL is able to reproduce the transition from sugar to flowers on February 2–3, 2020. Figure 2a-e shows 192×192 km^2 snapshots from GOES-16 along the trajectory on which the simulation is based. Figure 2f-j and Movie S2 show the cloud state

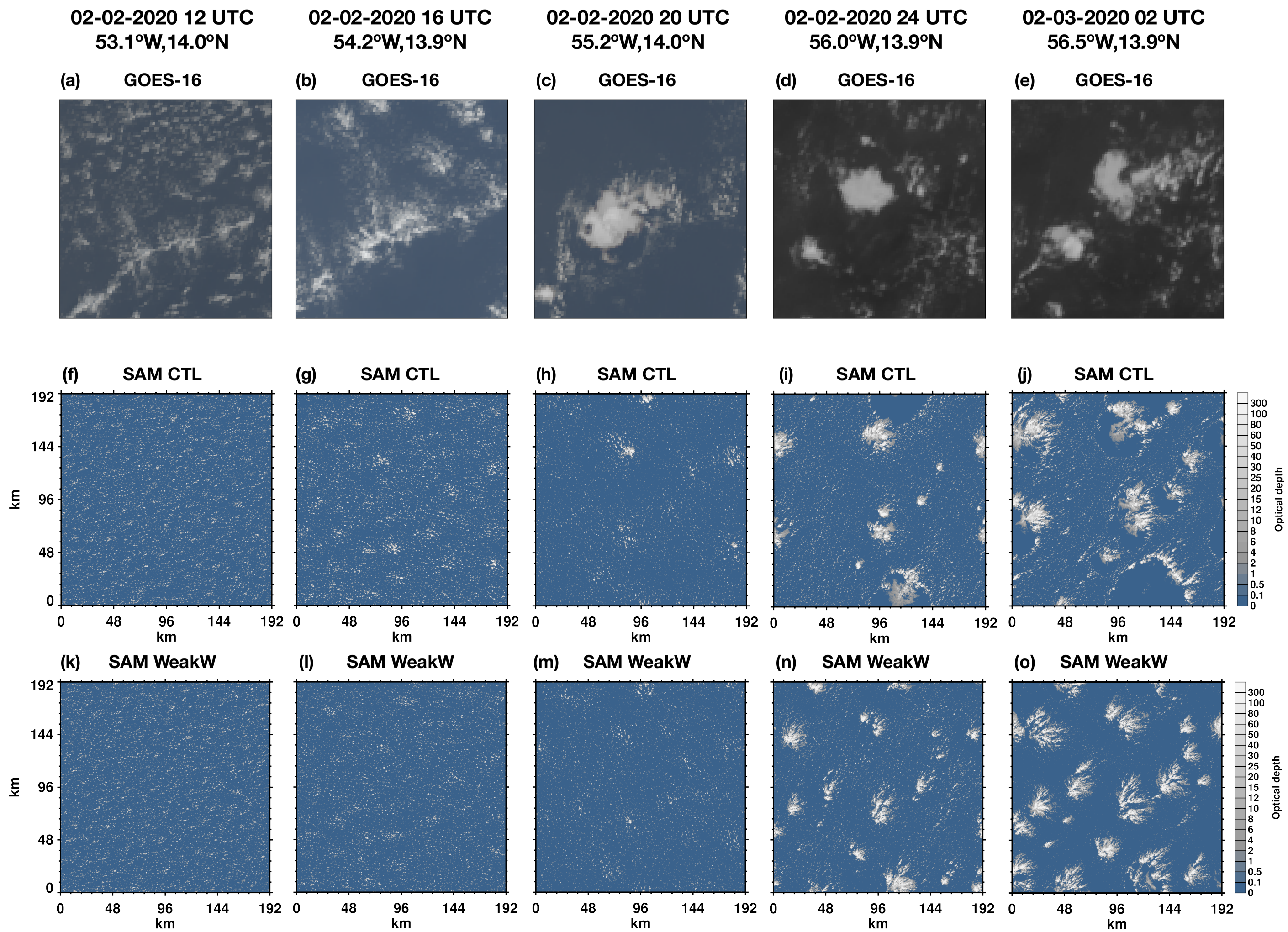

Figure 2. Comparisons of GOES-16 and SAM simulations over a 192×192 km^2 domain at 12, 16, 20, and 24 UTC on February 2, and 2 UTC on February 3, 2020. (a-e) Satellite images from GOES-16, centered on the trajectory presented in Figure 1. (f-j) Snapshots of total (cloud+rain) optical depth from SAM control simulation (CTL). (k-o) As in Panels (f-j) but for the weaker vertical velocity simulation (WeakW).

evolution from CTL. A comparison between the snapshots from GOES-16 and CTL shows that SAM reproduces the nature of the transition well, although there are some disagreements between the satellite images and the simulation. In particular, the satellite imagery shows greater variability in cloud structure over the same area compared to the simulation domain.

The sugar-to-flowers transition in CTL occurs between 8 UTC and 18 UTC, consistent with GOES-16 except the satellite shows larger cloud clusters forming along a line toward the south. During this time, the sugar cloud fields in CTL develop into contiguous aggregates and expand laterally to mature into flowers. As the initial sugar clouds organize, some interspersed cumulus clouds are suppressed while the ones that have aggregated persist and grow. After 24 UTC the simulated cloud clusters expand and catch up with those captured by GOES-16. The aggregated flowers in CTL produce precipitation, which partially evaporates before reaching the surface, resulting in cold downdrafts that produce cold pools adjacent to the flowers.

Potential reasons for the discrepancy between SAM and GOES-16 could result from disagreements in ERA5 profiles and sea surface temperature, and the model physics. Furthermore, unlike regional models, SAM (and other LES) represent conditions at one particular location rather than the entire region of the satellite images. SAM operates with spatially invariant top, bottom, and lateral boundary conditions, the latter of which are periodic. However, in reality the area covered by the simulation domain experiences spatial variability in boundary conditions, and lateral boundary conditions are not periodic. Hence, we expect variability in the simulations to be smaller compared to reality over the simulated area, with the simulation capturing the real cloud state only within a limited sub-region of the area seen in the satellite imagery. Nonetheless, the mean states from SAM are still consistent with the observations, as shown in Figure 1b-e. Because the simulation still faithfully captures the general nature of this transition as seen in the satellite, the analysis is representative of what happens in reality.

3.1 Multiscale Partitioning

Although the simulations are run at 100 m grid spacing, it is helpful to coarse-grain the outputs into larger tiles. This approach partitions the results into contributions from the large-scale, mesoscale, and cumulus-scale processes (BB2017). Coarse-graining filters out the details at the smaller scales that may be associated with shallow convection but are not relevant to the organization. Similar to the approach taken by Honnert et al. (2011), the variance of total water path is computed at different scales (Appendix B). Total water path (TWP) is defined as the sum of vertically integrated water vapor, cloud, and rain (Fig. C1). A tile size of 16×16 km^2 is chosen for this study as it represents the horizontal variability of moist patches associated with flower shallow cumuli in the simulations.

The partitioning of total water mixing ratio (q_t) is given by:

$$q_t = \overline{q_t} + q_t'' + q_t''' \quad . \tag{1}$$

The overline is the domain-mean, the double prime is the perturbation coarse-grained to 16×16 km^2 tiles, representing variability associated with the mesoscale (≥16 km). The triple prime represents variability associated with cumulus-scale processes (<16 km). The partitioning is detailed in Appendix D1.

The coarse-grained outputs are sorted by TWP and binned into quartiles. Quartile 1 (Q1) represents the driest and cloud-free areas while Quartile 4 (Q4) represents the moistest and cloudiest areas of the simulation. The 16×16 km^2 tiles in each quartile are not necessarily adjacent to one another.

3.2 Shallow Convection Organization

Figure 3 shows the time series of the simulations. The thick solid lines represent the results from CTL. Sea surface temperature (SST) increases as the trajectory moves southwestward, and remains constant as the trajectory moves westward. The deepening of the cloud layer in CTL occurs after 6 UTC and becomes more obvious after 10 UTC, when the domain-mean vertical velocity ($\overline{w}$) shifts from negative to positive, helping the cloud layer to deepen (Fig 3b). After 20 UTC, the cloud depth remains constant as the boundary layer encounters large-scale subsidence.

The domain-mean TWP increases as the cloud layer deepens during the transition (Fig. 3d and Fig. C1). As the organization strengthens after 12 UTC, the TWP distribution becomes more asymmetrical; the moist areas become moister while the dry areas become drier (Fig. 3e). The variance of TWP normalized by the mean can be used as a proxy for the organization strength (Fig. 3f). The full 100-m resolution variance (black)

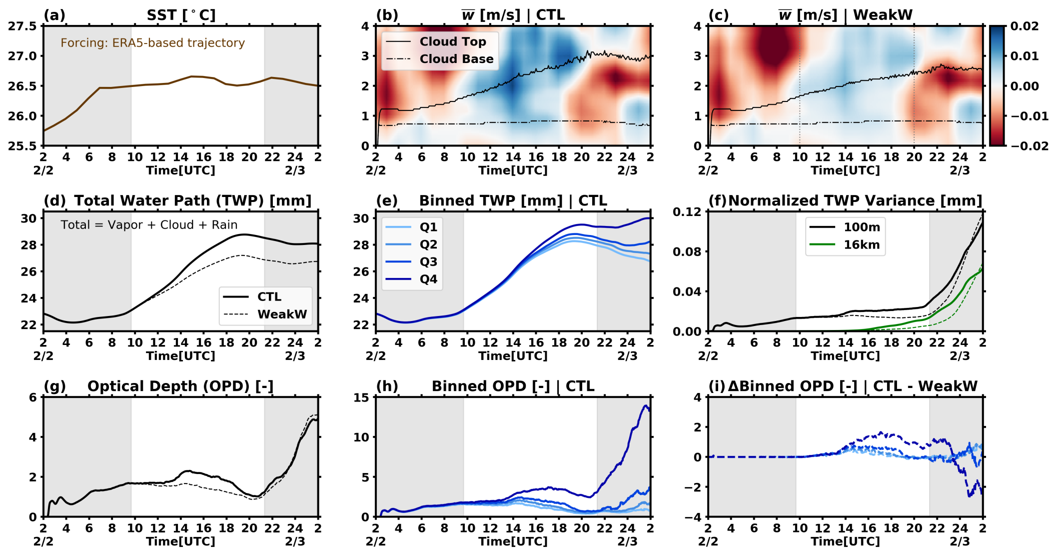

Figure 3. Time series of: (a) domain-mean sea surface temperature; (b) domain-mean vertical velocity, and cloud top and base heights, from CTL; (c) as in Panel (b) but for WeakW; (d) domain-mean total water path (TWP) of both CTL (solid) and WeakW (dash); (e) TWP sorted into quartiles from CTL; (f) variances of TWP computed at the full resolution (black) and the 16 km coarse-grained resolution (green), from both CTL (solid) and WeakW (dash); (g) domain-mean optical depth (OPD) from both simulations; (h) OPD from CTL binned by TWP into quartiles; (i) the change in OPD, binned by TWP, between CTL and WeakW. Gray shading is applied between the daylight hours of 5:48 am and 17:23 pm (local time), when the top-of-atmosphere incoming shortwave radiation exceeds zero in SAM.

increases first at 12 UTC, followed by the coarse-grained variance (green) which increases around 16 UTC; both of them increase rapidly after 22 UTC. This indicates that the organized moist patches first strengthen gradually, and later the organization accelerates. During the transition, the total optical depth (OPD) increases, except for a dip around 20 UTC (Fig. 3g-h), when the small isolated sugar clouds disappear while the larger cloud clusters have yet to aggregate and grow (Fig. 2h). After 20 UTC, the OPD also increases rapidly as the organization strengthens further. The first cold pool is observed at 22 UTC (Movie S2). Because the shallow cumuli in CTL do not precipitate until 20 UTC (Fig. C1c), approximately 4 hours after the mesoscale organization starts to take place, precipitation is not essential for organization in the considered case. This finding is consistent with BB2017, but different from Seifert and Heus (2013) who found that cold pool formation is a dominant mechanism leading to cloud cluster formation.

Figure 4 shows the vertical profiles at two different times, during and after the sugar-to-flowers transition. At 16 UTC on February 2, the domain-mean cloud fraction ($\overline{CF}$) and cloud fraction binned by TWP quartiles ($[CF]$) are bottom-heavy, with slightly enhanced cloudiness near the cloud top in Q4. The enhanced cloudiness near cloud top indicates that the clouds begin to transition from the sugar state to the flower state. At 2 UTC on February 3, the profiles become top-heavy, showing stratiform cloudiness, which is a distinct feature of the flower clouds (Bony et al., 2020; Rasp et al., 2020; Stevens et al., 2020). The stratiform cloudiness near the shallow cumulus cloud top is associated with pronounced longwave radiative cooling (Fig. C2a,c), consistent with previous studies (Vogel et al., 2020).

At both times, regardless of the cloud states and the large-scale vertical velocity ($\overline{w}$), the binned mesoscale vertical velocity perturbations (w'') are positive in the cloud and subcloud layers and negative in the inversion layer of the moistest quartile (Q4). In the drier quartiles (Q1-Q2), the signs of w'' are opposite. The moist quartiles also have positive mesoscale total water perturbations (q_t''). These mesoscale perturbation profiles exhibit similar behaviors to those in BB2017, except with larger magnitudes at 2 UTC. Figure C2b,d further shows that the longwave radiative heating perturbations (R_{LW}'') are negative (more cooling) in the inversion layer of the moistest quartile where q_t'' is also positive and large, and positive (more heating) in the cloud and subcloud layer. This suggests that longwave radiation generates relatively more buoyant air in the cloud plume and less buoyant air in the inversion aloft, contributing to the mesoscale circulation be-

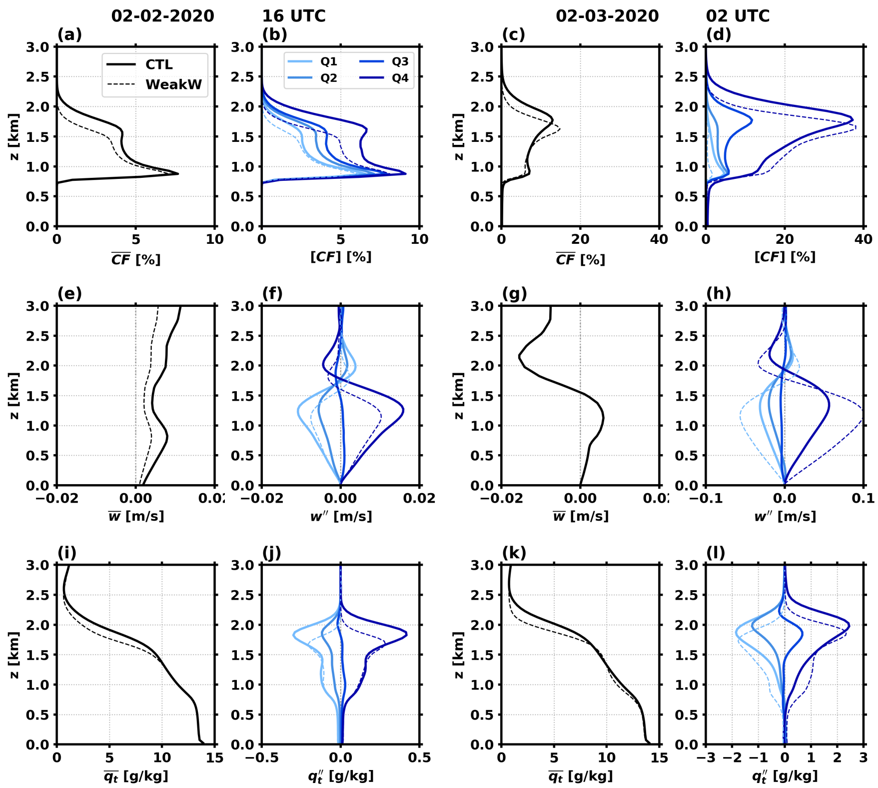

Figure 4. Vertical profiles of various variables at 16 UTC on February 2 (two left columns) and 2 UTC on February 3 (two right columns) of both CTL (solid) and WeakW (dash): (a,c) domain-mean cloud fraction ($\overline{CF}$); (b,d) cloud fraction binned by TWP quartiles ($[CF]$); (e,g) vertical velocity ($\overline{w}$); (f,h) mesoscale perturbations of vertical velocity binned by TWP quartiles (w''); (i,k) domain-mean total water mixing ratio ($\overline{q_t}$); and (j,l) mesoscale perturbations of total water (q_t''), binned by TWP quartiles. For the binned profiles, only Q1 and Q4 from WeakW are shown.

tween the moist and dry regions. During the daytime, the longwave radiation is almost balanced by the shortwave radiation (Fig. C2e-f), resulting in a negligible radiative contribution in the boundary layer, similar to BB2017. In the moist regions, there is also more latent heating in the subcloud and cloud layers due to more condensation, and more evaporative cooling in the inversion layer (Fig. C2j,l), which also contributes to w'', consistent with BB2017.

Mass continuity requires that in the moist and cloudy regions, where w'' is positive (negative) in the subcloud (inversion) layer, there is a local convergence (divergence) below (aloft) (see also BB2017). The profiles at both times have the same signs, but larger magnitudes at 2 UTC on February 3. This is because the cloud clusters are larger at the later time; therefore, coarse-graining does not wash out the variability associated with larger cloud clusters Although cold pools are observed at the later time, at this stage of cold pool development, there is no significant difference in the dynamics (w'') compared to the stage prior to their formation. The same underlying mechanism associated with the mesoscale circulation still dominates. The following section will show that this local circulation is key to redistributing the total water, leading to mesoscale organization.

4 The Mechanism of Transition

This section analyzes the budget of mesoscale total water perturbations q_t'' in the four TWP quartiles to determine a mechanism responsible for the transition. In each TWP quartile, the mesoscale tiles are not necessarily adjacent to one another and they can change location in time based on the mesoscale TWP. Based on Equation 12 of BB2017 and the derivation in Appendix D, the budget of q_t'' at each level can be written as:

$$\frac{\partial q_t''}{\partial t} = A + B + C + S_q'' \quad . \tag{2}$$

Each term on the right hand side of Equation (2) is described as follows: The first term is the advection of mesoscale variability due to trajectory-relative large-scale wind ($\overline{\boldsymbol{v}}$) and mesoscale perturbations of the wind velocity ($\boldsymbol{v}''$):

$$A = -(\overline{\boldsymbol{v}} + \boldsymbol{v}'') \cdot \nabla q_t'' \quad . \tag{3}$$

Let [ ] denote coarse-graining of the cumulus-scale field inside the brackets to a mesoscale region of 16×16 km^2, and let ρ denote the reference density profile. The second term represents the vertical and horizontal gradients of the cumulus-scale q_t flux coarse-grained to 16×16 km^2:

$$B = B_v + B_h = -\frac{1}{\rho}\frac{\partial}{\partial z}[\rho w''' q_t'''] - \nabla_h \cdot [\boldsymbol{v}''' q_t'''] \quad . \tag{4}$$

Eq. (4) was derived with the anelastic approximation used in SAM. The third term is the mesoscale vertical advection of large-scale q_t:

$$C = -w'' \frac{\partial \overline{q_t}}{\partial z} \quad . \tag{5}$$

Finally, the fourth term is the source term of q_t'', which represents the mesoscale perturbations of the precipitation mass flux (F_p) divergence:

$$S_q'' = (-\frac{1}{\rho}\frac{\partial F_p}{\partial z})'' \quad . \tag{6}$$

Figure 5(a-h) shows vertical profiles of A, B_v, B_h, and C binned by TWP quartiles from CTL at 16 UTC on February 2 (two left columns) and 2 UTC on February 3 (two right columns). In each panel, the vertically integrated value of the respective quantity between 0 and 3 km (denoted by $\langle \quad \rangle$) is also shown. (The S_q'' profiles and their vertically integrated values are much smaller and hence negligible even at 2 UTC on February 3, when the clouds precipitate, as shown in Figure C3a.) A positive quantity means the respective term is responsible for moistening the region, a source term for q_t''.

According to BB2017, A is small and tends to dry out the boundary layer in Q4. Although this is true at 16 UTC on February 2 (Fig. 5a), A has a non-negligible magnitude in the cloud layer at 2 UTC on February 3 (Fig. 5c). Nonetheless, $\langle A \rangle$ still dries out Q4, and A is not a major term in the q_t'' budget.

Although B_v is large at both times, $\langle B_v \rangle$ is negligible in all quartiles. This is expected because the vertical cumulus-scale flux transfers total water vertically from the cloud layer to the inversion layer but not horizontally. When coarse-grained within 16×16 km^2 regions, B_h is small and negligible at 16 UTC on February 2, but $\langle B_h \rangle$ is non-negligible at 2 UTC on February 3 and contributes to drying in Q4, albeit secondary to $\langle A \rangle$.

At both times, the magnitude of C is larger than that of A and B_h, and $\langle C \rangle$ is the only term that moistens the boundary layer in Q4, in which flower clouds aggregate. Because $\frac{\partial \overline{q_t}}{\partial z}$ is always negative (Fig. 4i,k), the sign of C always follows the sign of w''. Due to mass continuity, a positive C in the cloud layer of Q4 is associated with horizontal total water convergence below the cloud plumes, and divergence in the inversion. A positive $\langle C \rangle$ indicates a net total water convergence in the lower troposphere of the moistest quartile.

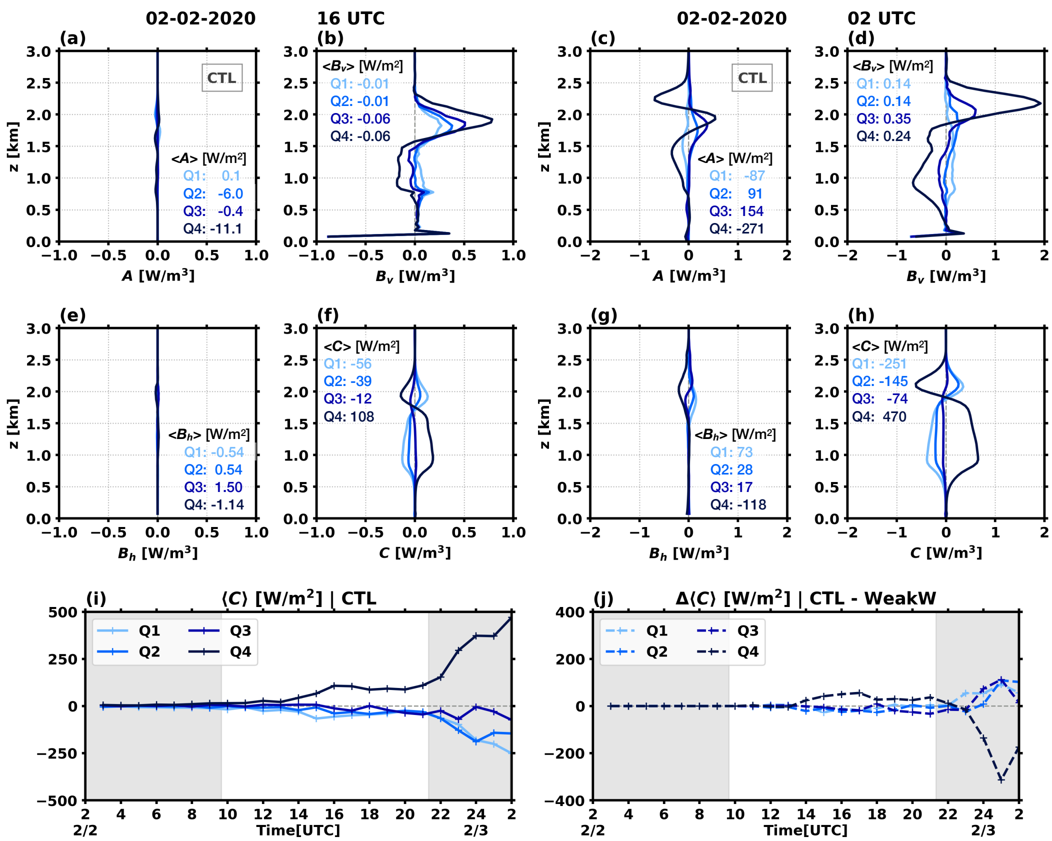

Figure 5. Vertical profiles of: (a,c) large-scale and mesoscale advection of q_t'' (A); (b,d) vertical gradient of the cumulus-scale vertical q_t flux (B_v); (e,g) horizontal gradient of the cumulus-scale horizontal q_t flux (B_h); and (f,h) mesoscale vertical advection of the large-scale q_t (C), at 16 UTC on February 2 (two left columns) and 2 UTC on February 3 (two right columns) from CTL, all coarse-grained to 16×16 km^2 tiles and binned by TWP. The vertically integrated values between 0 and 3 km are also shown, denoted by $\langle \quad \rangle$. (i) Hourly time series of $\langle C \rangle$ binned by TWP quartiles from CTL. (j) The change in $\langle C \rangle$ time series between CTL and WeakW.

To demonstrate that $\langle C \rangle$ drives moistening in Q4 and drying in Q1 through Q3, Figure 5(i) shows the hourly time series of $\langle C \rangle$ binned by TWP quartiles from CTL. This provides the evidence that the net convergence and divergence of total water due to mesoscale circulation renders the moist and cloudy patches moister, and the dry and cloud-free patches drier.

5 The Role of Large-Scale Upward Motion

To examine the role of large-scale vertical velocity for the sugar-to-flower transition, an additional simulation is performed and analyzed. Simulation WeakW has a 50 % weaker $\overline{w}$ during the period of strong upward motion, i.e., between 10 UTC and 20 UTC which is referred to as the intermediate state of the sugar-to-flower transition (Fig. 3c). WeakW produces a shallower cloud layer and lower TWP than CTL. Figure 2k-o and Movie S3 show the cloud field evolution in WeakW. Simulation CTL exhibits a more rapid transition from the sugar to the flower cloud state than WeakW. It has greater normalized TWP variance and optical depth, especially in Q4 where flowers aggregate (Fig. 3f,i).

Although mesoscale organization forms more rapidly in CTL compared to WeakW during the intermediate state of the sugar-to-flower transition, the same mechanisms take place in both simulations. Moist areas become moister and dry areas become drier. Figure 4f,j shows that with stronger upward motion, the w'' and q_t'' profiles of CTL during the transition period have the same structure as those in WeakW, except with larger magnitudes. In other words, the stronger upward motion assists the aggregation of total water on the mesoscale, accelerating organization.

The final organization state in WeakW is stronger than CTL, despite a slower transition and weaker organization during the intermediate state. After 23 UTC, when the organization in WeakW catches up with CTL, w'' becomes stronger in WeakW than in CTL (Fig. 4l). This is consistent with the change in $\langle C \rangle$, which is greater in Q4 of CTL compared to WeakW between 10 UTC and 23 UTC (Fig. 5j), and smaller thereafter. A possible explanation is that the cloud clusters in WeakW are initially smaller and thus barely precipitate, whereas in CTL the clouds precipitate sooner and more strongly, so more and larger cold pools form in CTL (Fig. 2i-j,n-o and Fig. C1c). Therefore, more but smaller flowers form at the end of WeakW, as opposed to fewer but larger flowers with cold pools at the end of CTL.

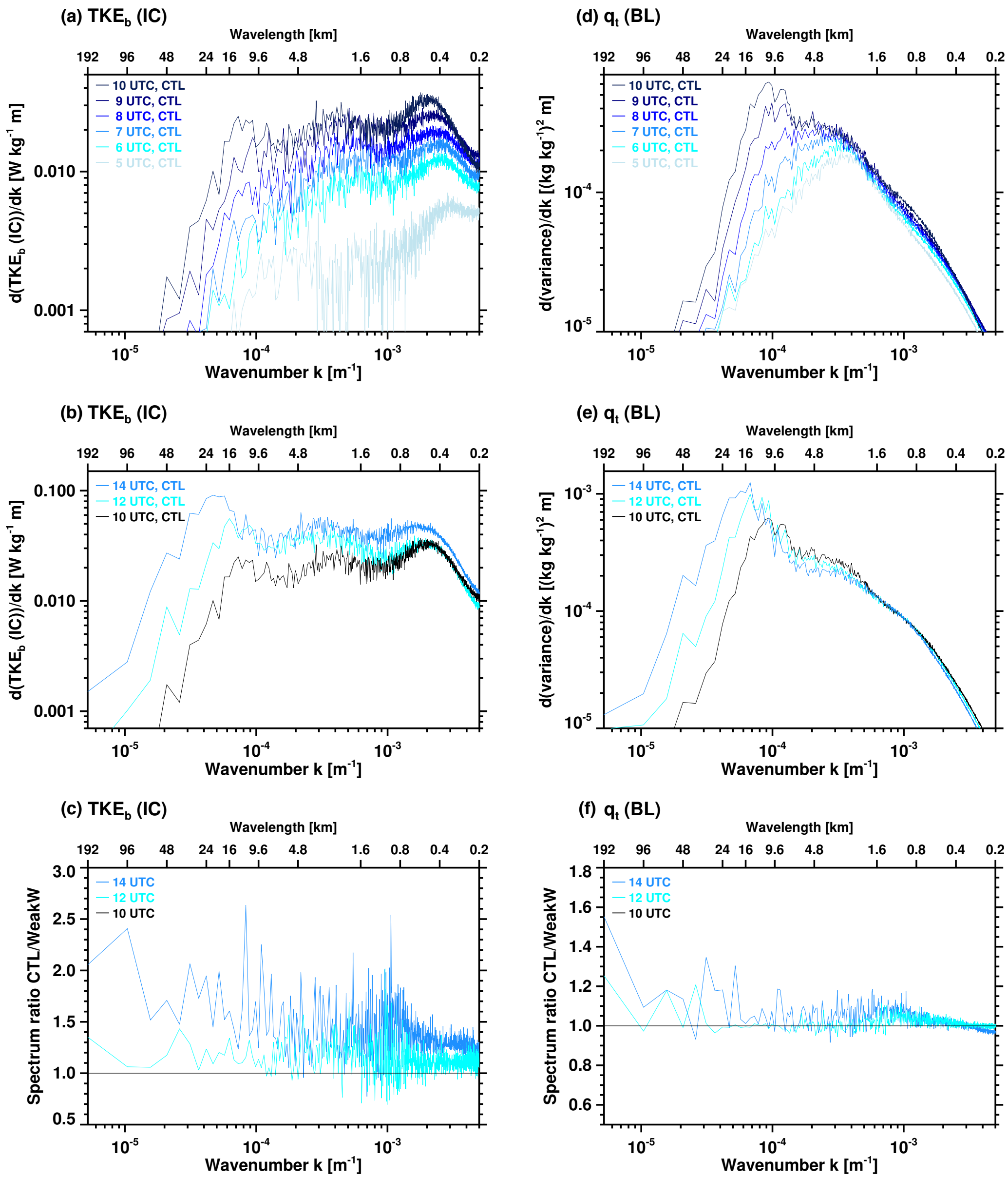

Figure 6. (a-b) Spectra of buoyant turbulence kinetic energy production in the cloud layer (TKE_b (IC)), expressed in units of W kg^{-1} of boundary-layer mass, plotted hourly from 5 UTC to 10 UTC and bi-hourly from 10 UTC to 14 UTC, respectively. (c) Ratio of the TKE_b (IC) spectra in CTL and WeakW plotted at 10, 12, and 14 UTC. (d-f) As in panels (a-c) but for total water mixing ratio in the boundary layer (q_t (BL)).

Figure 6 shows spectra of buoyant turbulence kinetic energy (TKE) production in the cloud layer (TKE_b (IC)) and of boundary-layer total water variance (q_t (BL)) derived from CTL, as well as the ratios of the spectra in CTL and WeakW. Circulation on the mesoscale and aggregation of moisture emerge in the form of peaks between 9.6 and 16 km that are clearly discernible by 10 UTC (Fig. 6a,d) and continue to grow upscale as the clouds transition to the flower state (Fig. 6b,e). Up to 10 UTC, CTL and WeakW have the same $\overline{w}$, hence the spectra are identical and the ratios of TKE_b (IC) and q_t (BL) spectra are 1 (Fig. 6c,f).

In the following hours, the ratio of TKE_b (IC) spectra increases (Fig. 6c), suggesting that the stronger large-scale upward motion renders TKE production stronger in CTL compared to WeakW. The subcloud layer, on the other hand, consumes TKE production at specific mesoscale wavelengths (see Appendix C and Fig. C4). This indicates that the mesoscale circulation that emerges in the sugar-to-flower transition is predominantly driven by TKE production in the cloud layer. Finally, the ratio in the q_t (BL) spectra remains noisy at 12 UTC and increases at 14 UTC (Fig. 6f), albeit at a smaller magnitude than the TKE_b (IC) spectra. This is evidence that stronger large-scale upward vertical motion strengthens both the mesoscale TKE production and the moisture aggregation, the former more than the latter.

Figure 7 shows the ratio of integrated TKE_b (IC) and q_t (BL) spectra in CTL and WeakW. The spectra are integrated at three different wavelength bands, 0-4.8 km, 4.8-16 km, and 16-48 km. From the moment the two simulations diverge, i.e., 10 UTC, the ratio of the TKE production at the mesoscale (4.8-16 km and 16-48 km) exceeds the ratio of the TKE production at the smaller scale (0-4.8 km). This disproportionate strengthening of cloud-level mesoscale TKE production relative to other scales, due to the more positive $\overline{w}$ in CTL compared to WeakW, increases and persists over the period during which $\overline{w}$ differs between the simulations. Additionally, the increase in the ratio of the TKE production leads a corresponding increase in the ratio of the QT variance delayed by approximately three hours, which indicates a causal relationship between the TKE production and the redistribution of the moisture. Therefore, it is the strengthening of cloud-level mesoscale TKE production in CTL relative to WeakW that strengthens aggregation of moisture on the mesoscale and accelerates the sugar-to-flower transition in response to a more positive $\overline{w}$.

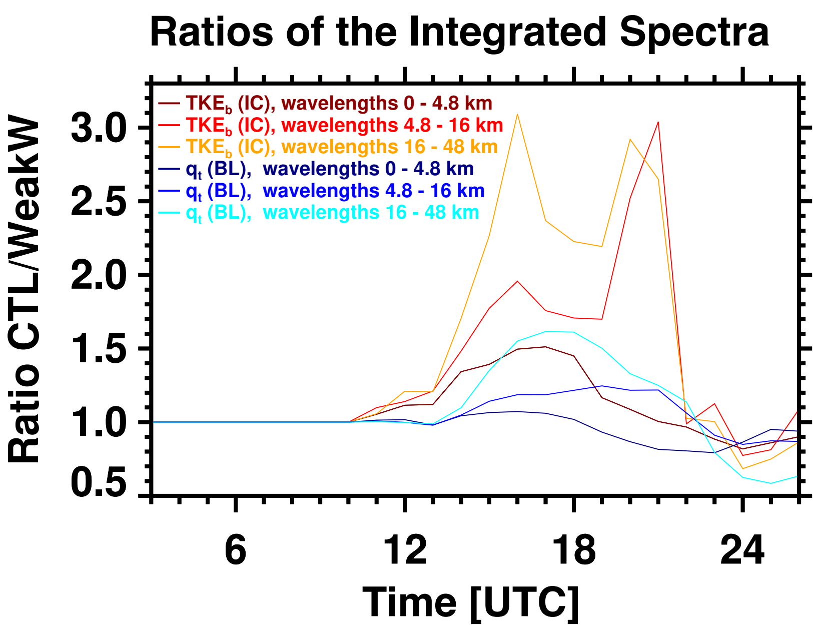

Figure 7. Time series of the ratio of integrated TKE$_b$ (IC) spectra (warm colors) and the ratio of integrated q$_t$ (BL) spectra. The ratio is between simulations CTL and WeakW. The spectra are integrated at three different wavelength bands: 0-4.8 km (small-scale), 4.8-16 km (meso-γ-scale), and 16-48 km (meso-β-scale).

6 Conclusions

The ATOMIC and EUREC^{4}A field campaign took place in the Atlantic Ocean east of Barbados in January–February 2020, with a goal of better understanding the relationship between shallow cumuli and large-scale meteorological and oceanic conditions. On February 2–3, a transition of trade cumulus organization from sugar to flowers was observed. This study shows that a Lagrangian LES following a boundary-layer airmass trajectory can reproduce the transition. During the sugar-to-flowers transition, the clouds become organized, and the cloud layer deepens and moistens.

Although the large-scale vertical motion helps deepen the cloud layer, the mesoscale wind drives the sugar-to-flowers transition. The mesoscale circulation, driven by local ascending (descending) air inside (above) the shallow cumulus plumes, leads to a net moisture convergence in the moist patches, in which the clouds aggregate. This renders the moist patches moister and dry patches drier.

It is shown that large-scale vertical velocity regulates the sugar-to-flower transition by modulating cloud-layer buoyant TKE production at the mesoscale, and the mesoscale circulation by which moisture aggregates. In the considered case, stronger large-scale upward motion accelerates the sugar-to-flower transition by strengthening cloud-layer mesoscale TKE production.

Given the broad interest in the vertical structure of subsidence engendered by ATOMIC and EUREC^{4}A, a follow-on study examining how the structure of the large-scale vertical velocity impacts the mesoscale organization is warranted. Because of the presence of mineral dust, a follow-on study examining the sensitivity of the shallow cumulus organization to mineral dust will be conducted. Precipitation and cold pools may also affect the rate of mesoscale organization and the cloud cluster sizes; hence, a future study will also explore these relationships.

Appendix A The Initialization of Sea Salt and Mineral Dust

Sea salt and mineral dust are initialized at the beginning of both the CTL and WeakW simulations (see Section 2.2 and Fig. A1). The details on the initialization are as follows.

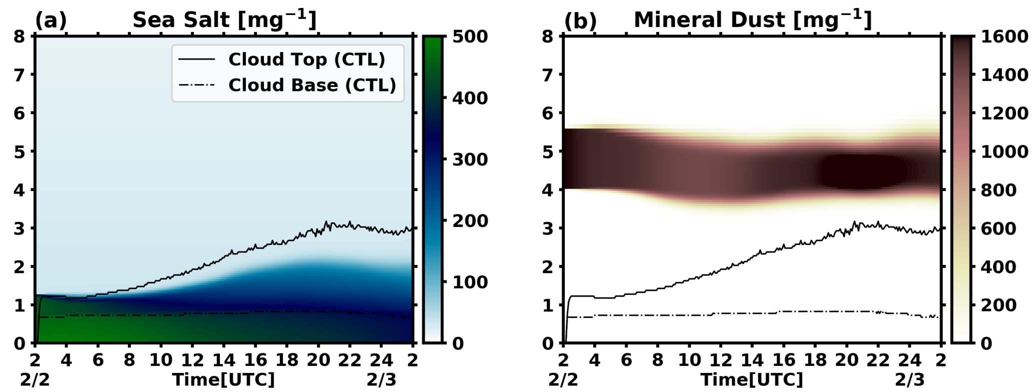

Figure A1. Time series of the domain-mean (a) sea salt and (b) mineral dust concentration from CTL. In both panels, the solid and dash-dot lines indicate the cloud-top and cloud-base heights of the simulation.

A1 Sea-Salt Particles

The sea-salt particles in the boundary layer are initialized based on in-situ aerosol data measured from the RHB averaged between 0 UTC and 4 UTC on February 2. The aerosol size distribution is bimodal and fitted with lognormal functions (Fig. A2). The first peak has a geometric mean diameter (D_g) and geometric standard deviation (σ_g) of 0.128 μm and 1.71, respectively, and the initial concentration (N) is 400 mg^{-1}. The second peak's D_g and σ_g are 0.961 μm and 1.73, respectively, and N is 13 mg^{-1}. The sea-salt particles in the free troposphere have initial N of 32 mg^{-1}, consistent with the EUREC^{4}A measurements from the Ultra-High-Sensitivity Aerosol Spectrometer (UHSAS) and the Cloud Droplet Probe (CDP-2) on the French ATR-42 research aircraft (personal communication with Pierre Coutris, September 30, 2020). The sea salt is coupled with the cloud microphysics scheme.

A2 Mineral Dust

Mineral dust was present in an elevated layer east of Barbados between January 31 and February 3. Therefore, a mineral dust layer is placed in the simulation between 4 and 5.5 km, colocated with an elevated moist layer, based on a previous study which showed that the long-ranged transported Saharan air layer carries mineral dust and moisture from Africa to the Caribbean (Gutleben et al., 2019). The initial mineral dust concentration inside the layer is 1,600 mg^{-1}. Dust optical properties are calculated based

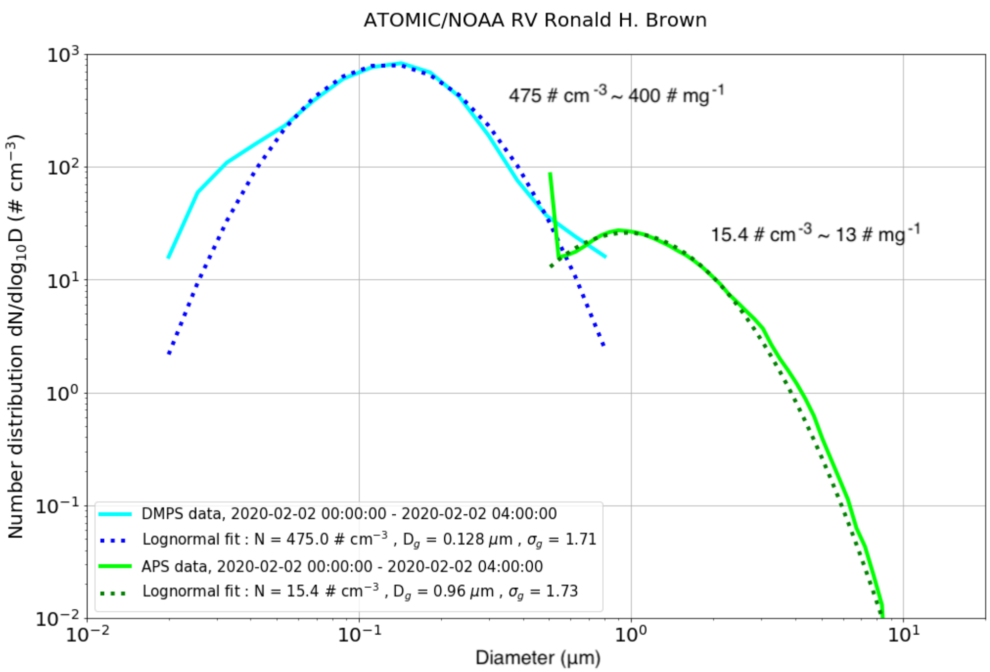

Figure A2. Aerosol size distribution (solid lines) measured from the RHB, averaged between 0 UTC and 4 UTC on February 2, 2020, used to initialize sea-salt aerosol in the simulations. The aerosol size distribution is bimodal and fitted with lognormal functions (dotted lines).

on the assumed size distribution and refractive indices in d'Almeida et al. (1991). The single scattering albedo is approximately 0.85. As a result, the aerosol optical depth of the mineral dust is approximately 0.35, consistent with the MODIS observation during the period of interest. The mineral dust is coupled with the radiation scheme, but not with the cloud microphysics, as the dust remains in the free troposphere in this simulation.

To confirm that the mineral dust configuration described above is consistent with the observation, two additional Eulerian simulations are performed. Figure A3 shows that the clear-sky surface radiations in SAM are more consistent with the in-situ measurements when the mineral dust is included. Since the RHB was stationary between February 1-2, during which there is a cloud-free period, the additional simulations' domain is fixed at the RHB location. The forcings are driven with ERA5, similar to the Lagrangian simulations presented in the main manuscript, except the large-scale horizontal advection tendency of the temperature and humidity is included. These additional simulations are configured with 50 m horizontal grid spacing and a horizontal domain extent of 40×40 km^2. The vertical grid spacing, domain top height, and cloud microphysics and radiation schemes of these Eulerian simulations are the same as those of the Lagrangian simulations. During the cloud-free period, the implemented mineral dust layer increases the surface downward shortwave radiation by approximately 70 W/m^2, making it more consistent with the observation from the RHB. The contribution of the mineral-dust layer on the surface longwave radiation is small, albeit in the right direction.

Appendix B Determining the Tile Size for Coarse-Graining

The ratio of total water path variance is used to determine the tile size for coarse-graining. The ratio is between TWP coarse-grained to different tile sizes ($\mathrm{Var(TWP)}_{\mathrm{Tile}}$) and TWP at the full 100 m resolution ($\mathrm{Var(TWP)}_{\mathrm{100m}}$), and is referred to as the 'TWP variance ratio' for short. (See Honnert et al. (2011) for examples of this approach being applied to other variables.) Figure B1 shows the TWP variance ratio from 4 UTC on February 2, 2020 to 2 UTC on February 3, 2020, plotted every 2 hours from CTL. The tile sizes are multiples of the horizontal grid spacing, from 200 m to 64 km. The TWP variance ratio is 1 if the tile size is 100 m (the horizontal grid spacing), and reduces to smaller values as the tile sizes become larger. When the TWP variance ratio is below the e-folding value (horizontal gray line), the tile size is too coarse to represent the vari-

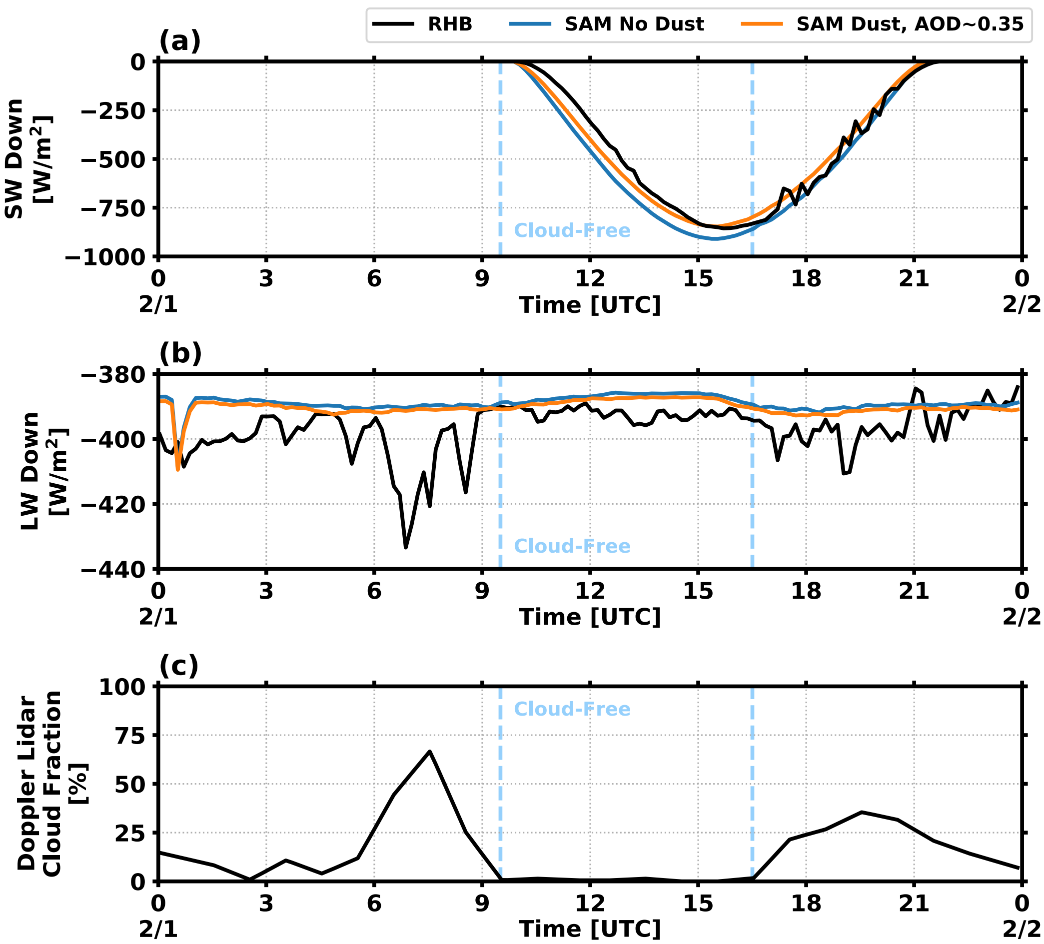

Figure A3. (a) A comparison of the downward shortwave radiation from the RHB in-situ measurement (black) and the Eulerian simulations with mineral dust (orange) and without mineral dust (blue). (b) As in panel (a) but for the downward longwave radiation. (c) Time series of the cloud fraction measured by the Doppler lidar at the RHB.

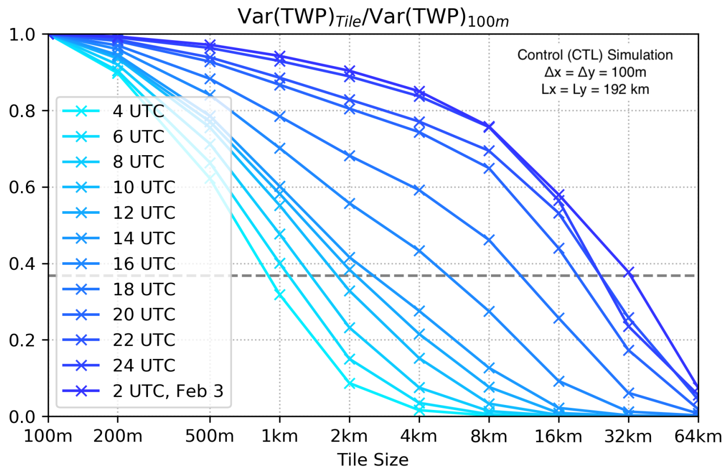

Figure B1. The TWP variance ratio, or the ratio of the variance of total water path coarse-grained to different tile sizes ($\mathrm{Var(TWP)_{Tile}}$) to the variance of 100-m resolution total water path ($\mathrm{Var(TWP)_{100m}}$), computed at different tile sizes from 200 m to 64 km for CTL. The horizontal gray dash line indicates the *e*-folding value. See text in Section 2 above for details.

ability of TWP within the domain on the scale represented by the tile. Since the mesoscale organization strengthens rapidly after 20 UTC, as measured by the normalized TWP variance (Fig. 3f), we look for the tile sizes that can still represent the variability of TWP within the domain after that time. The TWP variance ratio from CTL is above the *e*-folding value between 20 UTC on February 2 and 2 UTC on February 3 for the tile size of 16 km. Therefore, we pick 16 km as the tile size for coarse-graining in CTL.

Appendix C Additional Figures

This section provides additional figures for the discussion in Sections 3 through 5 of the main manuscript.

Figure C1 shows the time series of the vertically integrated water vapor, cloud water, and rain water, also known as precipitable water, cloud water path, and rain water path. The time series are from simulations CTL and WeakW. The sum of these quantities equals the total water path (Fig. 3d).

Figure C2 shows the vertical profiles from simulation CTL: (top) longwave radiative heating rate, (center) shortwave radiative heating rate, and (bottom) latent heat-

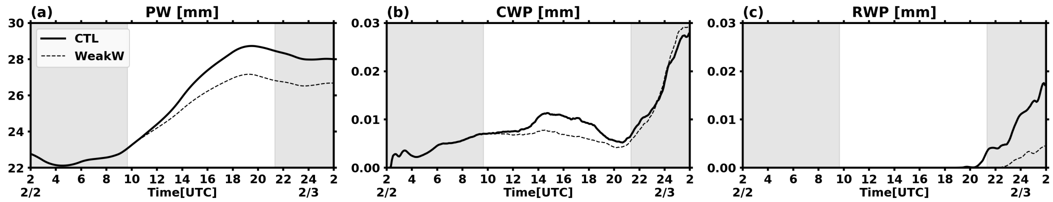

Figure C1. Time series of domain-mean: (a) water vapor path or precipitable water, (b) cloud water path, and (c), rain water path from CTL and WeakW. The sum of these three quantities are total water path, shown in Figure 3d in the main manuscript.

ing rate associated with net evaporation and condensation. See Section 3.2 and figure caption for details.

Figure C3 shows the vertical profiles from simulation CTL of the mesoscale perturbations of the precipitation mass flux divergence at 2 UTC on February 3, and the central difference of the mesoscale total water mixing ratio perturbations about 2 UTC. Since the 3D outputs are saved every 15 minutes, $\Delta t = 30$ min and $\langle \frac{\Delta q_t''}{\Delta t}|_{30min}\rangle$ does not necessarily equal the sum of the right hand side of Equation (2) in the main manuscript because of the large time interval. But the approximation

$$\langle \frac{\Delta q_t''}{\Delta t}|_{30min}\rangle \approx \langle A\rangle + \langle B_v\rangle + \langle B_h\rangle + \langle C\rangle + \langle S_q''\rangle$$

still holds, and the moister quartiles get moister and the drier quartiles get drier.

Figure C4 shows the spectra of buoyant TKE production in the subcloud layer (TKE_b (SC)). The spectra are expressed in the unit of W kg^{-1} of boundary layer mass, enabling a comparison of the spectra in the subcloud layer with the cloud layer (Fig. 6a-b) not only in terms of shape, but also magnitude. After 10 UTC, the TKE_b (SC) spectra decrease with time and is negative at the mesoscale (approximately 9.6-24 km wavelength). The negative spectra do not appear on the logarithmic axis. This indicates that the subcloud layer consumes TKE at specific mesoscale wavelengths. It is the TKE production in the cloud layer that drives the mesoscale circulation which emerges in the sugar-to-flower transition.

Appendix D Mesoscale Tracer Budget Derivation

This section explains the derivation of the budget of a tracer on a (mesoscale) region in detail. The derivation in Section D3 makes no assumptions simplifying the Navier-

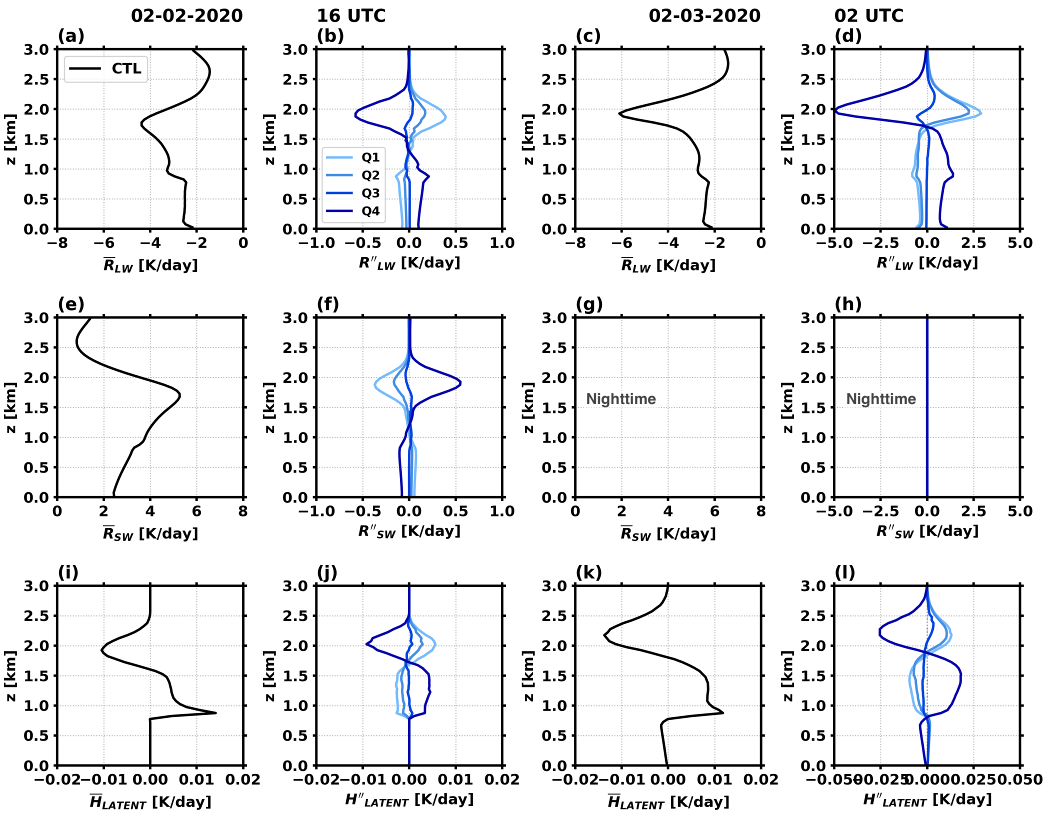

Figure C2. Vertical profiles of various variables at 16 UTC on February 2 (two left columns) and 2 UTC on February 3 (two right columns) from CTL: (a,c) domain-mean longwave radiative heating rate ($\overline{R}_{LW}$); (b,d) mesoscale longwave radiative heating perturbations binned by TWP quartiles (R''_{LW}); (e,g) domain-mean shortwave radiative heating rate ($\overline{R}_{SW}$); (f,h) mesoscale shortwave radiative heating perturbations binned by TWP quartiles (R''_{SW}); (i,k) domain-mean latent heating rate due to net evaporation and condensation at the particular time step ($\overline{H}_{LATENT}$); and (j,l) mesoscale latent heating perturbations binned by TWP quartiles (H''_{LATENT})

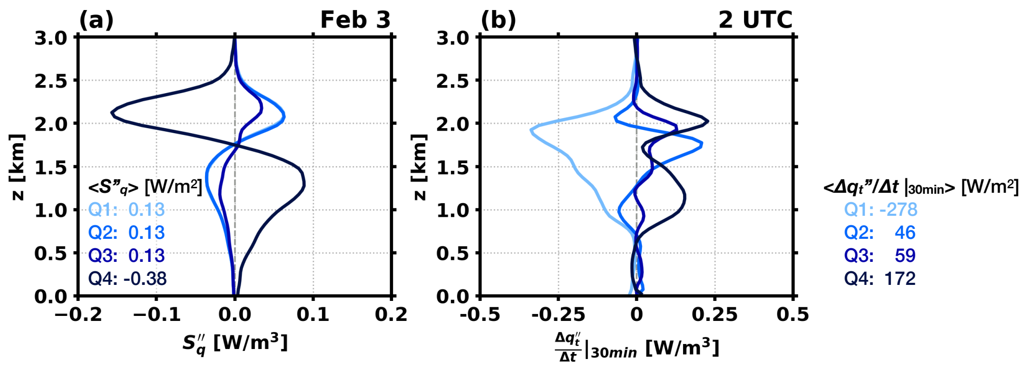

Figure C3. Vertical profiles of (a) mesoscale perturbations of the precipitation flux divergence binned by TWP quartiles at 2 UTC on February 3, and (b) central difference of the mesoscale total water mixing ratio perturbations (q_t'') about 2 UTC.

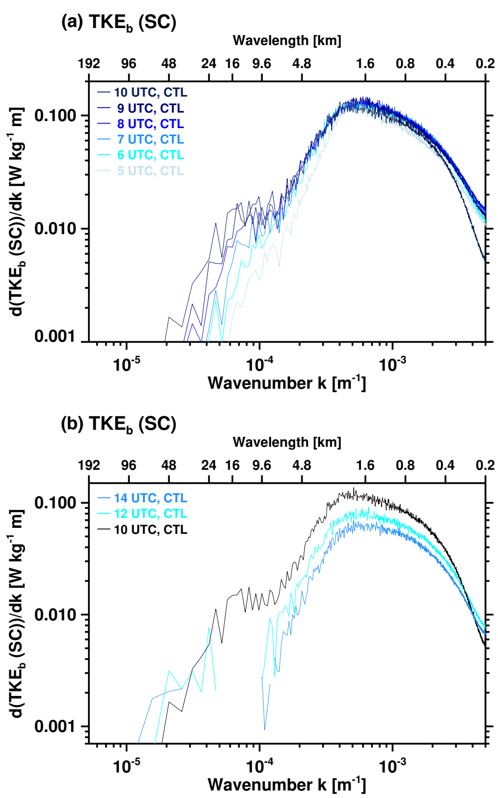

Figure C4. Spectra of buoyant turbulence kinetic energy production in the subcloud layer (TKE$_b$ (SC)), plotted (a) hourly from 5 UTC to 10 UTC and (b) bi-hourly from 10 UTC to 14 UTC.

Stokes equations. The anelastic approximation and a scale-separation approximation are applied in Section D4 to obtain the budget of a tracer on a (mesoscale) region derived by BB2017.

D1 Definitions

Let f be a function that is defined on the locations x_i, y_j, z_k and times t_l of the simulation domain

$$f \doteq f(x_i, y_j, z_k, t_l) \quad . \tag{D1}$$

Decompose f into its domain horizontal mean $\overline{f}$ and the local deviation f' from this mean:

$$f \doteq \overline{f} + f' \tag{D2}$$

Now consider a horizontal, rectangular (mesoscale) region covering $m \times n$ locations in the x and y dimensions, and let the square brackets [ ] denote the horizontal mean over the region:

$$[f] \doteq \frac{1}{mn} \sum_{m,n} f(x_i, y_j, z_k, t_l) \quad . \tag{D3}$$

(See Section 2 in the SI for how the size of the region is determined for the simulation presented in the manuscript.) We decompose f into

$$f \doteq \overline{f} + f'' + f''' \quad . \tag{D4}$$

f'' is the deviation of the region mean from the domain mean,

$$f'' \doteq [f] - \overline{f} \quad , \tag{D5}$$

and f''' the local deviation from the region mean:

$$f''' \doteq f - [f] \quad . \tag{D6}$$

D2 Identities

The following identities are used in the derivation of the mesoscale tracer budget. Firstly,

$$f' = f'' + f''' \quad . \tag{D7}$$

Since $[f]$ is constant over the region, we find

$$[[f]] = [f] \quad . \tag{D8}$$

Applying the horizontal mean over the region [ ] to (D6) gives

$$[f'''] = 0 \quad . \tag{D9}$$

The relationships

$$[f'] = [f''] \quad , \tag{D10}$$

$$[f''] = f'' \quad , \tag{D11}$$

$$f'' = [f'] \quad . \tag{D12}$$

are elementary. Furthermore, we note that because $\overline{f}$ and f'' are constant over the region, for a function $g \doteq g(x_i, y_j, z_k, t_l)$,

$$[\overline{f}g] = \overline{f}[g] \quad , \tag{D13}$$

$$[f''g] = f''[g] \quad , \tag{D14}$$

and

$$[\overline{f}g'''] = \overline{f}[g'''] = 0 \quad , \tag{D15}$$

$$[f''g'''] = f''[g'''] = 0 \quad . \tag{D16}$$

From the definition of the horizontal mean over the region [ ] we obtain

$$[\nabla f] = \nabla [f] \quad . \tag{D17}$$

The identities above hold for vectors in place of the scalars f or g. Then, because g'' and therefore $\nabla g''$ are constant over the region,

$$[\boldsymbol{v}''' \cdot \nabla g''] = [\boldsymbol{v}'''] \cdot \nabla g'' = 0 \quad . \tag{D18}$$

Based on the definition (D6) and using (D17),

$$[\nabla f'''] = [\nabla f] - [\nabla [f]] = [\nabla f] - [[\nabla f]] = [\nabla f] - [\nabla f] = 0 \quad . \tag{D19}$$

We did not make use of the identity $[f'''] = 0$ (Eq. D9), because in general, $[g] = 0$ does not imply $[\nabla g] = 0$.

Because $\overline{\boldsymbol{v}}$ and $\boldsymbol{v}''$ are constant over the region, we obtain

$$[\overline{\boldsymbol{v}} \cdot \nabla f'''] = \overline{\boldsymbol{v}} \cdot [\nabla f'''] = 0 \quad , \tag{D20}$$

$$[\boldsymbol{v}'' \cdot \nabla f'''] = \boldsymbol{v}'' \cdot [\nabla f'''] = 0 \quad . \tag{D21}$$

D3 Derivation of the mesoscale tracer budget

The continuity equation for a scalar with the mixing ratio q is

$$\frac{\partial(q\rho)}{\partial q} = -\nabla \cdot \boldsymbol{F}_q + \tilde{S}_q \quad , \tag{D22}$$

where ρ is the air mass density, and $\boldsymbol{F}_q$ the flux and $\tilde{S}_q$ the source of q, respectively. Using the mass continuity equation and the air velocity $\boldsymbol{v} = (u, v, w)$, it can be written as

$$\frac{\partial q}{\partial t} = -\boldsymbol{v} \cdot \nabla q + S_q \quad , \tag{D23}$$

where we set $S_q \doteq \tilde{S}_q/\rho$. Using the decomposition (D2) for q and S_q, so that

$$q = \overline{q} + q' \quad , \tag{D24}$$

and

$$S_q = \overline{S}_q + S_q' \quad , \tag{D25}$$

and noting that

$$\frac{\partial \overline{q}}{\partial t} = \overline{S}_q \quad , \tag{D26}$$

we obtain

$$\frac{\partial q'}{\partial t} = -(\boldsymbol{v} \cdot \nabla q' + w' \frac{d\overline{q}}{dz}) + S_q' \quad . \tag{D27}$$

Applying the horizontal mean over the region [ ] on both sides of (D27), and using the identity (D12) produces

$$\frac{\partial q''}{\partial t} = -[\boldsymbol{v} \cdot \nabla q' + w' \frac{d\overline{q}}{dz}] + S_q'' \quad , \tag{D28}$$

which simplifies to

$$\frac{\partial q''}{\partial t} = -[\boldsymbol{v} \cdot \nabla q'] - w'' \frac{d\overline{q}}{dz} + S_q'' \quad . \tag{D29}$$

Expanding the first term on the right hand side gives:

$$\begin{aligned} [\boldsymbol{v} \cdot \nabla q'] &= [(\overline{\boldsymbol{v}} + \boldsymbol{v}'' + \boldsymbol{v}''') \cdot \nabla(q'' + q''')] \quad , & \text{(D30)} \\ &= [(\overline{\boldsymbol{v}} + \boldsymbol{v}'') \cdot \nabla q''] + [\boldsymbol{v}''' \cdot \nabla q''] + [(\overline{\boldsymbol{v}} + \boldsymbol{v}'') \cdot \nabla q'''] + [\boldsymbol{v}''' \cdot \nabla q'''] \quad . & \text{(D31)} \end{aligned}$$

With suitable identities, this simplifies to

$$[\boldsymbol{v} \cdot \nabla q'] = (\overline{\boldsymbol{v}} + \boldsymbol{v}'') \cdot \nabla q'' + [\boldsymbol{v}''' \cdot \nabla q'''] \quad . \tag{D32}$$

Inserting (D43) into (D29) produces the budget of a tracer on a (mesoscale) region

$$\frac{\partial q''}{\partial t} = -(\overline{\boldsymbol{v}} + \boldsymbol{v}'') \cdot \nabla q'' - [\boldsymbol{v}''' \cdot \nabla q'''] - w'' \frac{d\overline{q}}{dz} + S_q'' \quad . \tag{D33}$$

On the right hand side, the first term is associated with advection of mesoscale variability. The second term represents sub-mesoscale processes, such as individual cumulus clouds. The third term is associated with mean mesoscale vertical advection of the large scale vertical tracer gradient. The last term, the tracer source, can represent non-advective transport, such as sedimentation. When the tracer q is total moisture, then

$$S_q'' = (-\frac{1}{\rho}\nabla \cdot \boldsymbol{F}_p)'' = (-\frac{1}{\rho}\frac{\partial F_p}{\partial z})'' \quad , \tag{D34}$$

is the precipitation flux divergence, with the precipitation flux $\boldsymbol{F}_p = (0, 0, F_p)$. As shown in Figures 5 and C3, for shallow cumuli that barely precipitate, the term S_q'' is much smaller than the other terms on the right hand side of Eq. (D33).

D4 Anelastic approximation

In the anelastic approximation of the Navier-Stokes equations,

$$\frac{\partial \rho}{\partial t} = \nabla \cdot (\rho \boldsymbol{v}) \doteq 0 \quad , \tag{D35}$$

and

$$\frac{\partial \rho}{\partial x} \doteq \frac{\partial \rho}{\partial y} \doteq 0 \quad . \tag{D36}$$

Then, for a scalar $f = f(x_i, y_j, z_k, t_l)$, we obtain from (D35)

$$\nabla \cdot (\rho \boldsymbol{v} f) = \rho \boldsymbol{v} \cdot \nabla f \quad . \tag{D37}$$

This also holds for $f = q'''$:

$$\nabla \cdot (\rho \boldsymbol{v} q''') = \rho \boldsymbol{v} \cdot \nabla q''' \quad , \tag{D38}$$

or, equivalenty,

$$\boldsymbol{v} \cdot \nabla q''' = \frac{1}{\rho}\nabla \cdot (\rho \boldsymbol{v} q''') \quad . \tag{D39}$$

Decomposing $\boldsymbol{v} = \overline{\boldsymbol{v}} + \boldsymbol{v}'' + \boldsymbol{v}'''$ and applying the horizontal mean over the region $[\quad]$ gives

$$[(\overline{\boldsymbol{v}} + \boldsymbol{v}'' + \boldsymbol{v}''') \cdot \nabla q'''] = \frac{1}{\rho}[\nabla \cdot (\rho(\overline{\boldsymbol{v}} + \boldsymbol{v}'' + \boldsymbol{v}''')q''')] \quad . \tag{D40}$$

On the right hand side of (D40), the brackets $[\quad]$ commuted with $\frac{1}{\rho}$ because of (D36). Using suitable identities, we obtain

$$[\boldsymbol{v}''' \cdot \nabla q'''] = \frac{1}{\rho}[\nabla \cdot (\rho \boldsymbol{v}''' q''')] \quad . \tag{D41}$$

Inserting (D41) into (D33) yields the budget of a tracer on a (mesoscale) region in which the sub-mesoscale term was converted using the anelastic approximation:

$$\frac{\partial q''}{\partial t} = -(\overline{\boldsymbol{v}} + \boldsymbol{v}'') \cdot \nabla q'' - \frac{1}{\rho}[\nabla \cdot (\rho \boldsymbol{v}''' q''')] - w'' \frac{d\overline{q}}{dz} + S_q'' \quad . \tag{D42}$$

Expanding the second term on the right hand side of (D42) with $\boldsymbol{v} = (u, v, w)$ gives

$$\frac{1}{\rho}[\nabla \cdot (\rho \boldsymbol{v}''' q''')] = \frac{\partial}{\partial x}[u''' q'''] + \frac{\partial}{\partial y}[v''' q'''] + \frac{1}{\rho}\frac{\partial}{\partial z}[\rho w q'''] \quad . \tag{D43}$$

Using the scale separation approximation (BB2017, Eq. (28))

$$\nabla_h \cdot [\boldsymbol{v}''' q_t'''] = \frac{\partial}{\partial x}[u''' q'''] + \frac{\partial}{\partial y}[v''' q'''] \ll \frac{1}{\rho}\frac{\partial}{\partial z}[\rho w''' q'''] \tag{D44}$$

gives

$$\frac{\partial q''}{\partial t} = -(\overline{\boldsymbol{v}} + \boldsymbol{v}'') \cdot \nabla q'' - \frac{1}{\rho}\frac{\partial}{\partial z}[\rho w''' q'''] - w'' \frac{d\overline{q}}{dz} + S_q'' \quad . \tag{D45}$$

This is the budget of a tracer on a (mesoscale) region in the anelastic approximation derived by BB2017, in their Eq. (31).

In the main manuscript, the full budget of the mesoscale tracer (Eq. (D42)) prior to applying the scale separation approximation is used. This is because because toward the end of the simulations, the scale separation approximation or Eq. (D44) does not hold true.

Therefore, Eq. (D42) can be written as:

$$\frac{\partial q''}{\partial t} = -(\overline{\boldsymbol{v}} + \boldsymbol{v}'') \cdot \nabla q'' - \frac{1}{\rho}\frac{\partial}{\partial z}[\rho w''' q'''] - \nabla_h \cdot [\boldsymbol{v}''' q_t'''] - w'' \frac{d\overline{q}}{dz} + S_q'' \quad , \tag{D46}$$

which is consistent with Equations (2) - (6) in the main manuscript.

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Supporting Information for "From Sugar to Flowers: A Transition of Shallow Cumulus Organization During ATOMIC"

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Additional Supporting Information (Files uploaded separately)

- Captions for Movies S1 to S3

Introduction

This is the Supporting Information (SI) for the manuscript "From Sugar to Flowers: A Transition of Shallow Cumulus Organization During ATOMIC," which contains the captions for Movies S1 to S3.

Additional Supporting Information (Files uploaded separately)

Movies S1 to S3

- **Movie S1**: An animation of hourly satellite images from the Geostationary Operational Environmental Satellite-16 (GOES-16) displaying the region of the trade cumulus organization transition from 8 UTC on February 2, 2020 to 2 UTC on February 3, 2020. The yellow dots represent hourly coordinates of the airmass-following trajectory on which the Lagrangian simulation is based. The red boxes indicate the simulation's (192-km)^2 domain extent, which passes over the Ronald H. Brown research ship (RHB) or 54.5°W and 13.9°N (green '×') at 17 UTC.

- **Movie S2**: An animation of cloud and rain optical depths from the control simulation (CTL). The snapshots are plotted every minute from 10 UTC on February 2, 2020 to 2 UTC on February 3, 2020.

- **Movie S3**: As in Movie S2 but for the weaker vertical velocity simulation (WeakW).