

What controls the mesoscale variations in water isotopic composition within tropical cyclones and squall lines? Cloud resolving model simulations

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Abstract

One way to test our understanding of the impact of convective processes on the isotopic composition of water vapor and precipitation is to analyze the isotopic mesoscale variations during organized convective systems such as tropical cyclones or squall lines. The goal of this study is to understand these isotopic mesoscale variations with particular attention to isotopic signals in near-surface vapor and precipitation that may be present in observations and in paleoclimate proxies. With this aim, we run cloud resolving model simulations in radiative-convective equilibrium in which rotation or wind shear is added, allowing us to simulate tropical cyclones or squall lines. The simulations capture the robust aspects of mesoscale isotopic variations in observed cyclones and squall lines. We interpret these variations using a simple water budget model for the sub-cloud layer of different parts of the domain. We find that rain evaporation and rain-vapor diffusive exchanges are the main drivers of isotopic depletion within cyclones and squall lines. Horizontal advection spreads isotopic anomalies, thus reshaping the mesoscale isotopic pattern. Variations in near-surface relative humidity and wind speed have a significant impact on d-excess variations within tropical cyclones, but the evaporation of sea spray is not necessary to explain the observed enrichment in the eye. This study strengthens our understanding of mesoscale isotopic variability and provides physical arguments supporting the interpretation of paleoclimate isotopic archives in tropical regions in terms of past cyclonic activity.

Abstract

One way to test our understanding of the impact of convective processes on the isotopic composition of water vapor and precipitation is to analyze the isotopic mesoscale variations during organized convective systems such as tropical cyclones or squall lines. The goal of this study is to understand these isotopic mesoscale variations with particular attention to isotopic signals in near-surface vapor and precipitation that may be present in observations and in paleoclimate proxies. With this aim, we run cloud resolving model simulations in radiative-convective equilibrium in which rotation or wind shear is added, allowing us to simulate tropical cyclones or squall lines. The simulations capture the robust aspects of mesoscale isotopic variations in observed cyclones and squall lines. We interpret these variations using a simple water budget model for the sub-cloud layer of different parts of the domain. We find that rain evaporation and rain-vapor diffusive exchanges are the main drivers of isotopic depletion within cyclones and squall lines. Horizontal advection spreads isotopic anomalies, thus reshaping the mesoscale isotopic pattern. Variations in near-surface relative humidity and wind speed have a significant impact on d-excess variations within tropical cyclones, but the evaporation of sea spray is not necessary to explain the observed enrichment in the eye. This study strengthens our understanding of mesoscale isotopic variability and provides physical arguments supporting the interpretation of paleoclimate isotopic archives in tropical regions in terms of past cyclonic activity.

Plain Language Summary

Water molecules can be light (one oxygen atom and two hydrogen atoms) or heavy (one hydrogen atom is replaced by a deuterium atom). These different molecules are called water isotopes. In large, long-lived, severe storms such as tropical cyclones or squall lines (thunderstorms that organize into lines), the rain is observed to be more depleted in heavy isotopes. Several studies have exploited this property to reconstruct the past variations in the frequency of occurrence of tropical cyclones or severe thunderstorms based on isotope variations observed in speleothems. The aim of this study is to understand what controls the depletion of the rain in tropical cyclones and squall lines. With this aim, for the first time we use high-resolution simulations (2-4 km in horizontal) to simulate the internal dynamics of tropical cyclones and squall lines and their isotope composition. We design a simple model to interpret the results. We show that the depletion in heavy isotopes of the rain is mainly due to rain evaporation, which moistens the lower atmosphere with depleted water vapor.

1 Introduction

The isotopic composition of water vapor (HDO or $H_2^{18}O$) evolves along the water cycle as phase changes are associated with isotopic fractionation. The isotopic composition of precipitation recorded in paleoclimate archives has significantly contributed to the reconstruction of past hydrological changes across the tropics (Wang et al., 2001; Cruz et al., 2009). Indeed, over tropical oceans, the precipitation is usually more depleted in heavy isotopes as precipitation rate increases, an observation called the amount effect (Dansgaard, 1964). In concert with the precipitation, the water vapor over tropical oceans is also more depleted as precipitation rate increases according to satellite and in-situ observations (Worden et al., 2007; Kurita, 2013). Over tropical land, both the precipitation and water vapor are generally observed to be more depleted as the precipitation rate increases in average over the previous days before the observation of isotopic depletion and in average over some large-scale domain upstream of the region of depletion, for example in Western Africa (Risi et al., 2008; Tremoy et al., 2012), Southeast Tibetan Plateau (Gao et al., 2013), Southern India (Lekshmy et al., 2014; Sinha & Chakraborty, 2020), Southern tropical America (Vimeux et al., 2005; Vimeux et al., 2011) or the Mar-

69 itime Continent (Moerman et al., 2013; Conroy et al., 2016). In the tropics, the impor-
70 tance of precipitation rate, either at the local or at the regional scale, in controlling the
71 water isotopic composition of water vapor and precipitation is thus well established. How-
72 ever, the relationship between the water isotopic composition and precipitation rate can
73 vary temporally and spatially. For example, it may depend on the proportion of strat-
74 iform versus convective rain (Aggarwal et al., 2016), on the organization of convection
75 (Lawrence et al., 2004; Risi et al., 2008; Chakraborty et al., 2016) or on the shape of ver-
76 tical velocity profiles (Moore et al., 2014; Torri et al., 2017; Lacour et al., 2017). For a
77 more robust and quantitative interpretation of water isotopic archives in terms of past
78 hydrological changes or cyclonic activity, a better understanding of how the precipita-
79 tion rate impacts the isotopic composition of water vapor and precipitation is thus nec-
80 essary.

81 In the tropics, the main source of precipitation is deep convection (Houze, 2004).
82 It is associated with processes which deplete the water vapor in heavy isotopes. In par-
83 ticular, observational studies have highlighted the role of rain evaporation (Worden et
84 al., 2007), diffusive liquid vapor exchanges (Lawrence et al., 2004), meso-scale downdrafts
85 (Risi et al., 2010; Kurita, 2013) and microphysical processes in stratiform regions of con-
86 vective systems (Aggarwal et al., 2016). Modeling studies with high resolution simula-
87 tions have confirmed the key role of rain evaporation and of microphysical processes in
88 stratiform regions of convective systems, especially melting of depleted snow that sub-
89 sequently evaporates (Risi et al., 2021).

90 One way to test the importance of these processes is to investigate the observed
91 evolution of the isotopic composition of precipitation or near-surface water vapor within
92 “organized” convective systems (Risi et al., 2010). By organized, we mean that the con-
93 vective system has different parts, characterized by different convective or microphys-
94 ical processes, and connected through some meso-scale circulation. For example, squall
95 lines are elongated, propagative convective systems with a gust front in front, followed
96 by a convective region of intense rainfall, a transition region with a paused rainfall, and
97 a trailing stratiform region of light rainfall (Houze, 2004). The precipitation collected
98 during squall lines often features a W shape with more depleted rain in convective and
99 stratiform regions (Taupin & Gallaire, 1998; Risi et al., 2010). In the near-surface wa-
100 ter vapor, many squall lines show isotopic depletion in the convective and stratiform re-
101 gions (Tremoy et al., 2014). This pattern has been interpreted in terms of rain evapo-
102 ration and meso-scale downdrafts.

103 As another example, tropical cyclones are a spectacular manifestation of convec-
104 tive organization, with usually an eye at the center, surrounded by convective walls with
105 very intense rainfall and spiral rain bands reaching several hundreds of kilometers (Houze,
106 2010). The precipitation and near-surface water vapor collected in the vicinity of tropi-
107 cal cyclones often show stronger depletion towards the cyclone center, more depleted
108 water vapor in spiral bands than in between bands (Gedzelman et al., 2003; Xu et al.,
109 2019), and more enriched water vapor in the eye (Fudeyasu et al., 2008). The depletion
110 has been interpreted in terms of progressive rain out towards the center and rain-vapor
111 diffusive exchanges (J. R. Lawrence et al., 2002). The enrichment in the eye has been
112 interpreted in terms of sea spray evaporation (Fudeyasu et al., 2008).

113 The goal of this paper is to investigate the processes controlling the evolution of
114 near-surface water vapor and precipitation within squall lines and tropical cyclones. So
115 far, this question has often been addressed using observational studies or simple concep-
116 tual models. Here for the first time, we use three-dimensional high-resolution, isotope-
117 enabled simulations in which convective motions are explicitly represented. Using these
118 simulations together with an interpretative framework, we aim at quantifying the rel-
119 ative importance of the different processes that have been previously suggested in the
120 literature. Our simulations will be run in idealized conditions of radiative-convective equi-
121 librium. Therefore, we will focus on robust features that are observed in most squall lines

122 and tropical cyclones based on previous studies. No one-to-one comparison can be made
123 with any particular real observed system.

124 This study may also be useful to better understand how convective organization
125 could be recorded in paleoclimate archives. In particular, more organized convective sys-
126 tems, such as squall lines (Risi et al., 2008; Tremoy et al., 2014; Maupin et al., 2021) or
127 tropical cyclones (J. R. Lawrence & Gedzelman, 1996; Lawrence et al., 2004; Price et al.,
128 2008; Chakraborty et al., 2016), have been observed to be associated with water vapor
129 and precipitation that are more depleted in heavy isotopes than unorganized systems.
130 In particular, the depleted rain of tropical cyclones leaves a depleted imprint in surface
131 waters and can significantly affect long-term averages of isotopic composition of precip-
132 itation or surface waters (J. R. Lawrence, 1998; Baldini et al., 2016). This suggests that
133 the isotopic composition of precipitation recorded in speleothems could be used to re-
134 construct past cyclonic activity (J. Lawrence & Gedzelman, 2003; Frappier et al., 2007;
135 Chen et al., 2021). In the past few years, several studies have interpreted speleothems
136 in terms of cyclonic frequency (Nott et al., 2007; Medina-Elizalde & Rohling, 2012; Bal-
137 dini et al., 2016). Similarly, the depletion observed in Texan speleothems has been in-
138 terpreted as enhanced activity of large, long-lived, organized convective systems (Maupin
139 et al., 2021).

140 2 Model and simulations

141 2.1 Isotopic variables

142 The water content in heavy isotopes (HDO or $H_2^{18}O$) is expressed in ‰ as $\delta D =$
143 $(R_D/R_{D,SMOW} - 1) \times 1000$ and $\delta^{18}O = (R_{18O}/R_{18O,SMOW} - 1) \times 1000$, where R_D
144 and R_{18O} are the ratio of Deuterium over Hydrogen atoms and of ^{18}O over ^{16}O atoms
145 in the water, and SMOW is the Standard Mean Ocean Water reference. To first order,
146 δD variations are 8 times those in $\delta^{18}O$ (Craig, 1961), so we will focus on δD here. How-
147 ever, slight deviations in the $\delta D - \delta^{18}O$ relationship can be quantified by the second-
148 order parameter d-excess: $d = \delta D - 8 \cdot \delta^{18}O$. It reflects kinetic effects, i.e. associated
149 with diffusivity differences between the different water isotopologues. We will also show
150 some results for d-excess as it can reflect kinetic effects in rain evaporation or surface
151 evaporation.

152 2.2 Cloud Resolving Model

153 We use the same Cloud Resolving Model (CRM) as in (Risi et al., 2020), namely
154 the System for Atmospheric Modeling (SAM) non-hydrostatic model (M. F. Khairout-
155 dinov & Randall, 2003), version 6.10.9, which is enabled with water isotopes (Blossey
156 et al., 2010). This model solves anelastic conservation equations for momentum, mass,
157 energy and water, which is present in the model under six phases: water vapor, cloud
158 liquid, cloud ice, precipitating liquid, precipitating snow, and precipitating graupel. We
159 use the bulk, mixed-phase microphysical parameterization from Thompson et al. (2008)
160 in which water isotopes were implemented (Moore et al., 2016).

161 At the ocean surface, there is no representation of sea spray. Therefore, we do not
162 expect to simulate the possible impact of sea spray on the isotopic composition in the
163 eye (Fudeyasu et al., 2008).

164 2.3 Radiative-convective equilibrium with large-scale forcing

165 Simulations are three-dimensional, with a doubly-periodic domain. They are run
166 in radiative-convective equilibrium over an ocean surface. The sea surface temperature
167 (SST) is 30°C. There is no diurnal cycle.

168 Organized convection is typically observed in regions of large-scale ascent (Tan et
 169 al., 2013; Jakob et al., 2019). Therefore, we impose a large-scale vertical ascent with a
 170 cubic shape, reaching -60 hPa/d at 500 hPa and 0 hPa/d at the surface and above 100 hPa
 171 (Risi et al., 2020).

172 Simulations were also run without vertical ascent, and gave similar results except
 173 that the convective systems were smaller and with a less defined internal structure. For
 174 example, the tropical cyclone without ascent does not show any eye at the center. We
 175 thus focus on the simulations with large-scale ascent in the following.

176 The simulations are run during 50 days. The last 10 days of simulation are ana-
 177 lyzed with one three-dimensional output file every day.

178 **2.4 Set-up for the cyclone simulation**

179 We use a domain of 1024 km \times 1024 km with a horizontal resolution of 4 km and
 180 96 vertical levels. This horizontal resolution is sufficient to properly simulate the inter-
 181 nal structure of a cyclone (Gentry & Lackmann, 2010). Cyclones spontaneously develop
 182 in radiative-convective equilibrium simulations when some rotation is added (M. Khairout-
 183 dinov & Emanuel, 2013; C. J. Muller & Romps, 2018). Here the effect of rotation is added
 184 through a Coriolis parameter that corresponds to a latitude of 40°. Although no trop-
 185 ical cyclones are expected to form at such latitudes, a strong rotation allows us to sim-
 186 ulate a small cyclone (Chavas & Emanuel, 2014) that can fit our small domain. This al-
 187 lows the simulation to remain computationally reasonable.

188 The initial conditions are spatially homogeneous and one unique cyclone develops
 189 spontaneously through self-aggregation mechanisms after a few days. This is consistent
 190 with the time scale for cyclogenesis in other self-aggregation studies (C. J. Muller & Romps,
 191 2018).

192 **2.5 Set-up for the squall line simulation**

193 We use a domain of 256 km \times 256 km with a horizontal resolution is 2 km and 96
 194 vertical levels. Squall lines spontaneously develop in radiative-convective equilibrium sim-
 195 ulations when horizontal wind shear is added (Robe & Emanuel, 2001; C. Muller, 2013).
 196 We add a horizontally uniform wind in the x direction that reaches 10 m/s at the sur-
 197 face and linearly decrease to 0 m/s at 1 km. According to (Rotunno et al., 1988), this
 198 critical shear with our settings leads to the formation of a strong and long-lived squall
 199 line, perpendicular to the background wind. The uniform surface wind is subtracted when
 200 calculating surface fluxes, to avoid this simulation to have significantly higher surface
 201 fluxes. The radiative fluxes are imposed, because interactive radiation leads to some ra-
 202 diative feedbacks that disfavors the organization into squall lines.

203 The convection quickly organizes into a line, after about one day of simulation.

204 **3 Simulated patterns and qualitative comparison with observations**

205 **3.1 Tropical cyclone**

206 **3.1.1 Meso-scale structure**

207 To visualize the meso-scale structure of the tropical cyclone, in Figure 1 we plot
 208 maps of precipitation rate, near-surface air temperature, surface pressure anomaly, near-
 209 surface relative humidity, near-surface water vapor δD and surface rain δD for an ar-
 210 bitrary snapshot. The simulated cyclone exhibits features that are typical of observed
 211 cyclones (Houze, 2010). It exhibits a small eye with weak precipitation (Figure 1a) and
 212 warm air (Figure 1b), consistent with the subsidence in the eye. It is surrounded by an

213 eyewall and spiraling rain bands with very intense precipitation and strong cyclonic winds.
 214 Around the cyclone, strong compensating subsidence develops, leading to a very dry en-
 215 vironment and some scattered, isolated cumulus and cumulonimbus clouds and their cold
 216 pools (Figure 1a-b,d).

217 To better document the different parts of the tropical cyclone, we plot composites
 218 of meteorological and isotopic variables as a function of the distance r to the storm cen-
 219 ter (Figure 2 and 3). All 10 snapshots were used to compute the composites. The storm
 220 center is defined as the minimum surface pressure over the domain for each snapshot.
 221 The typical structure of a tropical cyclone is well captured.

- 222 • The eye is associated with minimum pressure (around 50hPa lower than in the en-
 223 vironment, typical of category 4 cyclones), a local minimum in precipitation, max-
 224 imum near-surface air temperature and relative humidity and weak winds (Figure
 225 2a-c). The eye is however too small to see the expected subsidence in Fig 2.
- 226 • The eyewall is associated with maximum precipitation and horizontal winds. The
 227 air is strongly ascending, almost saturated throughout the full troposphere (Fig-
 228 ure 3a), and condensation is very intense except in the shallow sub-cloud layer (Fig-
 229 ure 3c).
- 230 • Beyond the eyewall, rain bands are associated with significant but weaker precip-
 231 itation and winds. There is strong condensation, but the air is in average drier (Fig-
 232 ure 3a), allowing thick layers of snow sublimation and rain evaporation (Figure
 233 3c).

234 **3.1.2 Definition of sub-domains**

235 Based on the previous description of meso-scale structure, we divide all grid points
 236 into 5 sub-domains. These sub-domains are defined automatically based on some arbi-
 237 trary thresholds, to which results are not crucially sensitive. We define:

- 238 • the “eye” as grid points for which $r \leq r_{wall}$, where r_{wall} is the first r value for
 239 which the precipitation exceeds 20 times the domain-average precipitation (yel-
 240 low rectangles in Figure 2).
- 241 • the “eyewall” as grid points for which $r_{wall} < r \leq r_{band}$, where r_{band} is the first
 242 r value for which $r > r_{wall}$ and the precipitation is lower than 20 times the domain-
 243 average precipitation (blue rectangles in Figure 2).
- 244 • the “environment” as grid points for which $r > r_{env}$, where r_{env} is the first r value
 245 for which $r > r_{band}$ and the precipitation is lower than 0.8 times the domain-average
 246 precipitation (left in white in Figure 2).

247 In between the eyewall and the environment (pink rectangles in Figure 2), rain bands
 248 are not radially symmetric. Therefore, we define “rain bands” as grid points for which
 249 $r_{band} < r \leq r_{env}$ and precipitation exceeds 4 times the domain-average precipitation,
 250 and “in between rain bands” as the other points.

251 **3.1.3 Simulated isotopic evolution**

252 The water vapor is most enriched in the eye and in the dry environment (Figure
 253 1e-f, Figure 2e), and most depleted in the eyewall and spiraling rain bands. The water
 254 vapor d-excess is lower in the eye, and higher in the eyewall and rain bands (2e-f). Ar-
 255 eas in-between rain bands are associated with weaker depletion and higher d-excess (Fig-
 256 ure 2d-e, dashed black) than in rain bands.

257 The precipitation δD (δD_p) varies in concert with the water vapor δD (δD_v) where
 258 the precipitation is highest (Figure 2e, dashed black). The precipitation is slightly more

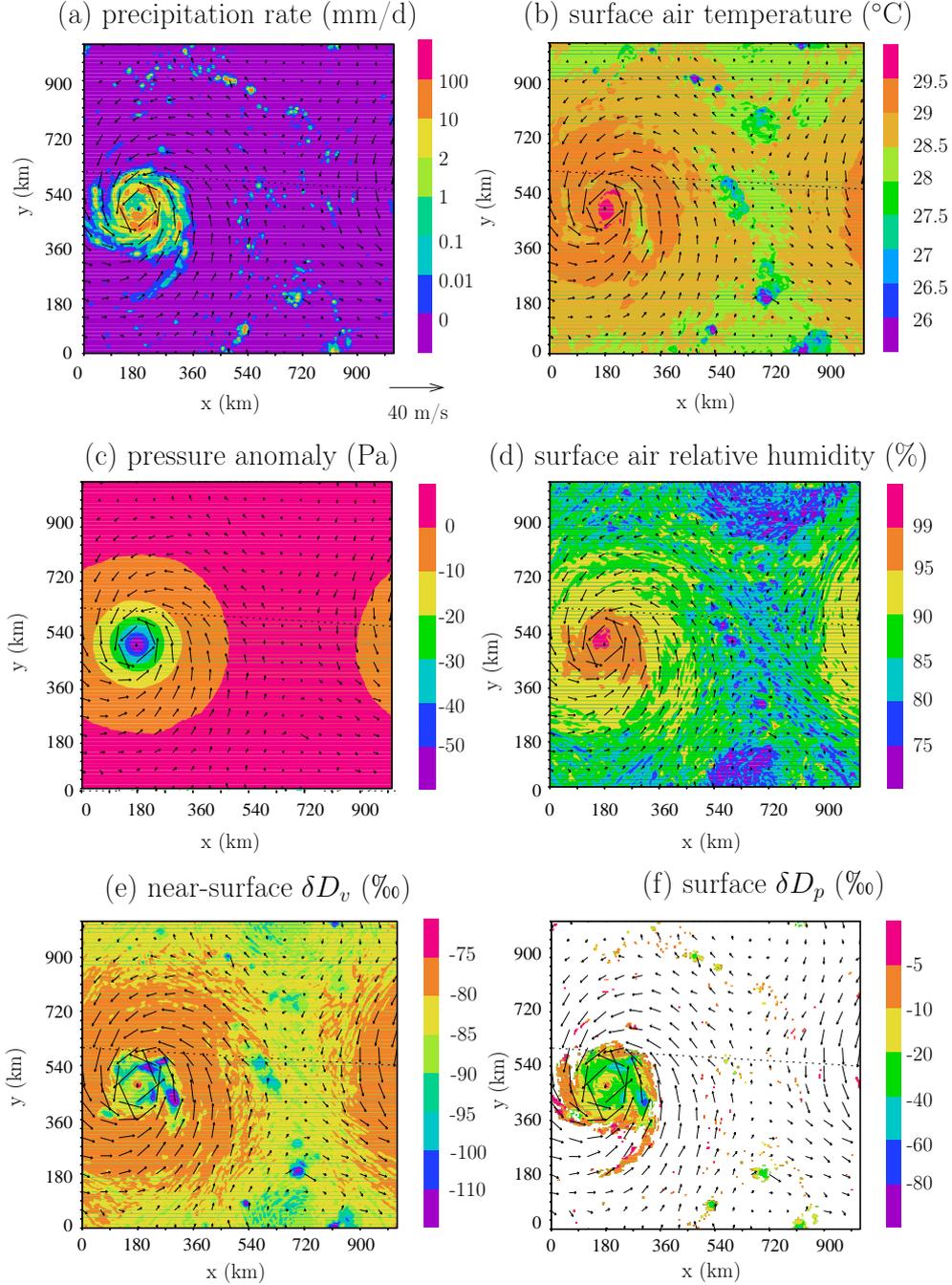


Figure 1. Maps for a snapshot of the cyclone simulation: (a) precipitation rate, (b) near-surface air temperature, (c) surface pressure anomaly with respect to the domain-mean, (d) near-surface relative humidity, (e) near-surface δD_v and (f) δD_p . The near surface winds are shown as arrows. Note that due to the doubly-periodic domain, the missing part of the cyclone on the left edge of the domain appears on the right edge of the domain. The snapshot was chosen as the one where the cyclone is the closest to the center of the domain, for easier visualization.

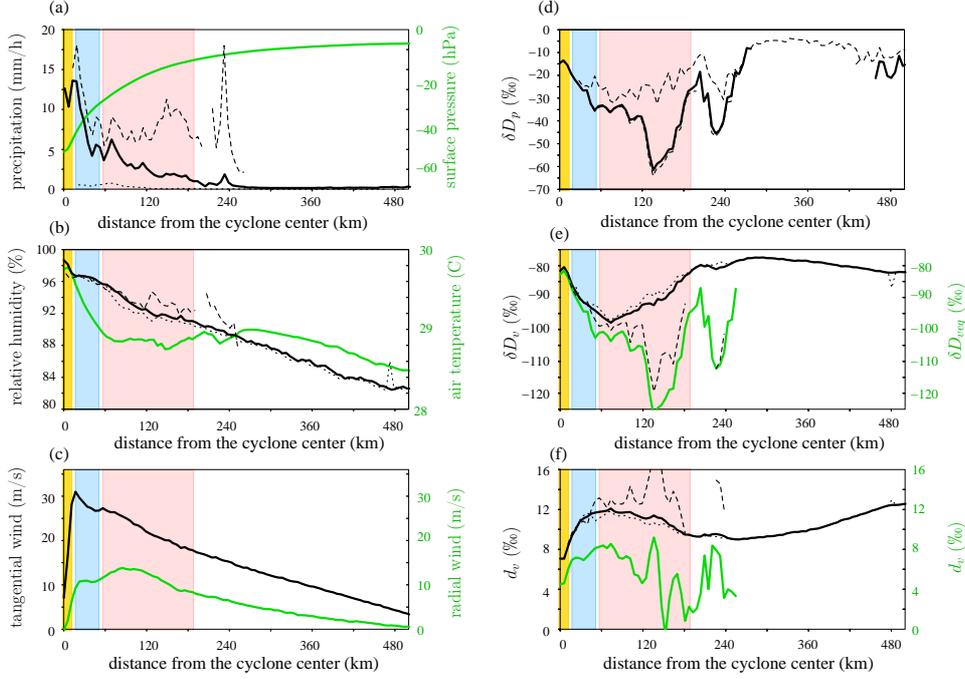


Figure 2. Evolution of surface variables as a function of distance to the storm center: Precipitation rate (a, black), surface pressure (a, green), near-surface air temperature (b, black), near-surface relative humidity (b, green), tangential (c, black) and radial (c, green) wind, surface precipitation δD (d), near-surface water vapor δD (e, black), water vapor δD that would be in equilibrium with the precipitation (e, green), near-surface water vapor d-excess (f, black) and precipitation d-excess (f, green). In d and e, dashed and dotted black lines indicate the same as black lines but for grid points where the precipitation rate is respectively higher and lower than 4 times the domain-mean precipitation, representing respectively the rain bands and in-between rain bands. The yellow, blue and pink rectangles indicate the eye, eyewall and rain band sub-domains respectively.

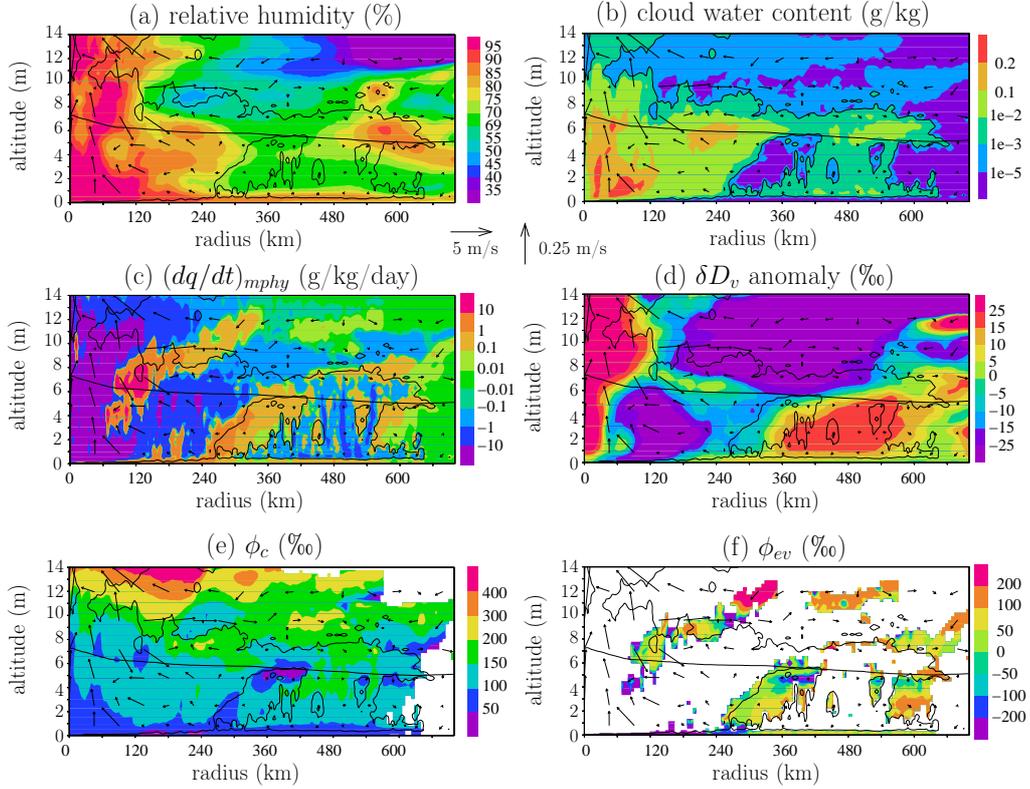


Figure 3. Variables as a function of altitude and of the distance r to the storm center: (a) Relative humidity; (b) cloud water content (cloud condensate and cloud ice); (c) specific humidity tendency due to phase changes (negative and positive values represent condensation and evaporation); (d) water vapor δD_v anomaly with respect to the domain-mean δD_v at each level; (e) relative enrichment $\phi_c = R_c/R_v$ of the isotopic ratio of the hydrometeors (cloud condensate, cloud ice, rain, graupel and snow) R_c relative to that in the vapor R_v ; (f) relative enrichment of the isotopic ratio of the hydrometeor evaporation relative to the water vapor isotopic ratio $\phi_{ev} = R_{ev}/R_v$. The vectors show the radial and vertical components of the wind. The nearly-horizontal black line shows the 0°C isotherm. The black contours highlights the 10^{-3} g/kg contour for cloud water content.

259 depleted than if in equilibrium with the vapor. This suggests that the rain forms in al-
 260 titude and undergoes little evaporative enrichment as it falls, consistent with the high
 261 relative humidity. In addition, it quickly falls to the ground without having the time to
 262 fully equilibrate isotopically with the vapor.

263 **3.1.4 Qualitative comparison with isotopic observations**

264 Observed isotopic patterns in tropical cyclones can be very diverse (Guilpart, 2018).
 265 However, some robust features emerge. The few studies that sampled water vapor or pre-
 266 cipitation in the eye found that it was relatively enriched (Gedzelman et al., 2003; Fudeyasu
 267 et al., 2008). Outside the eye, many studies have observed that the water vapor and pre-
 268 cipitation is more depleted towards the storm center (Gedzelman et al., 2003; Fudeyasu
 269 et al., 2008; Munksgaard et al., 2015; Jackisch et al., 2020; Skrzypek et al., 2019; Xu et
 270 al., 2019; Sanchez-Murillo et al., 2019). At a given distance from the storm center, the
 271 water vapor or precipitation is often more depleted in rain bands than in between (Munksgaard
 272 et al., 2015; Guilpart, 2018).

273 The observed d-excess in water vapor or precipitation is weaker in the eye (Fudeyasu
 274 et al., 2008), higher in the environment and higher in the rain bands than in-between
 275 (Munksgaard et al., 2015).

276 All these features are consistent with our simulation.

277 **3.2 Squall line**

278 **3.2.1 Meso-scale structure**

279 Figure 1 shows maps of precipitation rate, near-surface air temperature, surface
 280 pressure anomaly, near-surface relative humidity, near-surface water vapor δD and sur-
 281 face rain δD for an arbitrary snapshot. In presence of wind shear, the convection orga-
 282 nizes into lines of intense precipitation perpendicular to the imposed surface winds (Fig-
 283 ure 4a). The environment is very dry, with only a few isolated cumulonimbi. Under the
 284 squall line, a cold pool is driven by meso-scale downdrafts (Zipser, 1977; Gamache & Houze,
 285 1981). The cold pool has a very sharp edge at the front of the line, corresponding to the
 286 gust front, and a long trail due to the imposed rearward horizontal winds near the sur-
 287 face (Figure 4b).

288 To better document the different parts of the squall line, we plot composites of me-
 289 teorological and isotopic variables as a function of the along-x distance to the gust front
 290 (Figures 5 and 6). At each snapshot, for each row of the domain where the precipita-
 291 tion rate exceeds the domain-mean value, we select the x for which the along-x pressure
 292 gradient is maximum. If the pressure gradient exceeds 1.7 Pa/km, we assume that it is
 293 a gust front. This threshold was visually defined to optimally detect gust fronts. We de-
 294 fine a new x-axis and translate all rows so that all gust fronts of the different rows are
 295 aligned at $x_{gust}=30$ km. We arbitrary set $x_{gust}=30$ km so that the squall lines stand in
 296 the middle of the composite plots. Rows of the domain where the precipitation is lower
 297 than the domain mean, or where a gust front could not be identified, are considered “en-
 298 vironment” and are not taken into account in the composite.

299 The precipitation rate is maximum just after the gust front (Figure 5a), consistent
 300 with observations (Chong, 2009). The maximum precipitation locates where the along-
 301 x near-surface surface wind becomes null (Figure 5c), favoring the maintenance of strong
 302 updrafts (Rotunno et al., 1988). Elsewhere, the surface wind blows rearward. Near the
 303 gust front, the temperature drops and the relative humidity rises (Figure 5c). The re-
 304 covery to their environment value is slow due to the rearward advection.

Our simulated squall line shows only one precipitation peak. This is at odds with observations that often show two peaks, one for the convective region and one for the stratiform region, separated by a transition region (Biggerstaff & Houze Jr, 1991; Chong, 2009). In our simulation, the convective region transitions continuously to the stratiform region. Increasing the horizontal resolution to 1 km did not help to simulate a transition region.

In spite of this shortcoming, the convective and stratiform regions of the squall line can be identified from water vapor tendencies (Figure 6b). The convective region can be identified by its intense condensation throughout the full troposphere (Figure 6b, around 50-60 km). The stratiform region can be identified by the condensation restricted to the upper troposphere (the anvil) and evaporation below (meso-scale downdraft) (Figure 6b, around 60-80 km). This pattern of condensation and evaporation is consistent with what we know from the squall line water budgets (Gamache & Houze, 1983; Chong & Hauser, 1990).

3.2.2 Definition of the sub-domains

Based on the above description of the meso-scale structure, we divide the grid points into 4 sub-domains.

Given the continuous transition in our simulations, we define the convective and stratiform sub-domains based on a precipitation threshold. For rows where x_{gust} is defined, we define:

- the convective region for x between x_{gust} and x_{conv} , where x_{conv} is the first x values for which the precipitation comes back below 8 times the domain-average precipitation (yellow rectangle in Figure 5).
- the stratiform region for x between x_{conv} and x_{strati} , where x_{strati} is the first x values for which $x > x_{conv}$ and the precipitation is below the domain-average precipitation (blue rectangle in Figure 5).

The horizontal winds near the surface spread the cold pool rearward beyond the precipitating region. Therefore, we also define a sub-domain called “trailing”, for x between x_{strati} and x_{trail} , where x_{trail} is the x value for which $x > x_{strati}$ and $T(x) < T(x_{gust}) - 1$, where T is the near-surface temperature in K (pink rectangle in Figure 5). All grid points that are not categorized as “convective”, “stratiform” or “trailing” are called “environment” (left in white in Figure 5).

3.2.3 Simulated isotopic evolution

Simulated squall lines show a progressive depletion of the vapor in the convective region, maximum depletion at the end of the convective region, and a long recovery in the stratiform and trailing regions (Figure 5e). The δD_v reaches its environment value about 100 km after the convective peak.

The δD_p varies in concert with δD_v (Figure 5d). In the convective and stratiform regions, δD_p is more depleted than in equilibrium with the vapor (Figure 5e, red), consistent with a quick fall with little time to equilibrate and little evaporative enrichment. The weak precipitation that falls upwind of the convective region, where the air is dry, has a δD_p higher than that in equilibrium with vapor, indicating evaporative enrichment during rain evaporation.

D-excess is higher in the vapor in the convective, stratiform and trailing regions (Figure 5f). The low d-excess in the precipitation reflect the effect of evaporative enrichment, especially before the gust front and in the trailing region.

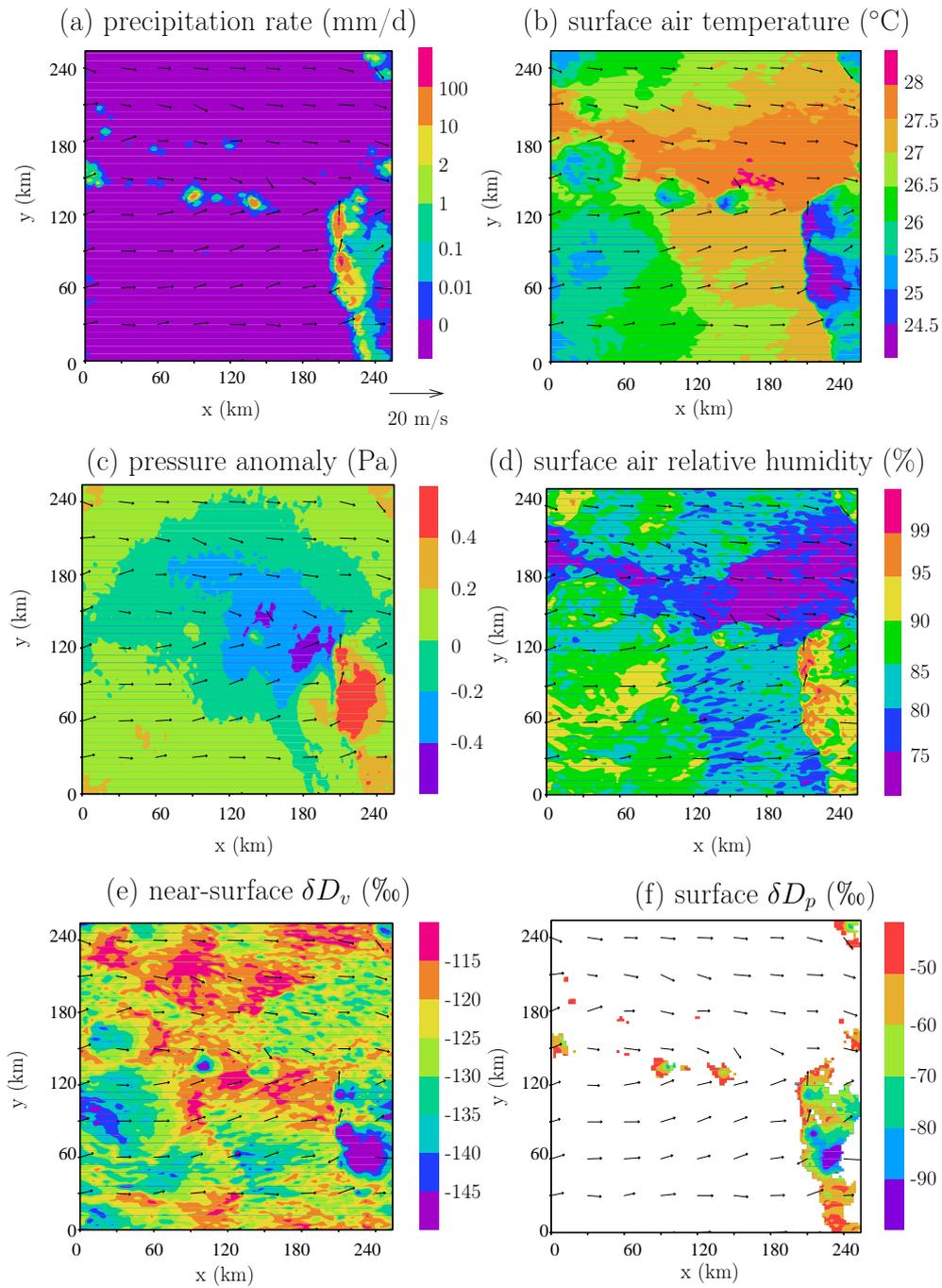


Figure 4. Same as Figure 1 but for the squall line. Note that due to the doubly periodic domain, the trailing region on the right edge of the domain continues on the left edge.

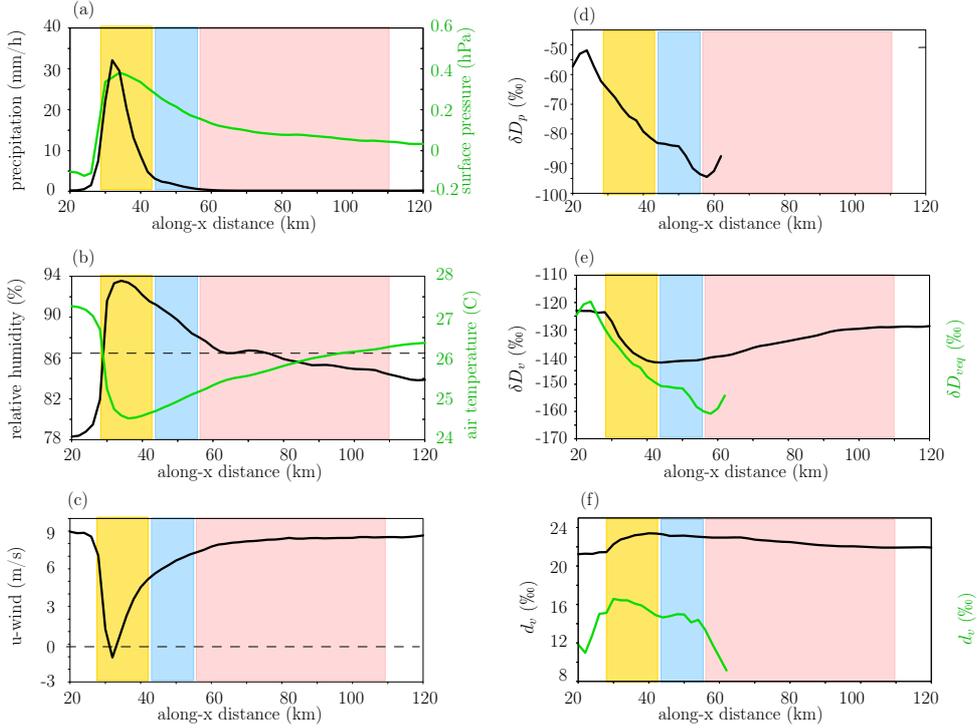


Figure 5. Evolution of surface variables as a function of distance along the x-axis, as a composite of all rows of all snapshots where a gust front could be defined (see text): Precipitation rate (a, black), surface pressure (a, green), near-surface air temperature (b, green), near-surface relative humidity (b, black), u-wind (c, black), surface precipitation δD (d), near-surface water vapor δD (e, black), water vapor δD that would be in equilibrium with the precipitation (e, green), near-surface water vapor d-excess (f, black) and precipitation d-excess (f, green).

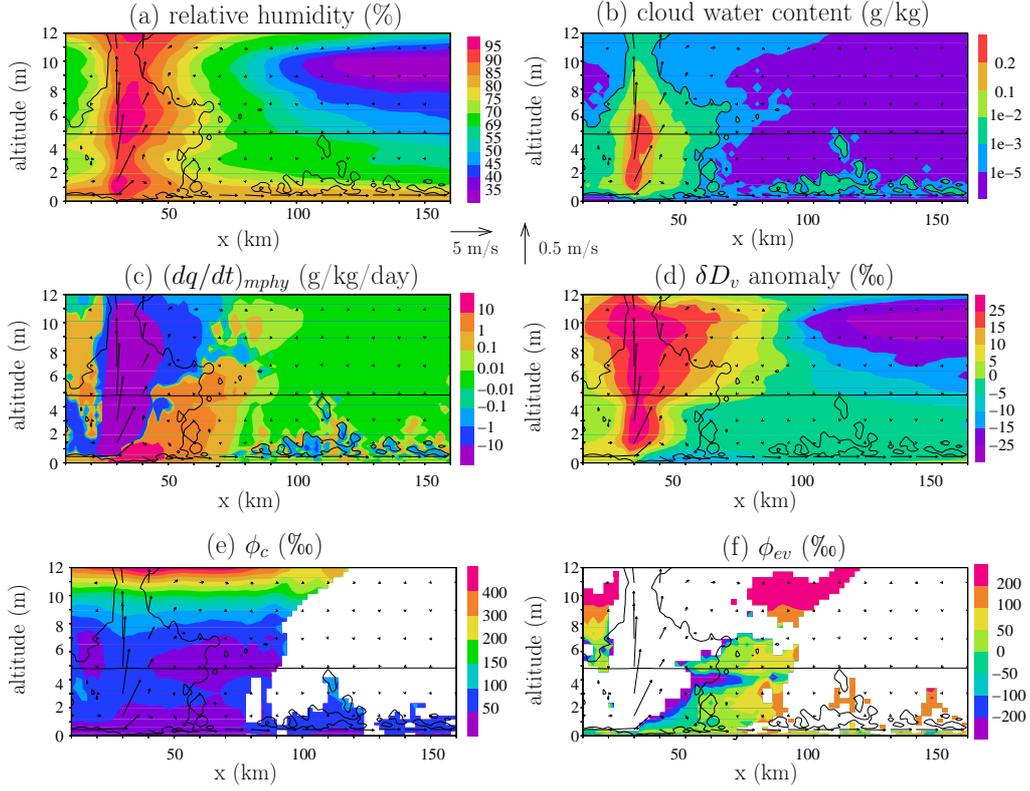


Figure 6. Relative humidity (a), specific humidity tendency due to phase changes (b; negative and positive values represent condensation and evaporation), water vapor δD anomaly (c) and the relative enrichment of the isotopic ratio of the hydrometeor evaporation relative to the water vapor isotopic ratio $\phi_{ev} = R_{ev}/R_v$ (d) as a function of altitude and of the distance along the x-axis. The vectors show the wind, with the vertical wind multiplied by 20 for better readability. The thick dashed horizontal black lines indicate the melting level.

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3.2.4 Qualitative comparison with isotopic observations

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Isotopic observations during squall lines often show a “W” shape with minimum δD_p in the convective and stratiform regions and a local maximum in the transition region (Taupin & Gallaire, 1998; Risi et al., 2010). Our simulation is consistent with this observation, except that since our simulation does not exhibit any transition region, it shows a “V” shape instead of a “W” shape.

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In the vapor, inspection of a large number of squall lines in the Sahel showed that the isotopic evolution can be very diverse, but some robust features emerge (Tremoy et al., 2014).

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- In 80% of 74 observed squall lines in (Tremoy et al., 2014), there is a depletion in the convective region compared to the environment before the squall line. This is consistent with our simulation.
- More than half of the observed squall lines show additional depletion in the stratiform region (Tremoy et al., 2014). This is also consistent with our simulation.
- For squall lines showing an isotopic depletion in the convective or stratiform region, the recovery from this depletion takes several hours after the end of the rain (Tremoy et al., 2014). Considering a propagation speed of about 20 m/s, this is consistent with the recovery distance of about 100 km in our simulation.
- In 78% of observed squall lines, the “W” shape often observed in the precipitation is not observed in the vapor (Tremoy et al., 2014). Our simulations are thus consistent with this majority of squall lines

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Our simulated isotopic evolution during the squall line thus captures the features that are most commonly observed in squall lines.

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Some squall lines may feature very different variations, and even enrichment in the convective and stratiform regions (Tremoy et al., 2014). To check whether we could capture such a diversity of isotopic variations, we performed many sensitivity tests, including simulations without large-scale ascent, with large-scale ascent peaking in the upper troposphere to favor stratiform development (Su et al., 2000), increased horizontal resolution, interactive radiation, reduced sublimation or reduced rain evaporation to favor the maintenance of the stratiform region (Yang & Houze Jr, 1995; Bryan & Morrison, 2012), bowling alley domain, or prescribed horizontal wind in the upper troposphere to favor the development of the stratiform region (Caniaux et al., 1994). Depending on the simulations, the stratiform region is more or less extended and the squall lines are more or less organized, but the meteorological and isotopic evolution is always very similar. We thus keep in mind that our simulations are relevant for the majority of squall lines, but not all of them. In addition, some features in some of the squall line observed over land might not be captured by our simulations with an oceanic setting.

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4 Understanding mesoscale isotopic variations

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4.1 Importance of rain evaporation

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Observational and modeling studies highlighted the key role of rain evaporation and rain-vapor exchanges in depleting the water vapor within organized systems (Lawrence et al., 2004; Tremoy et al., 2014; Xu et al., 2019). In both the cyclone and the squall line, very dry air in the environment favor thick layers of rain evaporation in the free troposphere (Figure 3a,c, 6a,c).

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In the simulated cyclone, they correspond to the two thick orange diagonals in Figure 3b. We notice that the δD pattern also shows a diagonal pattern of negative anomalies, descending inward and downward (Figure 3d), creating the depletion simulated near the surface in the eyewall and rain bands. For δD , the diagonal pattern is however much

399 smoother. This suggests that rain evaporation favors the isotopic depletion of water va-
 400 por, which accumulates as air moves inward.

401 Similarly, in the squall line, strong evaporation occurs in the stratiform region, be-
 402 tween 60 and 80 km (Figure 6b). Maximum evaporation occurs in the cold pool under
 403 the convective and stratiform region and coincides with the maximum depletion (Fig-
 404 ure 6c).

405 To analyze the isotopic effect of rain evaporation in more detail, we calculate $\phi_{ev} =$
 406 R_{ev}/R_v , where R_v and R_{ev} are the isotopic ratio in water vapor and in hydrometeor evap-
 407 oration. ϕ_{ev} represents the enrichment of rain evaporation relative to water vapor: if $(\phi_{ev} -$
 408 $1) \cdot 1000 > 0\text{‰}$, rain evaporation enriches the water vapor; if $(\phi_{ev} - 1) \cdot 1000 < 0\text{‰}$,
 409 rain evaporation depletes the water vapor. R_{ev} is calculated as $(dq_{HDO}/dt)_{mphy}/(dq/dt)_{mphy}$,
 410 where q_{HDO} is the mixing ratio for HDO , q is the water vapor mixing ratio, and $(dq/dt)_{mphy}$
 411 and $(dq_{HDO}/dt)_{mphy}$ are the water vapor and HDO tendencies associated with phase
 412 changes. The $(dq/dt)_{mphy}$ tendency is positive if dominated by rain or cloud water evap-
 413 oration or sublimation of ice, snow or graupel, and negative if dominated by cloud con-
 414 densation or deposition onto snow, cloud ice or graupel. R_{ev} is calculated only where $(dq/dt)_{mphy} >$
 415 0 .

416 We can see that near the rain bands of the cyclone and in the stratiform region of
 417 the squall line, there is a strongly depleting effect of rain evaporation just below the melt-
 418 ing level (Figure 3f,6f). This is because just below the melting level, most of the rain orig-
 419 inates from snow melt, which is very depleted (Figure 3e,6e) because it has formed high
 420 in altitude (Risi et al., 2021). The depleting effect of rain evaporation and diffusive ex-
 421 changes in stratiform regions of convective systems has already been highlighted in pre-
 422 vious studies (Kurita, 2013; Aggarwal et al., 2016), including in cyclones (Munksgaard
 423 et al., 2015).

424 There is also a depleting effect directly in the sub-cloud layer of the cyclone, prob-
 425 ably because intense rain falls so fast and the air is so moist that diffusive exchange be-
 426 tween the depleted rain and the vapor dominate and deplete the water vapor (Lawrence
 427 et al., 2004).

428 Elsewhere, rain evaporation has an enriching effect, especially where the air is dry
 429 and the rain rate is small (Tremoy et al., 2014). In the limit case where rain drops evap-
 430 orate totally, $\phi_{ev} = R_p/R_v$ which is close to the fractionation coefficient α_{eq} . This is
 431 reflected by the orange shades at the periphery of the cyclone and in the trailing region
 432 of the squall line.

433 4.2 Simulations with de-activated fractionation during rain evaporation

434 One way to quantify the effect of rain evaporation and rain-vapor diffusive exchanges
 435 is to run additional simulations in which they are de-activated (Field et al., 2010; Risi
 436 et al., 2021). The simulations are the same for meteorological variables, but the rain-vapor
 437 diffusive exchanges are suppressed and the rain evaporation is assumed not to fraction-
 438 ate.

439 Without fractionation during rain evaporation, the mesoscale δD_v variations are
 440 strongly reduced (Figure 7). In cyclones, in absence of fractionation during rain-vapor
 441 interactions, the δD_v would be almost flat, and the maximum depletion would be in the
 442 environment (Figure 7a), contrary to observations and to the full simulations. In squall
 443 lines, the difference between the δD_v in the stratiform region and in the environment is
 444 reduced by 80%, and the δD_v recovers much more quickly after the squall line (Figure
 445 7b).

446 This confirms the key role of rain evaporation and rain-vapor diffusive exchanges
 447 to deplete the low-level water vapor at the mesoscale scale.

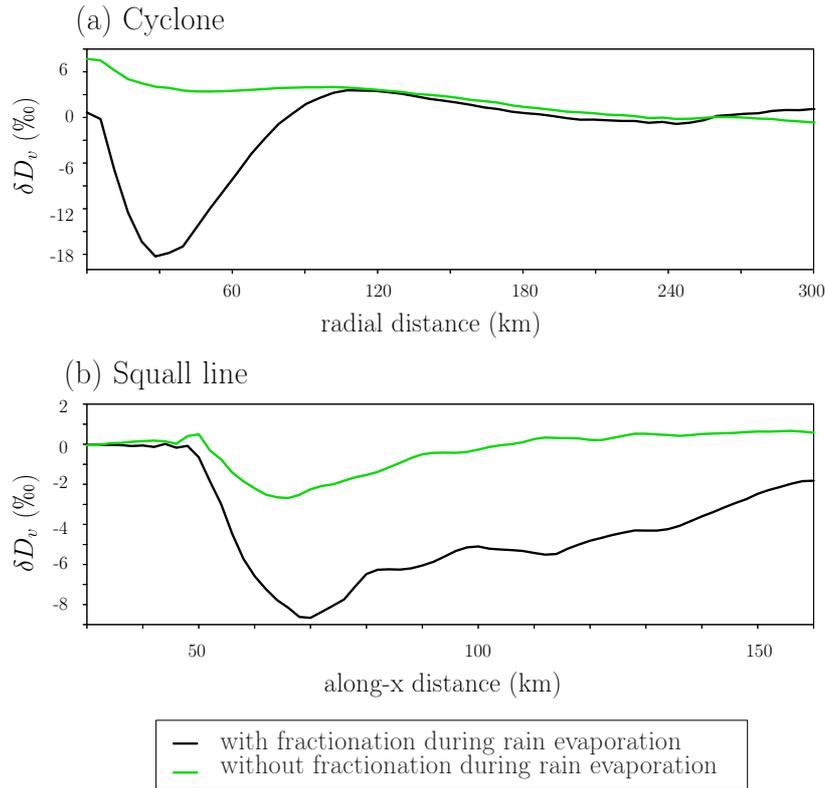


Figure 7. Evolution of near-surface δD_v as a function of r for tropical cyclones (a) and as a function of x for squall lines (b), in simulations in which rain evaporation and rain-vapor diffusive exchanges are activated (black) and de-activated (green).

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4.3 Decomposition method

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To quantify the relative importance of processes in determining the isotopic composition in the different parts of the domain, we design a simple box model for the sub-cloud layer (SCL) inspired from (Risi et al., 2020) (Figure 8a). The main difference is that here we account for horizontal advection and non-stationary effects, because the simple model will be applied in the different sub-domains of the simulation domains. Whereas the SCL is in quasi-equilibrium in the domain-mean, it is not in quasi-equilibrium in sub-domains. For example, the eye of the cyclone wanders across the domain and is thus never in quasi-equilibrium.

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The SCL is defined as the first atmospheric levels where the domain-mean cloud fraction remains below 10% of its maximum value. The water budget of the SCL in a given sub-domain writes (Figure 8a):

$$\frac{dW}{dt} = E_{sfc} + F_d(q_d - q) - F_u(q_u - q) + E_{horiz} + E_{ev} - E_c$$

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where W is the water mass in the SCL per area unit (in kg/m²), E_{sfc} is surface evaporation, F_d and F_u are the downward and upward mass fluxes at SCL top, E_{horiz} is the flux of water through horizontal advection, E_{ev} is the rain evaporation, E_c is some condensation that may occur if the SCL top is not horizontally uniform, q_u and q_d are the specific humidity in updrafts and downdrafts and q is the specific humidity near the surface. All these variables can directly be diagnosed from the simulations for each sub-domains.

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Similarly, the isotopic budget writes:

$$\frac{d(R \cdot W)}{dt} = R_{sfc} \cdot E_{sfc} + F_d(R_d \cdot q_d - R \cdot q) - F_u(q_u - R \cdot q) + R_{horiz} \cdot E_{horiz} + R_{ev} \cdot E_{ev} - R_c \cdot E_c$$

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where R is the isotopic ratio of the near-surface vapor, R_u and R_d are the isotopic ratios in updrafts and downdrafts, R_{sfc} , R_{horiz} , R_{ev} and R_c are the isotopic compositions of the surface evaporation, horizontal advection, rain evaporation and condensation fluxes.

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We define:

$$E_{res} = E_{horiz} - \frac{dW}{dt}$$

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It is the flux of water through both horizontal advection and non-stationary effects, and is calculated as a residual. For example, in the cyclone's eyewall where the air is very moist, we expect that horizontal advection will have a drying effect, i.e. $E_{horiz} < 0$. In addition, since the cyclone wanders across the domain, the eyewall often arrives in dry parts of the domain, i.e. $\frac{dW}{dt} > 0$. Therefore, both horizontal advection and non-stationary effects contribute to drying the eyewall, i.e. $E_{res} < 0$.

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Similarly, we define the isotopic ratio of the flux R_{res} :

$$R_{res} = \frac{R_{horiz} \cdot E_{horiz} - \frac{d(R \cdot W)}{dt}}{E_{horiz} - \frac{dW}{dt}}$$

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To solve the isotopic budget equation for R , the isotopic ratios R_{sfc} , R_d , R_u , R_{res} , R_{ev} and R_c are all expressed as a function of R . The isotopic ratio of surface evaporation is given by (Craig & Gordon, 1965):

$$R_{sfc} = \frac{R_{oce}/\alpha_{eq}(SST)}{\alpha_K \cdot (1-h)}$$

483 where R_{oce} is the isotopic ratio at the ocean surface, $\alpha_{eq}(SST)$ is the equilibrium
 484 fractionation coefficient at the sea surface temperature, α_K is kinetic fractionation co-
 485 efficient (Merlivat & Jouzel, 1979) and h is the relative humidity normalized at the SST
 486 and accounting for ocean salinity: $h = q/q_{sat}^{surf}(SST)$, $q_{sat}^{surf}(SST) = 0.98 \cdot q_{sat}(SST)$
 487 and q_{sat} is the humidity saturation as a function of temperature at the sea level pres-
 488 sure. We assume $\delta D_{oce} = 0\text{‰}$ and h is diagnosed from the CRM. The kinetic fraction-
 489 ation is a function of surface wind speed and is also diagnosed from the CRM.

490 The isotopic ratios in updrafts and downdrafts are assumed to follow logarithmic
 491 functions: $R_u = R \cdot \left(\frac{q_u}{q}\right)^{\alpha_u - 1}$ and $R_d = R \cdot \left(\frac{q_d}{q}\right)^{\alpha_d - 1}$ where R_u and R_d are isotopic
 492 ratios in updrafts and downdrafts, and α_u and α_d are the $q-\delta D_v$ steepness coefficients
 493 for updrafts and downdrafts (Risi et al., 2020). We set $R_{res} = \phi_{res} \cdot R$, $R_{ev} = \phi_{ev} \cdot R$
 494 and $R_c = \phi_c \cdot R$. All parameters α_u , α_d , ϕ_{res} , ϕ_{ev} and ϕ_c can be diagnosed from the
 495 simulation for each sub-domain.

496 We get:

$$R = \frac{R_{oce}/\alpha_{eq}(SST)}{h + \alpha_K \cdot (1-h) \cdot A} \quad (1)$$

497 where

$$A = \frac{((q_u/q)^{\alpha_u} - 1) + \frac{F_d}{F_u} \cdot (1 - (q_d/q)^{\alpha_d}) - \frac{E_{ev}}{qF_u} \cdot \phi_{ev} + \frac{E_c}{qF_u} \cdot \phi_c - \frac{E_{res}}{qF_u} \cdot \phi_{res}}{(q_u/q - 1) + \frac{F_d}{F_u} \cdot (1 - q_d/q) - \frac{E_{ev}}{qF_u} + \frac{E_c}{qF_u} - \frac{E_{res}}{qF_u}} \quad (2)$$

498 Note that the diagnostic of E_{res} and ϕ_{res} as residuals guarantees that the water
 499 and isotopic budgets of the SCL are closed. However, it does not guarantee that equa-
 500 tion 1 with input parameters diagnosed from the CRM simulations yields exactly the same
 501 isotopic ratios as those directly simulated by the CRM, because of the numerous sim-
 502 plifying assumptions underlying the simple model.

503 In each sub-domain of a simulation, we calculate R from equation 1 in 8 different
 504 ways, de-activating different effects one by one (table 1). By calculating the differences
 505 between these different simulations, we can decompose R into 7 contributions. We ex-
 506 plain below how these contributions are calculated, with names of calculations defined
 507 in table 1. We also explain the physical meaning of these contributions, which is illus-
 508 trated in Figure 8b:

- 509 1. Mean_wind-Mean_h represents the effect of near-surface relative humidity (Fig-
 510 ure 8b, red). Near-surface relative humidity impacts the kinetic processes during
 511 ocean surface evaporation (Merlivat & Jouzel, 1979).
- 512 2. Merlivat-Mean_wind represents the variations in the kinetic fractionation coeffi-
 513 cient α_K , which are mainly due to variations in surface wind speed (Merlivat &
 514 Jouzel, 1979) (Figure 8b, orange).
- 515 3. No_grad-Merlivat represents the effect of the horizontal humidity contrasts (Fig-
 516 ure 8b, green). When horizontal humidity contrasts between dry and moist zones
 517 of a sub-domain are larger, dry subsident regions import drier air and more depleted
 518 water vapor in the SCL, while ascending regions export moister air and more en-
 519 riched water vapor in the SCL. This has thus a depleting effect.
- 520 4. No_ev-No_grads represents the effect of variations in the steepness of the relation-
 521 ship between q and δD_v for updrafts and downdrafts. When the $q-\delta D_v$ steep-
 522 ness is larger, downdrafts import more depleted vapor into the SCL and updrafts

523 export more enriched vapor out of the SCL (Risi et al., 2021). The $q-\delta D_v$ steep-
 524 ness depends on the enriching or depleting processes that occur above the SCL.
 525 Typically, the dominant effect is rain evaporation above the SCL, which depletes
 526 the water vapor, especially near the melting level (Risi et al., 2021) (Figure 8b,
 527 blue). Hereafter for simplicity, we will call this contribution “Rain evaporation above
 528 the SCL” because this is the main process underlying this contribution. But we
 529 keep in mind that it might encompass in reality a wider range of processes (e.g.
 530 entrainment in cloud updrafts (Risi et al., 2021)).

- 531 5. No_cond-No_ev represents the effect of rain evaporation in the SCL (Figure 8b,
 532 purple).
- 533 6. No_adv-No_cond represents the effect of condensation in the SCL (Figure 8b, cyan).
- 534 7. Full-No_adv represents horizontal advection and non-stationary effects (Figure 8b,
 535 brown).

536 By construction, the sum of these 7 contributions yields Full-Mean_h, which corresponds
 537 to the sub-domain-mean anomaly relative to the domain-mean.

538 4.4 Water budget in each sub-domain

539 4.4.1 Cyclone

540 The cyclone in itself (sub-domains 1-4) covers less than 1% of the domain (Figure
 541 9a). In all sub-domains, the main source of water vapor is surface evaporation (Figure
 542 9b red). It is more than twice larger in the eyewall, in rain bands and in-between rain
 543 bands than in the environment, consistent with the maximum winds, and less than half
 544 in the eye, due to weak winds and very moist near-surface air. Rain evaporation is also
 545 a significant moistening term in the eyewall and in the rain bands (pink). Condensation
 546 is insignificant (Figure 9b cyan). Everywhere except in the eye, updrafts and downdrafts
 547 have a drying effect (green and blue), because updrafts are preferentially moister and
 548 downdrafts are preferentially drier. In the eye, updrafts and downdrafts slightly moisten
 549 the SCL because the core of the eye is descending and almost saturated whereas air parcels
 550 near the eyewall may be drier and ascending. Horizontal advection and non-stationary
 551 effects dry the cyclone and slightly moisten the environment (brown). This is because
 552 dry air from the environment converge towards to cyclone center (horizontal advection
 553 effect). In addition, the cyclone wanders across the domain and thus mixes with air that
 554 was previously in the dry portions of the domain (non-stationary effect). In turn, in the
 555 wake of the cyclone, the environment is left moistened.

556 4.4.2 Squall line

557 The squall line and its trailing region (sub-domains 1-3) cover about 15% of the
 558 domain (Figure 10a). Surface evaporation is the main source of water in the SCL and
 559 is approximately uniform in all sub-domains (Figure 10b red). The rain evaporation is
 560 a significant source in both the convective and stratiform parts (pink). In the convec-
 561 tive part, the main sink of water is the export of moist air through updrafts (green), con-
 562 sistent with the very vigorous updrafts. Horizontal advection and non-stationary effects
 563 moisten the convective zone by advecting air from the stratiform region moistened by
 564 rain evaporation, and dries the trailing region by advecting drier air from the environ-
 565 ment (brown).

566 4.5 Decomposition of the isotopic composition in each sub-domain

567 4.5.1 Cyclone

568 Regarding δD_v , the simple model is able to capture the main isotopic differences
 569 between the different sub-domains, especially the relatively more enriched eye, the max-

Table 1. Different calculations of the isotope ratio following equations 1 and 2, allowing us to de-activate different effects one by one. For each calculation, we give the values of different input parameters (columns 2 to 10). “sub” means that we use the values diagnosed from the CRM for each sub-domain. $\bar{\alpha}_z$ is the average $q - \delta D_v$ steepness over the full domain (Risi et al., 2021). The “Merlivat” calculation is identical to the traditional (Merlivat & Jouzel, 1979) closure. The “Full” calculation corresponds to the calculation with all 7 contributions included. In contrast, the “Mean_h” calculation includes none of the 7 contributions, and yields the same results for all sub-domains. The 7 contributions to the SCL water vapor isotopic ratio are then calculated by differences between these different calculations (last column).

Name of the calculation	h	α_K	q_u	q_d	α_u	α_d	E_{ev}	E_c	ϕ_{res}	Effect that it allows to isolate
Mean_h	domain-mean h	domain-mean α_K	q	q	$\bar{\alpha}_z$	$\bar{\alpha}_z$	0	0	1	Constant reference
Mean_wind	sub	domain-mean α_K	q	q	$\bar{\alpha}_z$	$\bar{\alpha}_z$	0	0	1	Mean_wind-Mean_h = near-surface relative humidity (#1)
Merlivat	sub	sub	q	q	$\bar{\alpha}_z$	$\bar{\alpha}_z$	0	0	1	Merlivat-Mean_wind = surface wind speed (#2)
No_grad	sub	sub	sub	sub	$\bar{\alpha}_z$	$\bar{\alpha}_z$	0	0	1	No_grad-Merlivat = horizontal humidity contrasts (#3)
No_ev	sub	sub	sub	sub	sub	sub	0	0	1	No_ev-No_grads = rain evaporation above the SCL (#4)
No_cond	sub	sub	sub	sub	sub	sub	sub	0	1	No_cond-No_ev = rain evaporation in the SCL (#5)
No_adv	sub	sub	sub	sub	sub	sub	sub	sub	1	No_adv-No_cond = condensation in the SCL (#6)
Full	sub	sub	sub	sub	sub	sub	sub	sub	sub	Full-No_adv = horizontal advection and non-stationary effects (#7)

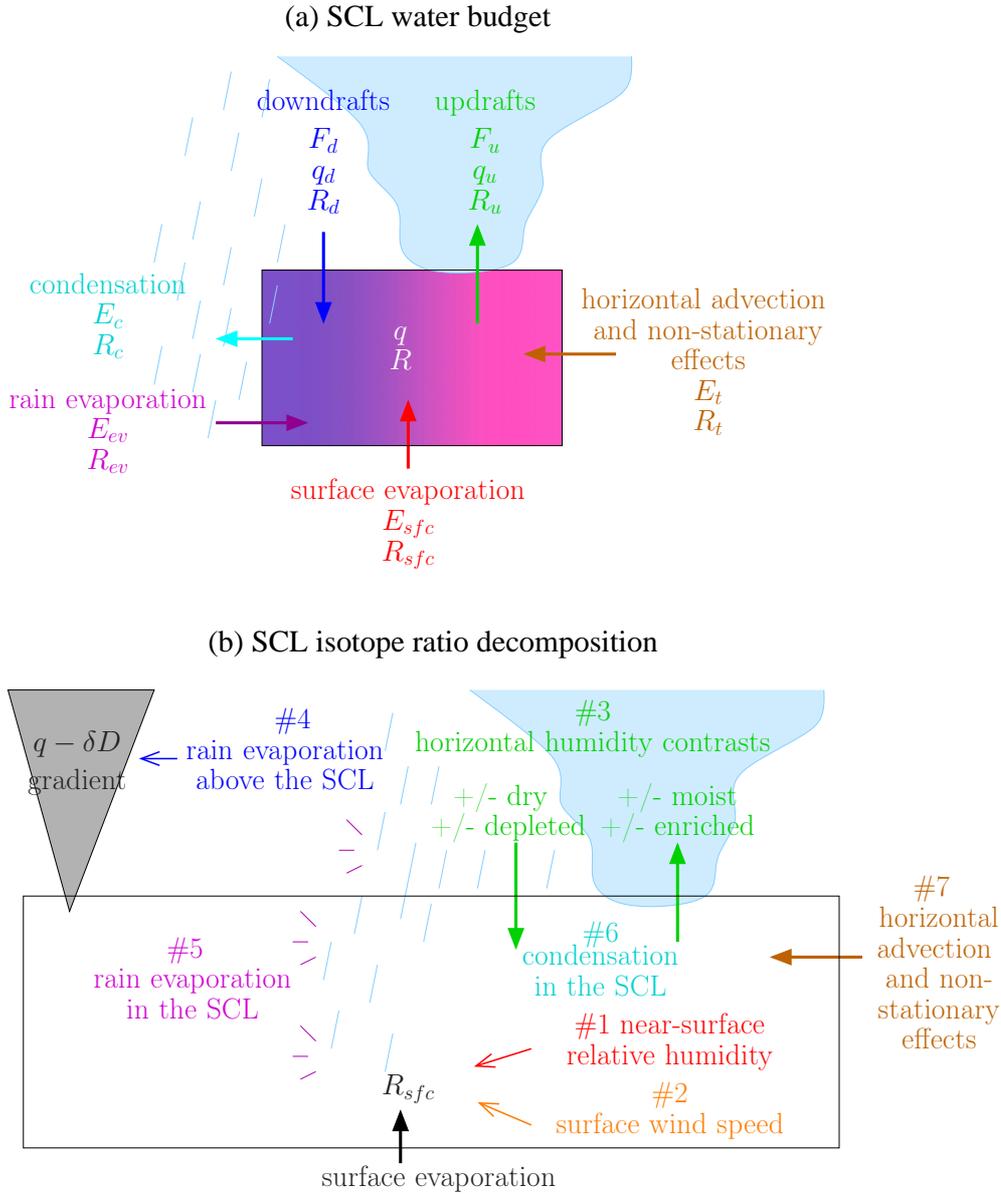


Figure 8. (a) Simple model to predict the SCL water vapor composition. It accounts for surface evaporation, rain evaporation, cloud condensation, updrafts and downdrafts at the SCL top, and horizontal advection and non-stationary effects quantified as a water budget residual. (b) Schematic illustrating the 7 contributions in the decomposition of the isotopic ratio: near-surface relative humidity (#1, red) and surface wind speed (#2, orange), which both contribute to control the isotope composition of the surface evaporation; horizontal humidity contrasts (#3, red) and rain evaporation above the SCL (#4, blue), which both contribute to the SCL depletion by vertical mixing; rain evaporation (#5, purple) and condensation (#6, cyan) within the SCL; and horizontal and non-stationary effects (#7, brown).

imum depletion in the eyewall, the relatively depleted rain bands and the relatively enriched environment (Figure 9c).

Rain evaporation and rain-vapor diffusive exchanges in the SCL (Figure 9d pink) are the main drivers of the depletion in the rain bands and in the eyewall. Alone, it would deplete the rain bands and the eyewall relative to the environment by about 7‰ and 28‰, greater than the total predicted depletion relative to the environment. This is due to the very depleted isotopic signature of rain evaporation in the SCL (Figure 3d), and this is consistent with the strong contribution of isotopic fractionation to rain evaporation (section 4.2).

The rain evaporation above the SCL (Figure 9d blue) also contributes to deplete the rain bands and in the eyewall relative to the environment, by about 9‰. This effect is consistent with the very depleted isotopic signature of rain evaporation near the melting level (Figure 3d), and also contributes to the strong contribution of isotopic fractionation to rain evaporation estimated (section 4.2).

These two effects are partially counter-balanced by the stronger humidity contrast (Figure 9d green) in the environment, reflecting drier and more depleted conditions in the mid-troposphere associated with the compensating subsidence in the environment.

Horizontal advection and non-stationary effects (Figure 9d brown) have a smoothing effect on the isotopic patterns mainly driven by rain evaporation. In particular between rain bands, they are the main depleting factor, contributing to a 10‰ depletion relative to the domain-mean. This is because horizontal winds bring depleted water vapor from the rain bands (Figure 9d). In the eyewall, horizontal advection and non-stationary effects contribute to a 2‰ depletion relative to the domain-mean, because horizontal winds bring depleted water vapor from rain bands. Horizontal advection has an enriching effect in rain bands, where the isotopic gradients are reversed: horizontal winds bring enriched water vapor from in-between rain bands.

The other contributions, including the effects of relative humidity and kinetic fractionation during surface evaporation and of condensation in the SCL, have a marginal impact on δD_v . The marginal impact of condensation is consistent with the absence of clouds in the SCL, and confirms that rain-out does not directly impact the SCL isotopic composition.

A relative enrichment inside the eye is simulated in spite of the neglect of sea spray in our simulations. In our simulation, this enrichment is explained by the weak rain evaporation and by the relatively weak horizontal advection into the eye (Figure 9b). Therefore, the simple model simulates an isotopic composition that is similar to that predicted by (Merlivat & Jouzel, 1979). This does not exclude the possibility for a role of sea spray in nature (Fudeyasu et al., 2008), but this role is not necessary to explain the enrichment in the eye.

Regarding d-excess, the simple model captures the maximum d_v in the rain bands (Figure 9e). This is mainly due to the rain evaporation in the SCL (Figure 9f, purple), which yields water vapor with very high d-excess because of the relatively larger diffusivity of HDO relative to that of $H_2^{18}O$. Alone, it would contribute to an increase in d-excess by more than 7‰ relative to the environment, i.e. more than 150% of the total d-excess difference. Rain evaporation also acts to increase d-excess in the eyewall.

The stronger winds, resulting in stronger kinetic fractionation during surface evaporation, also play a significant role (Figure 9f, orange). It increases the d-excess by about 2‰ in the eyewall, bands and in-between bands, relative to the environment.

618 The simple model also captures the weakest d_v values in the eye (Figure 9e). These
 619 weak values are due to the moist conditions in the eye that reduce the kinetic effects dur-
 620 ing surface evaporation (Figure 9f, red).

621 As for δD_v , horizontal advection acts to smooth the d-excess patterns (Figure 9f,
 622 brown).

623
 624 To summarize, the δD_v differences between the sub-domains are mainly explained
 625 by rain evaporation and rain-vapor diffusive exchanges inside the SCL, which deplete the
 626 eyewall and rain bands, consistent with previous studies (Gedzelman et al., 2003). The
 627 d-excess differences between the sub-domains are explained both by rain evaporation and
 628 by kinetic effects during surface evaporation. Horizontal advection plays a key role to
 629 smooth the isotopic patterns, contributing to the progressive depletion as the air con-
 630 verges towards the center of cyclones suggested in previous studies (Gedzelman et al.,
 631 2003; Xu et al., 2019).

632 **4.5.2 Squall line**

633 The simple model captures the maximum depletion in the stratiform region and
 634 the depletion in the convective and trailing regions (Figure 10c).

635 In both the convective and stratiform parts of the squall line, two terms mainly con-
 636 tribute to the depletion:

- 637 1. rain evaporation and rain-vapor diffusive exchanges in the SCL deplete the wa-
 638 ter vapor (Figure 10d, purple). Alone, it would deplete the convective and strat-
 639 iform regions by about -100 and -50 ‰ respectively, far exceeding the total dif-
 640 ference relative to the environment.
- 641 2. Rain evaporation above the SCL also contributes to the depletion (Figure 10d, blue).

642 These two processes are consistent with the depleting effect of rain evaporation both in
 643 the SCL and near the melting level (Figure 6d), and with the major effect of fraction-
 644 ation during rain evaporation on the isotopic evolution in squall lines (section 4.2).

645 In the convective region, the humidity contrast (Figure 10d, green) also contributes
 646 to the depletion relative to the environment. This may be due to the fact that the con-
 647 vective region is near the environment boundary, and thus experiences strong horizon-
 648 tal humidity gradients.

649 In the trailing region, where the precipitation is very small, the depletion is explained
 650 by horizontal advection and non-stationary effects (Figure 10d, brown). Alone, it would
 651 contribute to a 40‰ depletion relative to the domain mean. This reflects the effect of
 652 horizontal advection spreading the depleted water vapor from the stratiform region. The
 653 environment is similarly, but to a lesser extent, affected by this depleting effect of rear-
 654 ward horizontal advection. In contrast, the horizontal advection explains why the con-
 655 vective region is less depleted than the stratiform region: horizontal advection brings en-
 656 riched water vapor from the environment towards squall line front.

657
 658 Regarding d-excess, the slightly higher d_v in the stratiform region is mainly explained
 659 by rain evaporation both within and above the SCL (Figure 10d, purple and blue). Rain
 660 evaporation in the SCL strongly increases d_v in the convective region (Figure 10d, pur-
 661 ple), but this is compensated by the advection of vapor from the environment with a lower
 662 d_v (Figure 10d, brown).

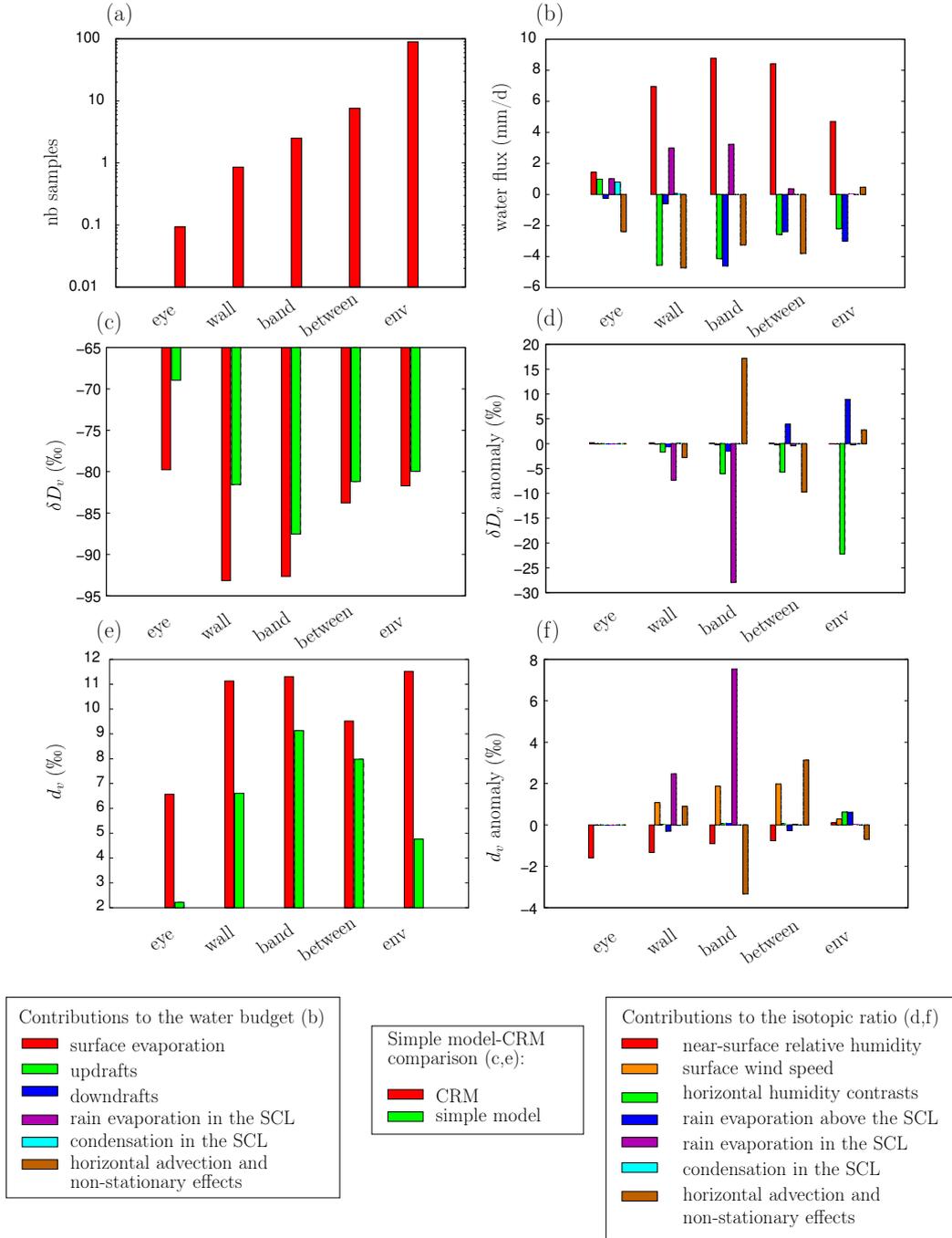


Figure 9. (a) fraction of the domain covered by the five sub-domains of the cyclone: eye, eye-wall (“wall”), rain bands (“bands”), in-between bands (“between”) and the environment (“env”). (b) Water fluxes contributing to the water budgets of the different sub-domains of the cyclone: Surface evaporation (red), updrafts (green), downdrafts (blue), rain evaporation (pink), condensation (cyan) and residual term associated with horizontal advection and non-stationary effects (yellow). (c) δD_v simulated by SAM (red) and by the simple model (green). (d) Decomposition of the δD_v difference between the sub-domain and the domain-mean into 7 contributions: near-surface relative-humidity (red), surface wind speed (orange), horizontal humidity contrasts (green), rain evaporation above the SCL (blue), rain evaporation within the SCL (purple), condensation within the SCL (cyan) and horizontal advection and non-stationary effects (brown). (e-f) Same as (c-d) but for d_v .

Variations in near-surface relative humidity and winds are smaller than in the cyclone simulations, so the contributions of these effects are marginal.

To summarize, the δD_v differences between the sub-domains are explained by rain evaporation and rain-vapor diffusive exchanges inside the SCL, and also probably above the SCL. This is consistent with previous studies (Risi et al., 2010; Tremoy et al., 2014). Horizontal advection then plays a key role in spreading the isotopic anomaly rearward.

4.5.3 Discussion

We find many common aspects for the mesoscale isotopic variability between cyclone and squall line simulations.

- In both cases, rain evaporation and rain-vapor diffusive exchanges both within and above the SCL (especially near the melting level) are the main drivers of isotopic depletion in the most depleted parts of the convective systems (eyewall and rain bands for the cyclone, convective and stratiform parts of the squall line). This is consistent with previous studies (Gedzelman et al., 2003; Tremoy et al., 2014; Xu et al., 2019). These processes have also a crucial impact on d-excess.
- In both cases, horizontal advection and non-stationary effects act to smooth the isotopic patterns. It leads to the gradual depletion towards the eyewall observed in tropical cyclones, and it spreads the isotopic anomalies rearward in the case of the squall line. This is consistent with previous studies (Xu et al., 2019).
- In both cases, condensation processes have no direct effect on the SCL water vapor. It only has an indirect effect through maintaining a vertical gradient in δD_v that allows the rain evaporation to have a depleting effect on the SCL water vapor. In tropical cyclones for example, the rain-out along trajectories has been suggested in some studies to explain the progressive depletion towards the eyewall. We saw here that this is not the case.

The main difference between the two simulations is in the effect of kinetic effects during surface evaporation. Strong winds and very moist conditions in tropical cyclones significantly impact the d-excess, whereas they have a marginal effect in squall lines.

5 Conclusion

Using cloud resolving model simulations of cyclones and squall lines, and a simple SCL budget model, we investigate how convective processes impact the isotopic composition of water vapor and precipitation at the meso-scale. Figure 11 summarizes our results. We show that the main factors depleting the water vapor at the meso-scale is rain evaporation, especially in the sub-cloud layer of rain bands and of the eyewall in tropical cyclones, and in the meso-scale downdraft of the stratiform region in squall lines. The meso-scale δD_v patterns are subsequently reshaped by horizontal advection. These mechanisms are overall consistent with those suggested in previous studies (Gedzelman et al., 2003; Tremoy et al., 2014; Xu et al., 2019). In contrast to previous studies however, we highlight that condensation has no direct impact and that the evaporation of sea spray is not necessary to explain the relative enrichment in the cyclone eye.

This study strengthens our understanding of mesoscale isotopic variability. It provides physical arguments for the more depleted rain in tropical cyclones or squall lines relative to the rain in their environment. Therefore, this study supports the interpretation of paleoclimate isotopic archives in tropical regions in terms of past cyclonic activity (Nott et al., 2007; Medina-Elizalde & Rohling, 2012; Baldini et al., 2016) or past

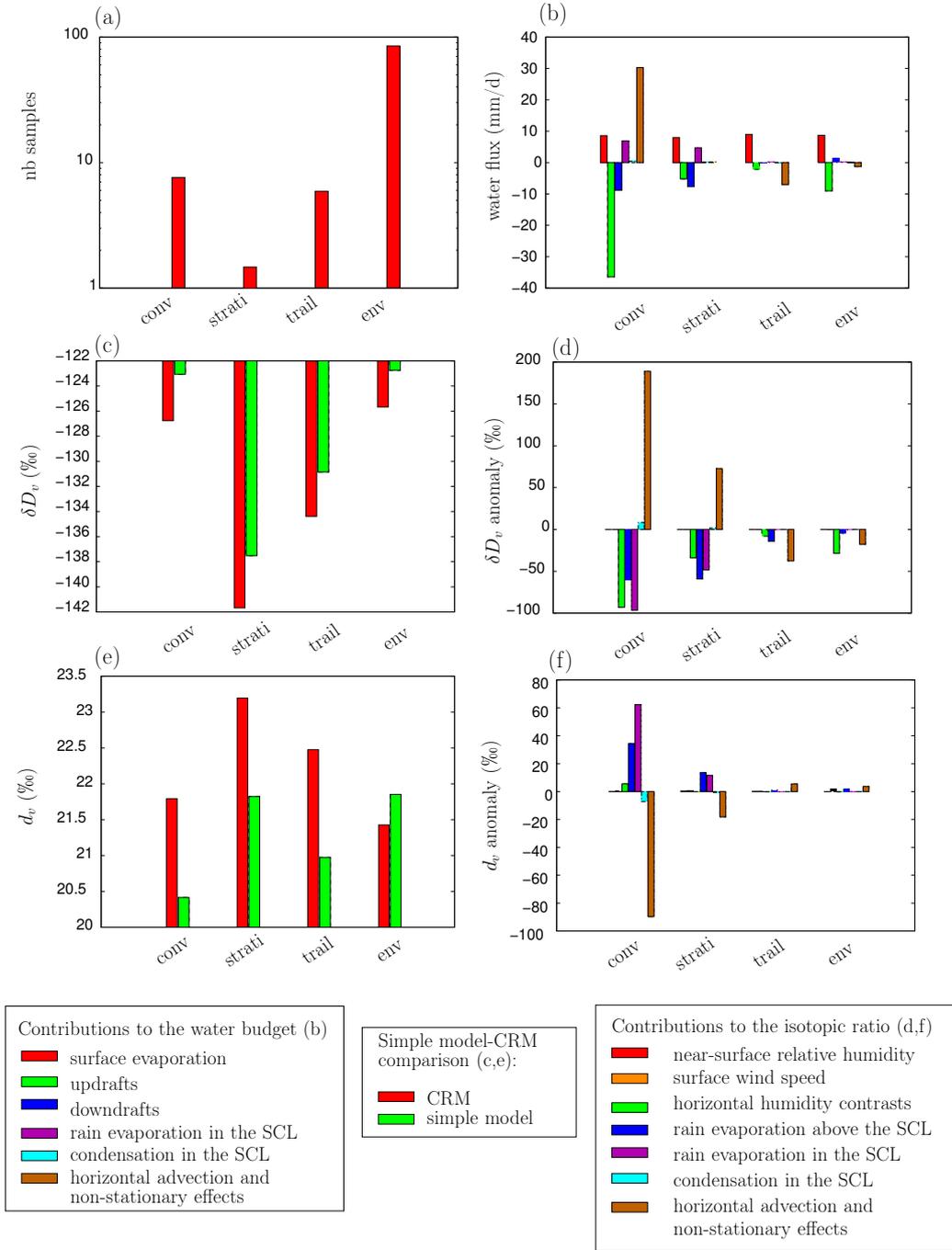


Figure 10. Same as Figure 9 but for the four sub-domains of the squall line: convective (“conv”), stratiform (“strati”) and trailing (“trail”) regions, and the environment (“env”).

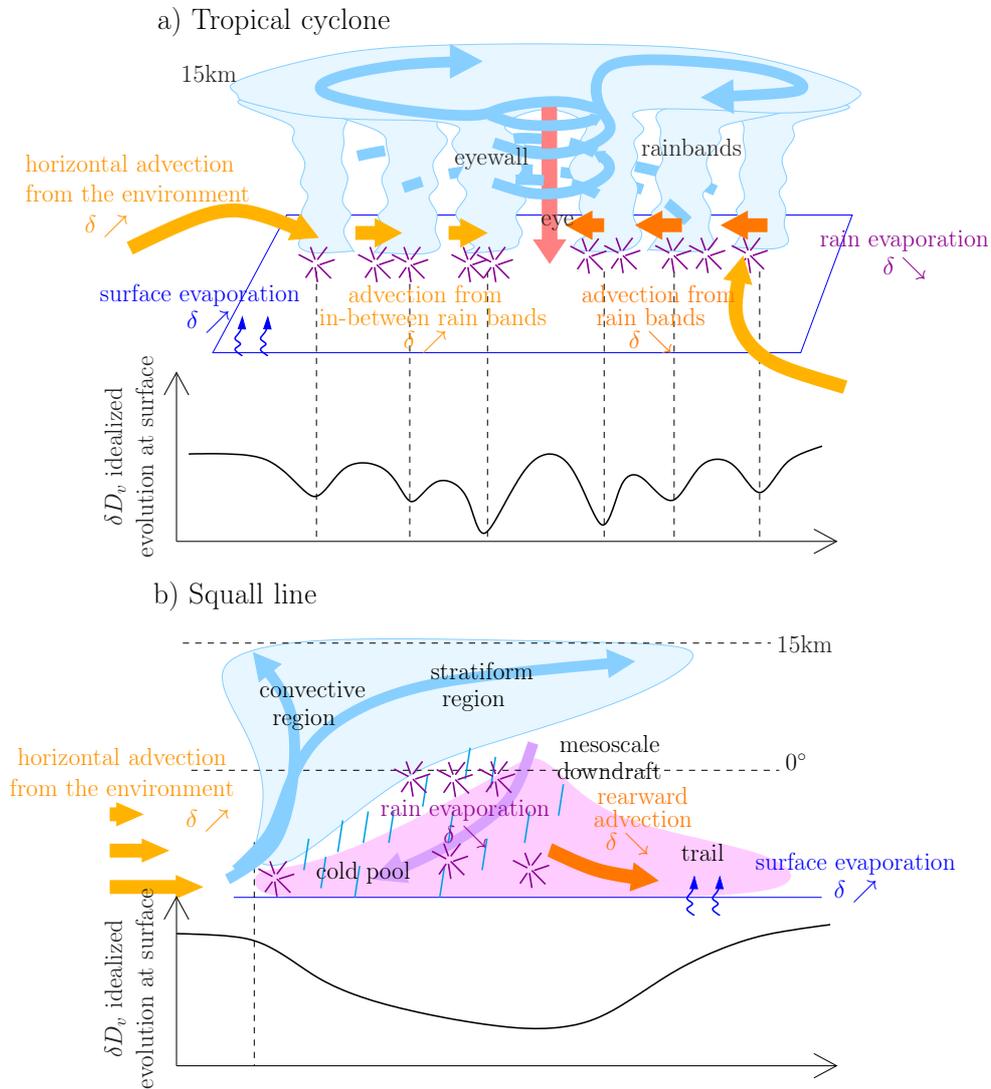


Figure 11. Schematic summarizing the processes controlling the water vapor composition inside tropical cyclones (a) and squall lines (b). The key driver is rain evaporation, indicated by purple stars. Rain evaporation deplete the water vapor in the rain bands and eyewall of tropical cyclones and in the convective and stratiform regions of squall lines. Horizontal advection then reshapes this pattern. Dark orange arrows indicate horizontal advection from depleted regions to less depleted regions, contributing to spread the depleted anomalies inward in cyclones and rearward in squall lines. Light orange arrows indicate horizontal advection from less depleted regions to depleted regions, limiting the depletion in most depleted regions.

709 frequency of large, long-lived, organized convective systems such as squall lines (Maupin
710 et al., 2021).

711 However, when considering paleoclimate records at the annual scale or larger, the
712 isotopic composition reflects an average over many convective systems of different organ-
713 ization types. In our simulations, this is equivalent to considering the domain-mean δD
714 in simulations of tropical cyclones or squall lines relative to the domain-mean δD in sim-
715 ulations of isolated cumulonimbi, rather than the δD in tropical cyclone or squall lines
716 relative to their environment in a given simulation. This paper focuses on mesoscale iso-
717 topic variations and does not discuss domain-mean values, because the realism of sim-
718 ulated mesoscale variations could be more easily assessed than the realism of domain-
719 mean values. In particular, we realized that the domain-mean δD in the precipitation
720 or water vapor of our tropical cyclone simulation was more enriched than that in sim-
721 ulations of squall lines or even of isolated cumulonimbi (Risi et al., 2020). This is at odds
722 with observations of depleted cyclonic rains in the tropics (Lawrence et al., 2004). This
723 discrepancy may be due to limitations in the radiative-convective equilibrium configu-
724 ration. In radiative-convective equilibrium, the cyclone maintains a strong subsidence
725 in its environment, which favors unrealistically dry conditions that allows enriched wa-
726 ter vapor in the SCL to accumulate. In reality, tropical cyclones propagate and are thus
727 not in equilibrium with their environment. Alternatively, this discrepancy may be due
728 to the misinterpretation of the observations. In observations, the isotopic depletion as-
729 sociated with tropical cyclones could be blurred by the effects of average precipitation
730 or large-scale circulation. To rigorously assess the role of convective organization, we would
731 need to compare isotopic observations for different kinds of convective organization but
732 for the same precipitation rate and large-scale context, as is now done for humidity (Tobin
733 et al., 2012). This will be the subject of a future study. This will allow us to rigorously
734 assess the realism of the domain-mean isotopic composition in our simulations, before
735 possibly analyzing it in more detail.

736 Finally, when considering paleoclimate implications, how many other processes need
737 to be investigated, including large-scale horizontal advection (Chen et al., 2021), land-
738 atmosphere interactions along the air mass trajectories, infiltration processes, processes
739 in the karstic systems and during calcite formation (Lases-Hernández et al., 2020). Our
740 study is a first step towards a more comprehensive understanding of water isotopic vari-
741 ations, focusing only on purely convective processes.

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756 Information on SAM can be found on this web page: [http://rossby.msrc.sunysb](http://rossby.msrc.sunysb.edu/~marat/SAM.html)
757 [.edu/~marat/SAM.html](http://rossby.msrc.sunysb.edu/~marat/SAM.html). The simulation outputs used in this article have been submit-

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 759 is: <https://issues.pangaea.de/browse/PDI-29361>.

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