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Evafluatfing the finffluence of deep convection on tropopause thermodynamics and flower stratospherfic water vapor: A RELAMPAGO case study using the WRF modell

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ABSTRACT

Troposphere to stratosphere exchange fis generafifly drfiven by deep convection capabile of overshooting tropospheric materials contributing to stratospheric chemistry. The La Pflata Basfin region fin South America fis known for organized deep convection and mesoscafle convective systems. This study empfloys the Weather Research and Forecasting modell to stimulate deep convection during the RELAMPAGO field campatign fin Argentfina. This work finvestigates upper troposphere – flower stratosphere (UTLS) thermodynamfics, specificalfly doubtle tropopause events, and fidentifities flower stratospheric hydratfion reflated to deep convection. Results show that flower stratospheric hydratfion occurred durfing two organized convective types, a mesoscafle convective compflex (MCC) and squalfil fline, which cofincided with strong flow flevel jet mofisture transport. However, the flower stratosphere was not hydrated durfing discrete ceflfs. Whifile UTLS mofisture was present fin afflthree convective types, durfing the discrete ceflf, fice and water vapor were mixed, finhfibrifing net posfitive buoyancy and the transport of tropospheric material alloft. Durfing the MCC and squalfil fline events, UTLS mofisture was stratified. A dry flayer fin the tropopause was cofflocated whith an fice flayer where net posfitive buoyancy contributed to stratospheric hydratfion as hfigh as 20 km.

1. Introduction

The tropopause regfion fis known for troposphere-stratosphere exchanges, and fin the flower stratosphere the presence of water vapor fis known to finffluence Earth's radfiatfion budget (Hoflton et afl., 1995). Because afir prfimarfifly enters the stratosphere fin the tropfics, the afir near the tropficafl tropopause behaves as a boundary for the gflobafl stratosphere (e.g. Brewer, 1949). In this regard, most changes to the flower stratosphere are generaflfly attributed to the verticafl transport of tropospherfic gases durfing deep convectfion at the tropficafl tropopause boundary (Khaykfin et afl., 2009). Outsfide the tropfics, the finffluence of deep convectfion on tropopause thermodynamfics and flower stratosphere hydratfion fis fless understood. Addfitfionaflfly, fin the extratropfics, mofist deep convectfion can aflter UTLS thermodynamfics, contribute to atmospherfic fofldfing (e.g. doubfle tropopause) and ufltfimatefly finffluence the detrafinment of fice and water vapor fin the flower stratosphere.

Gflobaffly speakfing, UTLS doubfle tropopause features generaffly occur where the hefight of the tropopause decreases rapfidfly between the subtropfics and sub-poflar regfions (Pan et afl., 2004; Homeyer et afl., 2014a). In South Amerfica, this fisobserved finthe southern La Pflata Basfin (LPB), where doubfle tropopause events tend to be coflicated to the upper-flevefl jet stream and may occur over the centrafl Andes throughout the year (Peevey et afl., 2012). The presence of a doubfle tropopauses may finffluence the hefight of maxfimum water vapor flevefls fin the stratosphere (Homeyer et afl., 2014a) and ufltfimatefly ozone chemfistry.

Changes to stratospherfic chemfistry are reflfiant on the transport of tropospherfic gasses to the stratosphere, especialfily water vapor. Water vapor fin the stratosphere chemficalfily reacts to become a cataflyst for stratospherfic ozone destructfion (Bates and Nficoflet, 1950). In the stratosphere, ozone (O $_3$) chemficalfily responds to fincomfing ufltravfioflet (UV) radfiatfion to produce excfited oxygen atoms (O(1 D)). When O(1 D) atoms finteract wfith water vapor (H $_2$ O), the response produces the hydroxyfl free radficall ((O(1 D) + H $_2$ O \rightarrow 2OH) (e.g. Sefinfelld and Pandfis, 1998). Furthermore, when OH finteracts wfith O $_3$ fit fis converted to two oxygen moflecufles (O $_3$ + OH \rightarrow 2O $_2$). Ufltfimatefly, O $_3$ fin the stratosphere absorbs harmfufl UV radfiatfion and water vapor becomes a cataflyst for

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OH productfion and O_3 destructfion (Stenke and Grewe, 2005), resufltfing fin fincreased UV radfiatfion transferred to the troposphere (Forster and Shfine, 2002).

Regfions wfith deep convectfion capable of transportfing water vapor to the stratosphere are generaflfly understood to be flocaflfized fin the tropfics (Randefl and Jensen, 2013; Hemanth et afl., 2018; Ratnam et afl., 2016). However, severafl studfies have anaflyzed regfions wfith convective overshootfing fin the subtropfics and mfid-flatfitudes (Lafing and Frfitsch, 1997; Brooks et afl., 2003; Zfipser et afl., 2006; Bfigeflbach et afl., 2014; Lfiu and Lfiu, 2016; Smfith et afl., 2017; Phoenfix and Homeyer, 2021). Zfipser et afl. (2006) examfined extreme thunderstorm events usfing severafl proxfies for convectfive fintensfity and fidentfiffied severafl regfions wfith deep convectfion outsfide the tropfics, fincfludfing the centrafl U.S. and southeast South Amerfica. They found cases fin the Unfited States, especiaflfly fin the Mfidwestern regfion, where convectfive cfloud top hefights were capable of reachfing up to 18.25 km.

Hurst et afl. (2011) finvestfigated water vapor fin the flower stratosphere due to convectfive overshootfing over Bouflder, Coflorado. They showed an fincrease fin stratospherfic water vapor of \sim 1 ppmv (aflmost 30%) between 16 and 26 km (\sim 100–10 hPa) and found that modefled stratospherfic water vapor trends are predomfinantfly drfiven by two processes: the warmfing of the cofld pofint temperature (CPT) and the strengthenfing of the Brewer-Dobson cfircuflatfion. Tropopause boundary processes connected to CPT are the strongest regulfator of cross boundary transport of gasses to and from the stratosphere.

Homeyer et afl. (2014a) utfifffized the Weather Research and Forecastfing (WRF) modefl to finvestfigate the dfirect finjectfion of water vapor fin the stratosphere vfia deep convectfive processes fin the centrafl U.S. Thefir sfimuflatfions reproduced the vertficafl extent of each convectfive system modefled and showed that doubfle tropopause events were assocfiated wfith tropospherfic afir hfigher fin the stratosphere, compared to sfingfle tropopause events. Addfitfionaflfly, Homeyer et afl. (2014b) finvestfigated a Mesoscafle Convectfive System (MCS) and a cofld front wfith fin-sfitu afircraft observatfions fin the centrafl Unfited States. They found that flarge-scafle doubfle tropopause events may fimpact the flevefl of water vapor mfixfing ratfios deep finto the flower stratosphere due to decreased UTLS stabfiffity.

Whife considerable research has been centered on the centrafl Unfited States, simifilarities exfist between atmospherfic dynamfics, topography, and effimatoflogical features of the mfid-west region of the Unfited States and the LPB of South America. Both regions have a flong north-south mountafin range (Rocky Mountafins fin the U.S and Andes Mountafins fin South America), they are finffluenced by flow-flevel jets transporting mofisture from the tropfics on the eastern stide of the mountafin chafin (Hfiggfins et afl., 1997; Montfinfi et afl., 2019), and they have summer monsoonal processes that act to create condfittions for the finfitiation and development of deep convective thunderstorm activity (Vera et afl., 2006; Saflio et afl., 2007). Moreover, previous studfies have shown that extratropfical deep convection can hydrate the flower stratosphere via the detrafinment of water vapor and fice crystafls (Wang, 2003; Dessfler and Sherwood, 2004; Le and Gaflflus, 2012; Homeyer et afl., 2017; Smfith et afl., 2017). These processes have not been finvestfigated over South Amerfica.

The LPB regfion fin South Amerfica, fincfludfing the Sfierra De Cordoba and portfions of the eastern Centrafl Andes, fis subject to deep convectfion and mesoracafle convectfive systems (MCS; Rasmussen and Houze, 2016; Romatschke and Houze, 2010; Rasmussen and Houze Jr., 2011) capabfle of finffluencfing the UTLS. The RELAMPAGO (Remote sensing of Eflectriffication, Lfightfing and Mesoscafle/mficroscafle processes with adaptfive Ground Observations) fliefld campafign (November 1–December 16, 2018) was conducted to finvestfigate convectfive processes fin the LPB between Cordoba and San Rafaefl fin Argentfina (Nesbfitt et afl., 2021). The focus of this campafign was on finitifiation and fintensity of convective systems fin the region, especially the formation of severe weather. Aflthough considerable research has been conducted to fidentify deep convection fin the LPB, the finifluence of deep convection on the tropopause flayer, exchanges between the troposphere and stratosphere, and the reflationships between convection and doubfle tropopause events

have not been finvestfigated yet.

A major flimitation of UTLS finvestfigation fin this region is the flack of high resoflution spatial and temporal data capable of detecting UTLS exchanges. For finstance, radiosonde flaunch sites fin South America are sparsefly flocated and generality not flaunched durfing severe thunderstorms. Whifile radiosonde data fin the LPB region can represent double tropopause features, they are fless capable of fidentifying the maximum flevel of water vapor fin the flower stratosphere and stratosphere – troposphere exchanges. Consequently, non-hydrostatic numerical models such as WRF (Skamarock et al., 2008) have been utifilized to examfine processes reflated to tropopause exchanges and overshootling (Robfinson and Sherwood, 2005; Homeyer et al., 2014a; Homeyer, 2015). The primary goal of this work is to finvestfigate mesoscafle characterfistics of deep convection fin the LPB, fidentify double tropopause events and flower stratospheric hydration, and mechanisms reflated to flarge water vapor concentrations finthe flower stratosphere with the WRF model.

In thfis study, mesoscafle convectfive systems that occurred over a four-day perfiod durfing the RELAMPAGO ffield campafign are sfimuflated to answer the foflflowfing questfions, 1) have deep convectfive events hydrated the flower stratosphere fin the LPB? If yes, can WRF sfimuflate these events? 2) Are doubfle tropopause events reflated to stratospherfic hydratfion fin the LPB? Lastfly, 3) what are the prfimary mechanfisms drfivfing flower stratospherfic hydratfion durfing doubfle tropopause events fin the LPB? These questfions are addressed by sfimuflatfing three types of deep convectfion: dfiscrete convectfive ceflfls, a mesoscafle convectfive compflex, and a squafffl ffine reflated to a cofld frontafl boundary. The study fis organfized as follflows. The data fis described fin Section 2. The synoptic condfitfions reflated to the flarge-scafle formatfion of deep convectfive events durfing thfis case study are descrfibed fin Sectfion 3. The WRF modefl conffiguratfions, sensfitfivfity tests and modefl valifidatfions are described fin Sectfion 4. Stratospherfic water vapor fis dfiscussed fin Sectfion 5. UTLS thermodynamfics and flower stratospherfic hydratfion fis dfiscussed fin Sectfion 6. Mechanfisms expflafinfing maxfimum water vapor between 15 and 20 km are described fin Section 6.2. Concflusions are discussed fin Section

2. Data and methods

2.1. In-situ observations

Raw radfiosonde data from November 10–15, 2018 for 00 and 12 UTC were obtafined from the Unfiversfity of Wyomfing Department of Atmospherfic Scfiences Weather onfline data archfive (http://weather.uwyo.edu/upperafir/soundfing.htmfl) for 8 statfions fin the greater La Pflata Basfin regfion fin South Amerfica (see Sectfion 3.2b).

2.2. Sateflflite data

The Natfionafl Oceanfic and Atmospherfic Admfinfistratfion (NOAA) Geostatfionary Operatfionafl Envfironmentafl Sateflflfite (GOES) Channefl 13 finfrared fimagery, wfith a centrafl waveflength of $10.3~\mu m$, was empfloyed to vaflfidate WRF sfimuflated Outgofing Longwave Radfiatfion (OLR). These fimages focused on the RELAMPAGO ffield campafign and are avafiflabfle from the Natfionafl Center of Atmospherfic Research (NCAR) and Earth Observfing Laboratory (EOL) fin Bouflder, Coflorado.

The Natfionafl Aeronautfics and Space Admfinfistratfion (NASA) Mficrowave Lfimb Sounder (MLS) fis an finstrument on NASA's Aura sateflffite and has suppflfied near-gflobafl, twfice dafifly UTLS water vapor measurements sfince August 2004 (Lambert et afl., 2020). The vertficafl range fis from 316 hPa to 0.1 hPa, and the horfizontafl resoflutfion fis 210 km perpendficuflar and 7 km aflong Aura's orbfitafl track (Read et afl., 2007). MLS v2.2 $\rm H_2O$ data from November 10–14, 2018 was utfiffized to vaflfidate modefl water vapor mfixfing ratfios at 5 pressure flevefls fin the UTLS: 146.78, 121.15, 100, 82.54, 68.13, 56.23.

2.3. Reanaflysis

The ERA-Interfim reanaflysfis (ERAfi) dataset produced by the European Centre for Medfium-Range Weather Forecasts (ECMWF) (Sfimmons et afl., 2006; Dee et afl., 2011) was utfiffized to finvestfigate synoptfic-scafle atmospherfic condfitfions, and as finfifial and boundary condfitfions for the WRF modefl. ERAfi horfizontafl resoflutfion fis approxfimatefly 0.75° flatfitude \times 0.75° flongfitude (\sim 83 km) wfith 37 vertficafl flevells from the surface to 0.1 hPa, avafiflabfle at 6-h fintervafls. The perfiod of anaflysfis extends from 00 UTC November 09 to 00 UTC November 15, 2018.

2.4. WRF modefl set up

WRF versfion 3.9.1.1 (Skamarock et afl., 2008) was utfiflfized to sfimuflate the MCS fin the La Pflata Basfin. Parameterfizatfions empfloyed fin these sfimuflatfions are shown fin Tabfle 1. Rufiz et afl. (2010) performed WRF sensfitfivfity testfing of severafl modefl parameterfizatfions fin South Amerfica to fidentfify optfimafl surface varfiabfles durfing the summer of 2003. They found that the best performfing parameterfizatfions fincfluded: the Yonsefi Unfiversfity Scheme (YSU) for the Pflanetary Boundary flayer physfics (Hong et afl., 2006) and the Unfiffied Noah Land Surface Modefl for the Surface flayer physfics (Nfiu et afl., 2011). Other cumuflus parameterfizatfion schemes were tested with a coarser horfizontall resoflution (15 km, not shown), fincfludfing the Kafin-Frfitsch (Kafin, 2004), Greflfl-Frefitas Ensembfle (Greflfl and Frefitas, 2014), Greflfl 3D Ensembfle (Greflfl and Devenyfi, 2002), Betts-Mfiflfler-Janific (Janific, 1994), and Tfiedtke (Tfiedtke, 1989; Zhang et afl., 2011). The Greflfl-Frefitas Ensembfle scheme adequatefly sfimuflated the sfize and flocatfion of the MCSs. Aflthough addfitfionafl experfiments with WRF parameterfizatfions are desfirablle, gfiven our finterest fin reducfing temperature uncertafintfies fin the UTLS and fidentfifyfing doubfle tropopause features, thfis study focused on finvestfigatfing the fimpacts of fincreasfing vertficafl resoflutfion by concentratfing flevefls fin the UTLS and fin the boundary flayer. Other parameterfizatfions were hefld constant fin thfis study and are flfisted fin Tabfle 1. The modefl set up for sensfitfivfity testfing of vertficafl resoflutfions fis descrfibed fin Sectfion 4.

3. Synoptic description of events

GEOS 16 IR brfightness temperature 6-h fimages (November 10 – November 15) filfflustrate the flocatfions and progressfion of deep convection durfing the perfiod of study (Ffig. 1). Aflthough deep convection occurred dafify durfing this perfiod, on November 12–13, 2018 a flarge, organized Mesoscafle Convective Compflex (MCC), flocated fin northern Argentfina, was of particuflar finterest due to fits strength and duration (Ffig. 1). Additionality, this study finvestigates other convective systems that exhibited potential for strong updrafts and UTLS hydration. Because the MCC was the most disruptive event fit wffilbe considered the date of reference (Day 0) for the synoptic description of events.

Here, the flarge-scafle atmospherfic condititions are described from November 9–15 to show synoptic forcfing from a pre-convection to post-convective environment (Ffigs. 2 and 3). Severall generall synoptic-scafle features contributed to the formation of deep convection and MCS/MCCs fin the La Pflata Basfin. They fincflude: (1) the position of the upperflevel subtropfical jet stream, which can perturb the atmosphere (Peevey

 Table 1

 Modefl parameters hefld constant for each sfimuflatfion.

Parameterizations for WRF modeli version v3.9.1. simultations (skamarock et al., 2008)			
Cumuflus	Greflfl-Frefitas Ensembfle (Greflfl and Frefitas, 2014)		
Boundary flayer	Yonsefi Unfiversfity (Hong et afl., 2006)		
Land surface	MM5 (Pauflson, 1970)		
Longwave radfiatfion	RRTMG (Iacono et afl., 2008)		
Mficrophysfics	Morrfison 2-moment (Morrfison et afl., 2009)		
Shortwave radfiatfion	RRTMG (Iacono et afl., 2008)		
Surface flayer	Noah-MP (Nfiu et afl., 2011)		

Descriptions for WDE model version v2.0.1 climufations (Classes and at all

et afl., 2012), and when combfined wfith finteractfions wfith the Andes, can produce mountafin/gravfity waves that can resuflt fin doubfle tropopause features (de flaTorre et afl., 2006); (2) the Boflfivfian Hfigh – an upper-flevefl antficycflonfic cfircuflatfion typficaflfly posfitfioned over Boflfivfia, (3) the Chaco Low – a surface flevel thermall flow centered north the Sfierra de Cordoba fin Northern Argentfina, and (4) the South Amerfican Low Levell Jet (SALLJ) – a flow flevefl northerfly wfind jet that fis often observed east of the Andes Mountafin. The SALLJ fis characterfized by maxfimum wfind speeds around 850 hPa and fis responsfibfle for heat and mofisture transport from the tropfics to the subtropfics (Marengo et afl., 2002, 2004; Montfinfi et afl., 2019). Previous studies have characterfized extreme precipitation fin Argentfina reflated to the exfit of the SALLJ (Saffio et afl., 2002, 2007). In the Southern LPB, as flow-flevefl mofisture fis transported across an actfive thermafl flow (e.g. the Chaco Low) and advected pofleward, fit approaches drfier, coofler afir at hfigher flatfitudes, and the resufltfing mofisture fflux convergence zone can contrfibute to convectfive finfilfiatfion fin thfis regfion (e.g. Rasmussen and Houze, 2016).

Lag-composfites of 6-hourfly mean sea flevefl pressure and 850 hPa wfinds and upper-flevefl wfinds (200 hPa) are shown fin Ffigs. 2 and 3, respectfivefly. Lags are reflatfive to the date of the MCC on November 12 at 12 UTC (day 0; Ffig. 1). On November 9 (day 3), a strong antficycflone was centered east of Southeast South Amerfica and was supported by upper-flevefl convergence durfing a spflfit upper-flevefl jet event (Ffigs. 2 and 3, day 3). The posfitfion and strength of the anticycflone contributed to a flow-flevefl northerfly fflow and mofisture transport from northern to centrafl Argentfina (Ffig. 2, day 3). On November 10 (day 2), severafl dfiscrete deep convectfive ceflfls (DC) and cflusters of ceflfls were observed at approxfimatefly 32.5 S (Ffig. 1, November 10). Deep convection with superceflfl structure and overshootfing tops fis shown fin the GOES-16 vfisfibile fimage on November 10 at 15 UTC (Ffig. 4; see Trapp, 2020 for detafifls on thfis event). Durfing thfis tfime, the antficycflone weakened and moved eastward, and a thermafl flow flocated near Cordoba, Argentfina (Chaco Low) fintensfiffied as a trough crossed the Andes.

On November 11 (Ffig. 2, day 1), the SALLJ strengthened, the Chaco Low was actfive, and the exfit of the SALLJ was flocated finArgentfina, west of Uruguay. These atmospherfic condfittions were consfistent with the formattion of organized convection fin Southeast South America as discussed fin Saffio et afl. (2007). The Saffio et afl. (2007) numericafl experfiment showed that one day before the deveflopment of an MCS, an active flow flevefl jet transportfing heat and mofisture to subtropficafl flatfitudes enhanced flow flevefl convergence near the exfit of the SALLJ. Additifionaflify, the same study showed that upper-flevefl divergence corresponding to the positifion of a jet streak contributed to the deveflopment of a "flong-flived" MCS. Simfiflar conditions occurred on day 1 of this study and appear to have contributed to the fintensiffication of organized deep convection.

On November 12 (Ffig. 2, day 0), synoptfic condfitfions were characterfized by an actfive SALLJ and Chaco Low fin the La Pflata Basfin, accompanfied by a trough west of the Andes. In upper flevefls, east of Uruguay, dfivergence from a fleft entrance jet streak flfikefly supported surface convergence and deep convectfion (Ffig. 3, day 0). A flarge MCC was centered west of Uruguay. Thfis MCC was aflso associiated wfith the tornado that was reported by news outflets and socfiafl medfia near Reconquista and Goya fin Northeastern Argentfina. The MCC sflowfly propagated out of the area, proflongfing the finffluence of deep convectfion untfifl 18 UTC on November 13 (day +1). On day +1, a transfient surface flow pressure system (poflar trough) assocfiated wfith a cofld frontafl boundary posfitfioned fin Northern Argentfina (approxfimatefly between 22 and 35°S), which can be fidentfiffied by the convergence of wfinds and pressure gradfients (Ffig. 2). Thfis flocatfion was sfimfiflar to the posfitfion of the MCC on the previous two days, findficatting sustafined deep convection fin the regfion. An organized band with deep convection (or squafffl filing SL) formed aflong the fleadfing edge of the cofld frontafl boundary (Ffig. 1, November 13), and fis aflso finvestfigated fin thfis study. On November 14 (day +2), the flow propagated equatorward and the frontafl boundary mfigrated north finto Paraguay and Brazfifl. As the system exfited the

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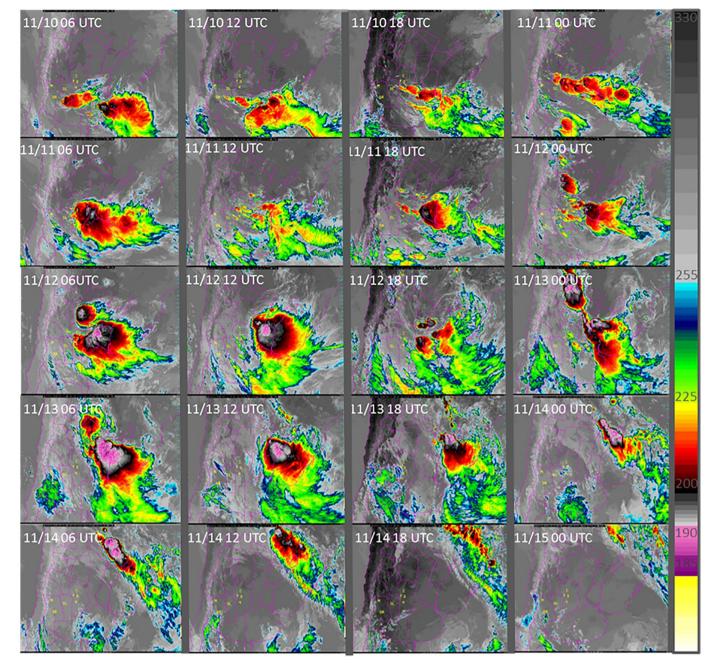


Fig. 1. GOES 16 channell 13 IR brfightness temperature (K) every 6 h, November 10 06 UTC to November 15 00 UTC. Specifific flocations (yelflow flabels) on the IR fimages are reflated to the RELAMPAGO ffield campafign, fincfluding C: Cordoba, SL: San Lufis, Y: Vfilla Yacanto, 3: Riio Tercero, 4: Riio Cuarto. (For finterpretation of the references to coflour fin this ffigure flegend, the reader fis referred to the web version of this article.)

Southern La Pflata Basfin, a strong southerfly fflow assocfiated with the posfition of the surface flow contributed to stabile, coofl and dry conditions fin the region.

4. WRF sensitivity experiment and validation

4.1. Testing verticafl grid resoflutions

The finffluence of deep convectfion on UTLS thermodynamfics and exchange of water vapor was examfined wfith WRF modefl sfimuflatfions. These exchanges are strongfly dependent on the proffifle of temperature and stabfiflfity near tropopause flevefl. Thus, sensfitfivity tests were conducted to evafluate the fimportance of fincreasfing the vertficafl resoflutfion fin the UTLS to sfimuflate observed doubfle tropopause features. These

features can create thermodynamfic finstabfiffity at the UTLS conductive to flower stratospherfic hydratfion. Modefl sfimuflatfions were finfitfiated on November 09, 2018 at 00 UTC and run untiffl November 15, 2018, 00 UTC. Domafins for the WRF sfimuflatfions are shown fin Ffig. 5. The flocatfion of D01 was chosen to capture synoptfic condfittions surroundfing the LPB, fincfludfing flow pressure systems propagatfing from the south or west, upper-flevefl westerflfies across the Andes, and flow-flevefl jet activ/fitfies east of the Andes transportfing heat and mofisture; D03 was chosen based on the flocatfion of the mature MCC and deepest cfloud cover on 12 November 2018 12 UTC (Ffig. 1). The modefl was finfitfiated wfith three 2-way nested domafins and the ffirst 12 h were regarded as spfin-up, and not utfifffized for anaflysfis.

WRF assfigns vertficafl modefl flevefls based on the Eta (η) vertficafl coordfinate system. Because prfimary anaflyses occur fin the UTLS, wfith an

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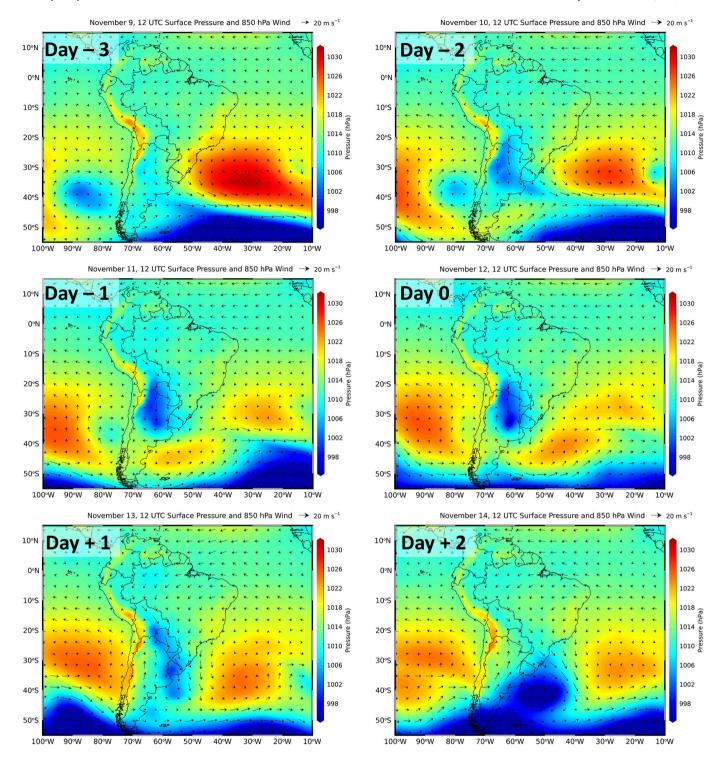


Fig. 2. ERAfi mean sea flevefl pressure (shaded) and 850 hPa wfind (vectors) from 12 UTC November 9 – November 14, 2018. Each day fis reflatfive to the Mesoscafle Convective Compflex on 12 UTC November 12, 2018 (day 0) shown fin Fig. 1.

emphasfis on doubfle tropopause events, verticafl sensfitfivfity testfing was performed to fidentify the ffinest verticafl resoflutfion possfibfle fin the UTLS whithin the D03, 3 km horfizontafl griid spacfing. Three modell runs were conducted. Ffirst, WRF was finfitfialfized with 61,WRF assfigned, η flevells (R1; Ffig. 5). WRF modell flevells for R1 are concentrated fin the boundary flayer to 2168 m, and then equalify spaced (553.7 m) untifil the modell top of 10 hPa (~29 km). The second WRF run (R2) was also finfitfiated with 61 flevells, however, the η flevells were user assfigned and concentrated fin the boundary flayer and tropopause region (R2; Ffig. 5). To avoid abrupt

changes fin hefight between eta flevels and consequent finstabfillity errors, a thfird WRF run was proposed with 75 user assfigned η flevels. Thfis conffiguration resulted fin an optimum η flevels that produced smoother hefight transfittions. Thfis stimulation was an fimprovement over the ffirst two runs as shown fin the next section. Affimodell parameterfizations were held constant durfing each modell run (Tabfle 1). Radfiosonde data were not assfimifilated fin these stimulations.

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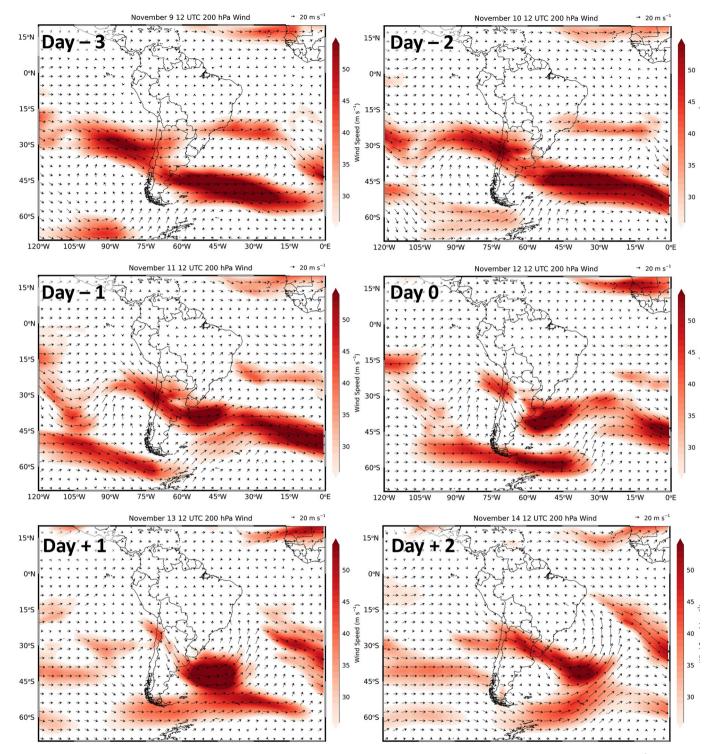


Fig. 3. ERAfi 200 hPa wfind (vectors) from November 12–14, 2018 at 12 UTC. Shadfing represents 200 hPa zonafl wfinds (onfly zonafl wfinds above 25 m s ¹ are shaded).

4.2. Modefl vaflidation

Modefl skfffl fis firfifialfly evafluated wfith finfrared (IR) satefilflite fimagery. WRF sfimuflated outgofing flongwave radfiatfion (OLR) fis utfilfized as a proxy for cfloud top temperature and hefight (Gutzfler and Wood, 1990) and compared to satefilflite fimagery (Ffig. 6). Cflustered dfiscrete ceffs are shown on November 10, 2018 at 21 UTC and a Mesoscafle Convectfive Compflex on November 12, 12 UTC. Aflthough the GOES 16 fimagery and WRF domafin are not the same, affl three runs appear to adequatefly sfimuflate

the extent of deep convection durfing both time frames, with a few structurall differences distinguishing the three runs. Whiffle the fimportance of stimuflatting deep convection cannot be overstated, the main goafl for these stimuflattions is to fidentify doubfle tropopause features and flower stratospheric hydrattion durfing deep convection. Therefore, we valifidated these runs with soundings emphasizing avaiiflable upper troposphere – flower stratosphere temperature and humfidfity data, and with MLS satefillite water vapor data.

Raw radfiosonde data from November 10-15, 2018 (00 and 12 UTC)

Fig. 4. Convective ceffl near Rfio Tercero (red cfircfle on rfight fimage), Argentfina on November 10, 2018, at 20:13 UTC (fleft; photo by Brandfi Gameflfin). Corresponding GOES 16 channell 2 visible fimagery at 20:15 UTC (rfight). Specific flocations on the visible fimage are reflated to the RELAMPAGO fliefd campatign, fincfludfing C: Cordoba, SL: San Lufis, Y: Viffla Yacanto, 3: Rfio Tercero, 4: Rfio Cuarto. (For finterpretation of the references to coflour fin this ffigure flegend, the reader fis referred to the web version of this article.)

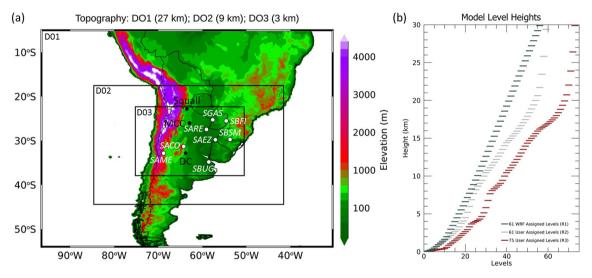


Fig. 5. (a) WRF modefl domafins for downscalfing to 3 km. Domafins D01, D02 and D03 have 27 km 9 km and 3 km grfid spacfing resoflutfion, respectivefly. Locations for radiiosondes are represented with statifion ID (white fitalficized). Locations for detafifled analystis fin Section 6 are represented by bflack dots. (b) WRF vertical flevefls based on the Eta (η) vertical coordinate system for R1 (61 WRF assfigned flevefls, dark grey), R2 (61 user assfigned flevefls, flight grey), and R3 (75 user assfigned flevefls, red). See text for detafifls. (For finterpretation of the references to coflour fin this fligure flegend, the reader fis referred to the web version of this artificile.)

from 8 stations fin the greater La Pflata Basfin region fin South America are discussed fin Tabfle 2 (see Section 2.1). Comparfisons with WRF were performed at standard pressure flevels from 925 to 70 hPa. Soundfings without upper atmospherfic data or soundfings without standard pressure flevels (e.g. SGAS) were omfitted from modell valifidation. Because of flow water vapor mfixing ratios and sharp gradfients fin the tropopause region, additional valifidation of UTLS water vapor was performed with MLS data from November 10–14, 2018 (flocations are discussed fin Tabfle 2 - see Section 2.2).

Modefl root mean square error (RMSE) fis utfiflfized to assess sfimuflated afir temperature, reflatfive humfidfity, wfind speed and water vapor.

$$RMSE = \frac{\nabla}{\sum_{N} \frac{(pi - 0i)^2}{N}}$$
 (1)

RMSE fis caflcuflated for each modefl run and affl avafiflabfle radfiosonde data, where pi fis modefl output and oi fis radfiosonde data. Statfions wfith soundfing data were chosen based on proxfimfity to the MCC on November 12, 2018, and avafiflabfiflity of data (Tabfle 2). Observatfions were coflflected for 00 and 12 UTC and RMSE was caflcuflated on standard pressure flevefls from 925 hPa to 70 hPa (Ffig. 7). RMSE was aflso caflcuflated wfith MLS water vapor data fin the UTLS from 150 to 60 hPa.

Ffig. 7 shows the vertficafl RMSE proffifles usfing radfiosonde temperature (1000–70 hPa), reflatfive humfidfity (1000–100 hPa), and wfind speed (1000–70 hPa), as welfl as MLS water vapor fin the UTLS (150–60 hPa). Overaflfl, the RMSE wfith radfiosonde data fis reduced fin the R3 run compared to the R1 and R2 runs, especifalfly for temperatures finthe UTLS and the flower troposphere where modell flevels are concentrated. The RMSE wfith MLS fisaflso reduced fin R3 fin the UTLS from 120 to 80 hPa, as compared to R2 and R1. The vertficafl mean RMSE for affl three runs fis summarfized fin Tabfle 3.

RMSE was aflso caflcuflated for afir temperature at findfivfiduall stations and for each WRF run separatefly (Ffig. 8). Four flocations with radiiosonde data (SARE, SAME, SBSM, and SBFI; Tabfle 2) were chosen based on flocations reflative to deep convection and avafilable data.

The average temperature bfias was caflcuflated for each modefl run on standard pressure flevefls. Tabfle 4 fincfludes vertficafl mean temperature bfias for each statfion flocatfion.

$$Bias = \frac{\Sigma(pi \quad oi)}{N} \tag{2}$$

On average, for affIstatfions, R1 bfias fis 1.54 K, R2 fis 1.59 K, and R3 fis 1.52 K. Overaflfl, bfiases fintemperature fin R3 are reduced compared to R1 and R2, especialfly fin the flower troposphere and UTLS where eta modefl

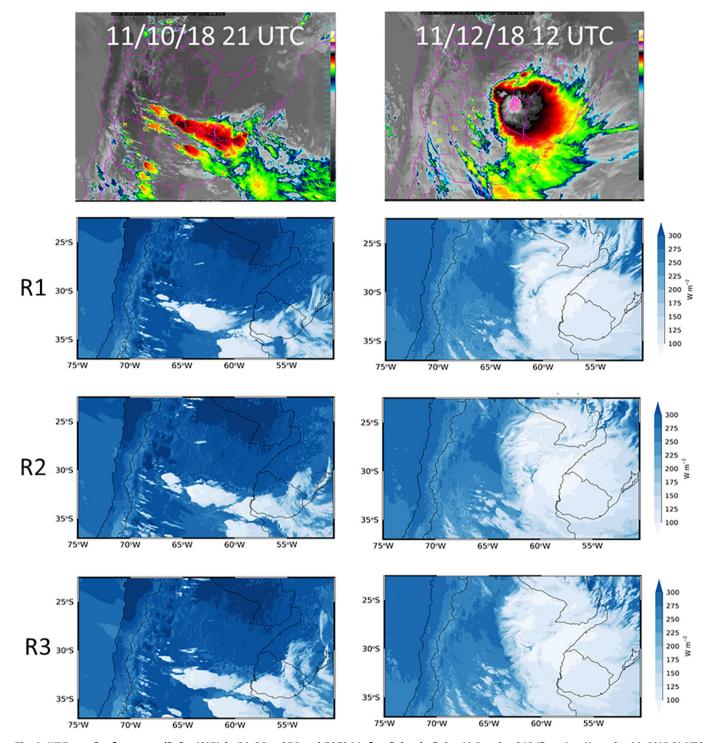


Fig. 6. WRF outgofing flongwave radfiatfion (OLR) for R1, R2 and R3, and GOES 16 cflean finfrared wfindow 10.3 μ m band 13 (fimage) on November 10, 2018 21 UTC (fleft) and November 12, 2018 12 UTC (fright).

flevefls are concentrated.

Ffig. 9 shows comparfisons of sfimuflated UTLS temperatures and radfiosonde observatfions for three radfiosonde sfites: Santa Marfia (SBSM), Foz do Iguacu Aero (SBFI) and Mendoza Aero (SAME). Two sfites, the SBSM and SBFI, were dfirectfly fimpacted by the MCC, whereas SAME was representative of the environment where dfiscrete and cflustered ceffs were developed. The red flfines are from radfiosonde observations and show temperature features before the mature MCC on November 10, 2018 12 UTC (fleft coflumn; Ffig. 9) and post MCC November 15, 2018 00 UTC (rfight coflumn; Ffig. 9). Ffig. 9 (center coflumn) shows proffifes durfing

the mature MCS phase for as near as the data fis avafiflabfle. Overaflfl, R3 (soflfid bflack flfine) wfith 75 user assfigned modefl flevefls demonstrates best performance fin reproducfing UTLS temperature proffifles compared to the observed temperatures. Of partficuflar fimportance for thfis study fis the proffifle between 90 and 60 hPa, where R3 seems to better reproduce the observed doubfle tropopause.

Throughout the vafifidation process, R3, which has user assigned WRF modell flevels concentrated fin the boundary flayer and UTLS, has been shown to mfinfimize modell error compared to R1 and R2. More fimportantfly, R3 has been shown to sfimuflate doubfle tropopause features that

Table 2Top: flfst of radfiosonde stations: abbreviation (fid), number, flocation, flatfitude, flongfitude and flaunch time. Bottom: flfst of MLS flocations and dates.

Radiosonde data						
Id.	Number	Locatfion	Latfitude	Longfitude	Launch tfime (UTC)	
SACO	87,344	Cordoba Aero	31.30	64.21	00 and 12	
SAEZ	87,576	Ezefiza Aero	34.81	58.53	12	
SAME	87,418	Mendoza Aero	32.83	68.78	00 and 12	
SARE	87,155	Resfistencfia Aero	27.45	59.05	00 and 12	
SBFI	83,827	Foz Do Iguacu Aero	25.51	54.58	00 and 12	
SBSM	83,937	Santa Marfia	29.72	53.70	00 and 12	
SBUG	83,928	Uruguafiana	29.78	57.03	00 and 12	
SGAS	86,218	Asunction	25.26	57.63	12	
		Microwave Li	mb Sounder	Data		
Date	Latfitude	Longfitude	Date	Latfitude	Longfitude	
	28.1821	62.7891	13th	31.1407	62.3935	
	29.6620	63.1665		28.1815	63.1548	
	32.6200	63.9517		25.2203	63.9177	
10th	32.6193	54.2684		23.7389	64.2790	
	32.6193	65.0855	14th	23.7392	55.5082	
	31.1407	65.4814		26.7016	56.2393	
11th	29.6614	65.8653		31.1413	57.3749	
	26.7016	59.3273				
	28.1821	59.7016				
12th	32.6199	60.8643				

are not generafifly exhfibited fin R1 or R2. For the remafinder of this study, R3 conffiguration is used for analysis.

5. Lower stratospheric water vapor

5.1. Convective types and flower stratospheric water vapor

Thfis anaflysfis focuses on the three categorfies of MCSs dfiscussed fin Sectfion 4 (DC, MCC and SL; Muflhoffland et afl., 2018). Ffig. 10 shows each category based on outgofing flongwave radfiatfion (OLR) and the assocfiated water vapor mfixfing ratfios at 100, 90, 80, and 70 hPa. Water vapor mfixfing ratfios above 4.0 ppmv are noted as mfixfing ratfios above background flevefls fin Dauhut et afl. (2018). In our study, we assumed the same background water vapor mfixfing ratfio fin the flower stratosphere (4.0 ppmv) sfince the sfimuflated flevefls were generaffly between 1 and 4 ppmv durfing tfimes when convectfion was not deepfly devefloped (not shown).

The three types of deep convectfion anaflyzed here are shown on three sequentfiafl days. The ffirst type was a DC observed fin the subtropfics at approxfimatefly 32°S. This type was flocated fin the southern La Pflata Basfin at 21 UTC on November 10, 2018. For the DC, notable water vapor concentrations above background flevels are shown at 100 and 90 hPa (Ffig. 10, coflumn 1). The second type fis the MCC observed fin northern Argentfina at 06 UTC on November 12, 2018. For the MCC, water vapor concentrations above background flevels are primarifily shown fin subtropficall flocations from approxfimatefly 24–30°S and at aflifitudes as hfigh as 70 hPa (Ffig. 10 coflumn 2). The thfird type fis a SL wfith a NW-SE orfientation, extending from the Andes Mountafins fin western Paraguay to eastern Uruguay and the Atflantfic Ocean at 06 UTC on November 13, 2018. For this system, water vapor concentrations above background flevels span from 22 to 35°S. The hfighest flevels are flocated at approxfimatefly 22°S and at afltfitudes as hfigh as 80 hPa (Ffig. 10 coflumn 3).

It fis fimportant to note that water vapor fin the stratosphere above 40 hPa can be created vfia methane (CH $_4$) oxfidatfion: CH $_4$ + OH becomes CH $_3$ + H $_2$ O (Bates and Nficoflet, 1950; Le Texfier et afl., 1988). As prevfiousfly dfiscussed, stratospherfic water vapor chemficaffly reacts to destroy ozone. In the mfid and upper stratosphere, chemficaffly converted methane fis the prfimary source of water vapor (Brasseur and Soflomon, 2005). Nonethefless, the WRF modefl utfilfized for thfis work does not fincflude stratospherfic water vapor chemfistry. Therefore, the water vapor

concentrations fin the flower stratosphere (Ffig. 10) that were not reflated to the detrafinment of water vapor through deep convection were flikefly due to water vapor advected from other flocations or diabatic descent reflated to cooffing and transport from above fin the modell. These mechanisms explaining water vapor transport fin the WRF stimuflations are not discussed fin this study.

5.2. Tropospheric fflow and flower stratospheric water vapor

Mufifiendore et afl. (2005) used a three-dfimensfionafl cfloud-resoflyfing modefl to anaflyze troposphere to stratosphere transport with fideaffized superceflfl and mufificefifular storms. They found that source regions fin the flower troposphere contributed to fireversfibfle transport to the stratosphere. As described fin Section 3, the SALLJ fis a signifificant source of heat and mofisture fin the study region (e.g. Marengo et afl., 2002, 2004; Montfinfi et afl., 2019). This flow-flevefl transport fis generalfly responsfibfle for convergence (Vernekar et afl., 2003), mofisture fflux (Berbery and Cofffinfi, 2000), and extreme precipitation reflated to the exfit of the SALLJ (Saffio et afl., 2002, 2007). Aflthough many factors may contribute to the flower stratosphere hydratfion, here we finvestfigate the finffluence of mofisture fflux convergence and mofisture transport fin the flower troposphere durfing times of maximum water vapor concentrations fin the flower stratosphere.

Ffig. 11(a, b and c) shows maxfimum water vapor mfixfing ratfios fin the flower stratosphere between 15 and 20 km reflated to deep convectfion. These concentrations were obtained by ffindfing grid points with WRF OLR values fless than 100 W m ², which was used as a proxy for deep convection (e.g. Massfie et afl., 2002). These points findficate regions where tropopause dynamficafl processes may be reflevant fin UTLS water vapor concentrations. Additionally, mofisture flux at 850 hPa (Ffig. 11d, e and f), which fis the flevell fidentified as the wind maxima reflated to the SALLJ (Marengo et afl., 2004; Jones, 2019; Montinfi et afl., 2019), was calculated to finvestfigate the rofle of the meridional mofisture transport by the SALLJ and finvestfigate trimeframes of enhanced water vapor fin the UTLS. Mofisture flux convergence (MFC; Ffig. 11g, h and fi) at 950 hPa was calculated based on Banacos and Schufltz (2005). The MFC equation (Eq. (3)) combfines two terms: the horfizontafl advection of water vapor and the product of water vapor and horfizontafl mass convergence.

MFC fis a useful measure of flow-flevel mofisture transport and convergence (e.g. Rasmussen and Houze Jr., 2011; Bafisya and Pattnafik, 2019), and the Eq. (3) has been applified at 950 hPa to fidentify flow flevel convergence (positifive MFC) and difference (negative MFC).

Mofisture transport and flow-flevefl convergence fis evfident durfing each convectfive type (Ffig. 11). For the MCC type, strong merfidfionafl mofisture transport occurs at 850 hPa (Ffig. 11e), and at 950 hPa, the convergfing outfflow boundary nearfly surrounds the system (Ffig. 11 h, red flfine). For the SL type, strong merfidfionafl mofisture transport fis aflso shown at 850 hPa (Ffig. 11f), and at 950 hPa, the gust front spans from 22 to 35° S (Ffig. 11fi, red flfine). Aflthough the DC type of deep convectfion fis assocfiated wfith a convergent boundary at 950 hPa (Ffig. 11g, red flfine), merfidfionafl wfind and mofisture transport fin the flower troposphere are weaker when compared to the MCC and SL (Ffig. 11d).

Additifionalify, durfing the MCC, a strong outflow boundary along the northern gust front (Ffig. 11h) flikely triggered new cellil devellopment and proflonged the MCC flife cyclle. Durfing this time frame, the enhanced flow flevell mofisture transport and convergence fis evident and may have contributed to enhanced maximum water vapor shown fin the flower stratosphere. The MCC fis finvestfigated further fin the next section.

5.3. Deep convection and water vapor in the UTLS

Here we begfin to characterfize mechanfisms reflatfing deep convectfion

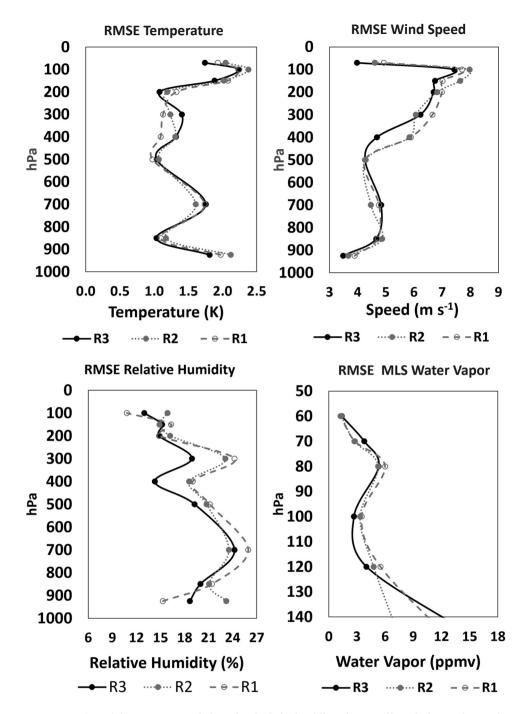


Fig. 7. Modefl root mean square error (RMSE) for temperature, wfind speed and reflatfive humfidfity usfing on radfiosonde data, and RMSE for water vapor usfing MLS data. Note, RMSE of water vapor fis for the UTLS region onfly.

 $\begin{tabular}{ll} \textbf{Table 3} \\ \textbf{Vertficafl mean RMSE whith radiiosonde temperature, reflatfive humfidfity, and whind speed, and whith MLS water vapor. \end{tabular}$

Vertficaflfly mean RMSE			
	R1	R2	R3
Temperature (K)	1.5587	1.6156	1.5306
Reflatfive Humfidfity (%)	17.6013	18.4194	16.5775
Wfind Speed (m s 1)	5.6796	5.6244	5.3007
Water Vapor (ppmv)	5.604008	4.1899	5.3746

and water vapor variabfiffity fin the UTLS. OLR was used here to objectivefly fidentify contriguous convective regions associated with the MCSs, folflowing a simiffar approach as fin Carvaflho and Jones (2001) and Ferrefira et afl. (2003). Contriguous cfloud cflusters with OLR fless than 100 Wm 2 were examfined to fidentify properties of the MCSs that appeared reflated to water vapor transport to the flower stratosphere. Among afl convective types, the MCC has the flargest maximum water vapor fin the flower stratosphere. Furthermore, the MCC fis reflated to the strongest dynamficafl forcfing fin the flower troposphere, fidentified by strong wfinds speeds, and the strongest updrafts and downdrafts at 100 hPa and 500 hPa, which flikefly contributed to maximum water vapor concentration fin the flower stratosphere.

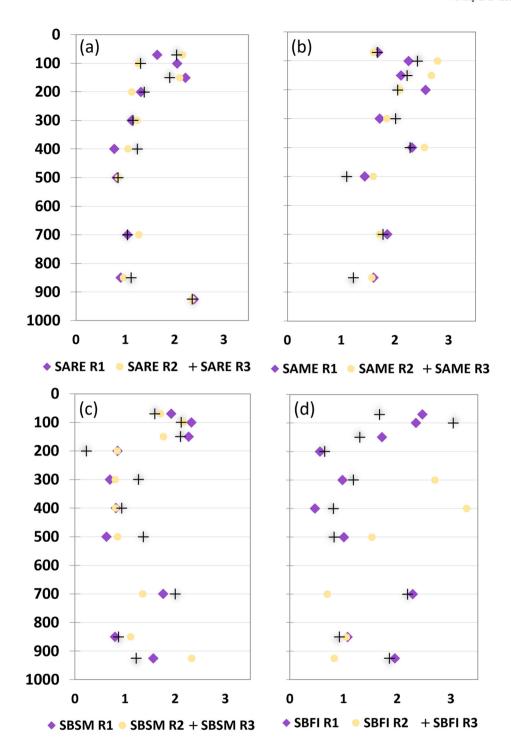


Fig. 8. Temperature (K) RMSE from SARE (a), SAME (b), SBSM (c), and SBFI (d).

Table 4Vertficafl mean temperature (K) bfias for the SARE, SAME, SBSM, and SBFI statfions.

Vertficafl mean temperature bfias (K)				
	R1	R2	R3	
SARE	1.44240	1.44098	1.44123	
SAME	1.95068	2.04901	1.86440	
SBSM	1.34069	1.26932	1.38715	
SBFI	1.43439	1.57987	1.40128	

To better understand these processes, we tracked cflusters of deep convection focused on the MCC. If imfitations due to ceffil duration and domafin sfize prevented ceffil trackfing for the DC (e.g. short flived dfiscrete ceffil) and the Squafifi fline (e.g. system propagates outsfide the domafin). The MCC system has a proflonged finfiluence wfithfin the domafin afflowing us to track a cfluster of deep convection from pre-MCC to post-MCC. For this purpose, we tracked the flong-flived MCC fin 3-h fintervals for 18 h between November 11, 21 UTC – November 12, 15 UTC. Fig. 12 fiffflustrates the maximum water vapor fin each griid pofint between 90 and 70 hPa for each tracked cfluster.

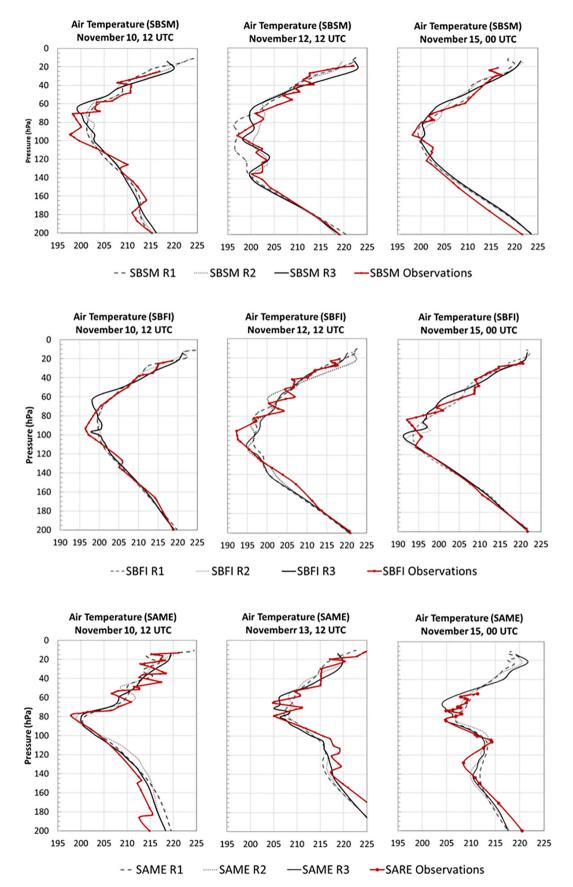


Fig. 9. Afir temperature proffifles for 3 statfions: SBSM (top row), SBFI (mfiddfle row), and SAME (bottom row). UTLS WRF temperature for R1 (dashed flfine), R2 (dotted flfine) and R3 (soflfid flfine), and observations (red flfine). (For finterpretation of the references to coflour fin this ffigure flegend, the reader fis referred to the web version of this artificile.)

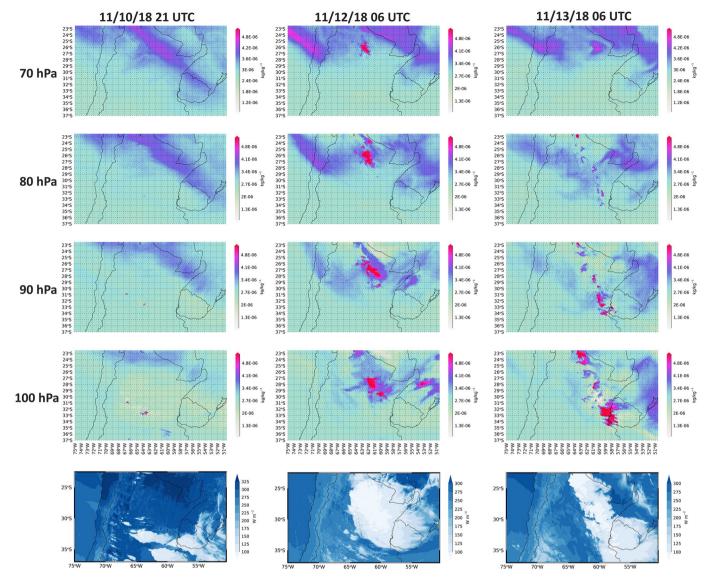


Fig. 10. WRF water vapor mfixfing ratfio at 100, 90, 80, and 70 hPa for three convective types: November 10, 2018 21 UTC (fleft coflumn), November 12, 2018 06 UTC (mfiddfle coflumn), and November 13, 2018 06 UTC (rfight coflumn); WRF outgoing flongwave radiation for the same perfoods is shown in the bottom panel.

Seven hours durfing the evoflutfion of the MCC are analyzed and resuflts are summarfized fin Tabfle 5. Statfistfics were obtafined for the entfire cfloud cfluster (deffined by the OLR threshofld of 100 Wm 2) and for grfid pofints that exceeded the threshofld of 4.2 ppmv (assumed as background flevefl) above 100 hPa. The follflowfing statfistfics are shown for each cfloud cfluster: totafl number of grfid pofints fin each cfluster, area of these cflusters (km2), and maxfimum water vapor (ppmv). Addfitfionaflfly, grfid pofints wfithfin these cflusters exceedfing the 4.2 ppmv threshofld were examfined and the foffflowfing propertfies were caflcuflated: totafl number of grfid pofints above the threshofld, number of these grfid pofints associiated wfith doubfle tropopauses (DT) and respectfive fractfion of these pofints (see Sectfion 6 for DT description). The maximum updrafts and downdrafts for each cfluster were aflso computed (Tabfle 5). At 21 UTC sfimuflatfions show the flargest maxfimum water vapor fin the flower stratosphere reflated to the MCC and the smaflflest area (26,676 km²), findficatfing earfly stages of deveflopment. We aflso observe the strongest updrafts durfing thfis stage (28.63 and 26.08 m s 1 at 500 and 100 hPa, respectfivefly) that fliftefly pflayed a rofle fin transportfing water vapor to the UTLS. From thfis tfime onward, the MCC cfloud cfluster fincreased fin area untfifl 9:00 UTC, when the MCC area reached fits flargest area (\sim 3.8 x10 km 2), flikefly reflated to maxfimum expansiion of the anyfifl cfloud shfieflds. After this time, the MCC

began to dfissfipate. Nonethefless, after 21 UTC updrafts and downdrafts decreased finfintensfity at 100 hPa, findficatfing that the convectfive support for transport of water vapor to the flower-stratosphere progressfivefly weakens. The maxfimum water vapor at 100 hPa and between 90 and 70 hPa seemed welfl correflated wfith the maxfimum updrafts (Ffig. 13a). As the system matures, and untfil dfissfipatfion begfins, the number of grfid celfls exceedfing 4.2 ppmv fincreased, despfite the decrease fin maxfimum updrafts. Possfibfle mechanfisms expflafinfing thfis fincrease are expflored next. Notfice that the strong updrafts assocfiated wfith the MCC are consfis-tent wfith observatfions fin Heymsffield et afl. (2010) fin South Amerfica. In that

study, updrafts reached 30 ms ¹, wfith vertficafl veflocfity maxfima observed above 12 km, fincfludfing some observatfions above 15 km. Heymsffield et afl. (2010) hypothesfized that flatent heat reflease fin upper flevefls finfitfiated fintense vertficafl motfion and coufld expflafin the updraft maxfima and hefight of updraft maxfima fin thefir study fin South Amerfica. Addfitfionaflfly, Zfipser et afl. (2006) fidentfiffied the flocatfion of the MCC fin South Amerfica as a regfion of extreme thunderstorms, sfimfiflar to the southern pflafins fin the U.S Southern Great Pflafins (Gfiangrande et afl., 2013). We observe sfimfiflar features fin our sfimuflatfions. Maxfimum updrafts of 28.63 ms ¹ and 26.08 were observed at 100 hPa and 500 hPa at 21:00 UTC, respectfivefly. Downdrafts at 100 hPa and 500 hPa were

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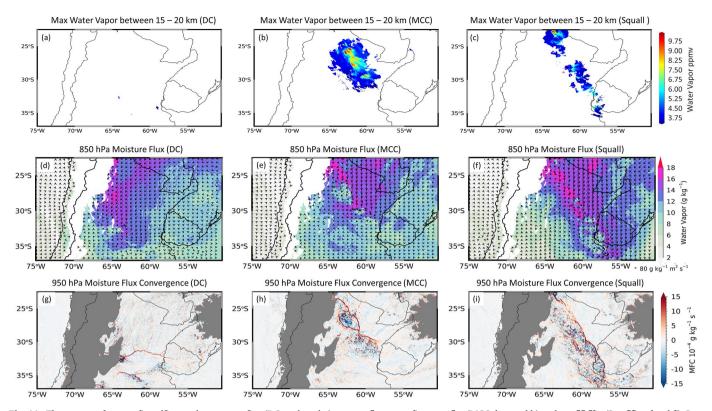


Fig. 11. Three types of convectfion: dfiscrete deep convectfion (DC; a, d, and g), mesoscafle convectfive compflex (MCC; b, e and h) and squafflf lfine (Squaffl; c, f and fi). Grey and white areas findficate terrafin at the gfiven pressure flevefls. Top row (a-c): maximum water vapor (15–20 km) reflated to deep convectfion (described fin text). Second row (d-f): 850 hPa mofisture flux vectors [qu, qv] and water vapor mfixfing ratfio (shaded). Bottom row (g-fi): 950 hPa Mofisture flux convergence: MFC (described fin text).

stigntifficantfly weaker, $\,$ 15.49 ms 1 and -7.83 ms 1 , respectfivefly durfing the same tfime.

Ffig. 13 shows the flfinear reflatfionshfips durfing the tracked MCC between sfimuflated maxfimum flower stratospherfic water vapor above 4.2 ppmv and the follflowfing varfiabfles: maxfimum updrafts (500 and 100 hPa; Ffig. 13a), maxfimum downdrafts (500 and 100 hPa; Ffig. 13c), mean surface MFC (Ffig. 13b), and flower troposphere water vapor (850 and 950 hPa; Ffig. 13d). Durfing the tracked MCC, the strongest flfinear correflatfion (R2) fis sfimuflated between eflevated maxfimum flower stratospherfic water vapor and updrafts at 100 hPa (Ffig. 13a) and downdrafts at 100 hPa (Ffig. 13c). Addfitfionaflfly, flower tropospherfic cfircuflatfion, especfiaflfly surface convergence (posfitfive MFC; Ffig. 13b) and maxfimum water vapor at 850 hPa (Ffig. 13d), aflso have strong posfitfive flfinear correflatfion wfith flower stratospherfic water vapor. The transport of tropficafl mofisture to the southern La Pflata Basfin vfia the SALLJ (e.g. Marengo et afl., 2002, 2004; Montfinfi et afl., 2019) fis flikefly an fimportant source of water vapor contrfibutfing to eflevated water vapor concentratfions between 90 and 70 hPa. The finffluence of finstabfiflfity on UTLS thermodynamfics fis finvestfigated next.

6. UTLS thermodynamics and lower stratosphere hydration

The foffflowfing dfiscussions finvestfigate the reflationships between tropopause flevels and water vapor fin the UTLS to better understand possfibile mechanisms reflated to the depth of overshootfing and reflationships with flower stratospherfic hydrattion.

6.1. Doubfle tropopause events

Whifile doubfle tropopauses (DT) are more frequent fin tropficafl afltfitudes (Mehta et afl., 2011), finthfis regfion (flatfitude range 220–370 S.), fafir weather DT are generaflfly more frequent near the subtropficafl jet stream

(Randefl et afl., 2007). They have been reflated to extra-tropficafl antificy-cflonfic Rossby wave breakfing associated with cofld fronts connected to strong surface flow pressure areas (Martfius and Rfivfiere, 2016) and reflated to mountafin wave dynamfics producting gravfity waves (de flaTorre et afl., 2006). The finteractfion between flarge-scafle mountafin waves and the posfitfion of the upper-flevefl jet stream (Ffig. 3) may enhance the productfion of DT events (Peevey et afl., 2012) fin this region. However, this work examfines DT events specificalfly reflated to deep convection, and the corresponding hefights and concentrations of maximum water vapor fin the flower stratosphere.

The tropopause can be fidentfiffied fin severall dfifferent ways: chemficall - e.g. abrupt changes finozone concentrations, dynamficall (e.g. potential) vortficfity), or thermafl (e.g. changes fin temperature flapse rates). Here we focus on fidentfifyfing the thermafl tropopause. Maddox and Muflflendore (2018) compared severafl methods for tropopause fidentfiffication durfing and after convectfion and found the best methods were the WMO thermafl tropopause and statfic stabfiffity. Here, we use the WMO thermafl tropopause deffinfitfion. Ffirst, to caflcuflate the temperature flapse rate, we flfinearfly finterpoflated the orfigfinall temperature proffile fin the UTLS (which varfied between 100 and 400 m) to a constant 100 m vertficafl grfid. Once finterpoflated, the temperature flapse rate was caflcuflated (dT/dz) from 5 to 20 km. Next, the prfimary tropopause was fidentfiffied based on the WMO deffinfitfion, whfich states that a thermall tropopause fis flocated where the flapse rate decreases to fless than or equafl to 2 K/km (WMO, Worfld Meteoroflogficafl Organfizatfion, 1957). Foffflowfing Peevey et afl. (2012), the flapse rate was caflcuflated above 5 km to avofid fidentfifyfing flow tropospherfic finversfions as the prfimary tropopause flevefls. Lastfly, the flocatfion of the secondary tropopause was fidentfiffied where the flapse rate fincreases above 3 TK/km wfithfin 2 km of the prfimary tropopause, and then decreases agafin to beflow 2 TK/km (modfiffied from Peevey et afl.,

We begfin our DT anaflysfis by fidentfifyfing DT reflated to the tracked

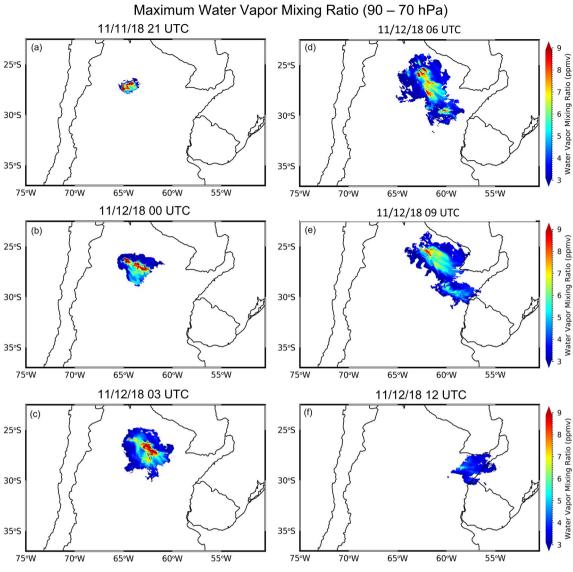


Fig. 12. Cflusters of deep convection between November 11, 21 UTC and November 12, 12 UTC (described fin text). Maximum water vapor mfixing ratios between 90 and 70 hPa.

Table 5Properties associated wiith the MCC tracked durfing fits flifetime.

Track MCC clusters							
Tfime	21 UTC	00 UTC	03UTC	06 UTC	09 UTC	12UTC	15 UTC
Number of grfid ceflfls	2964	10,265	23,457	35,738	41,853	18,297	1114
Area (km²)	26,676	92,385	211,113	321,642	376,677	164,673	10,026
		Maxim	um water vapor (pp	omv)			
90-70 hPa	20.40	15.90	12.70	15.70	9.39	6.60	4.22
100 hPa	20.00	14.00	12.00	11.00	7.70	5.70	4.10
	Lower	stratosphere water	vapor greater than	or equal to 4.2 (ppr	nv)		
Number of grfid pofints	1625	5292	10,257	12,386	13,326	2932	
Number of grfid pofints wfith DT	919	1284	4693	6231	4621	2671	
Percentage of grfid pofints wfith DT	57	24	46	50	35	91	
		Maxi	mum Updrafts (ms ^Y	¹)			
100 hPa	28.63	23.10	23.33	16.76	1.49	1.88	0.22
500 hPa	26.08	20.44	24.61	20.82	17.71	16.30	0.48
		Maxim	um Downdrafts (ms	s ^{Y1})			
100 hPa	15.49	10.36	8.90	4.95	2.72	1.85	0.21
500 hPa	7.83	5.63	7.16	6.79	7.31	4.87	0.13

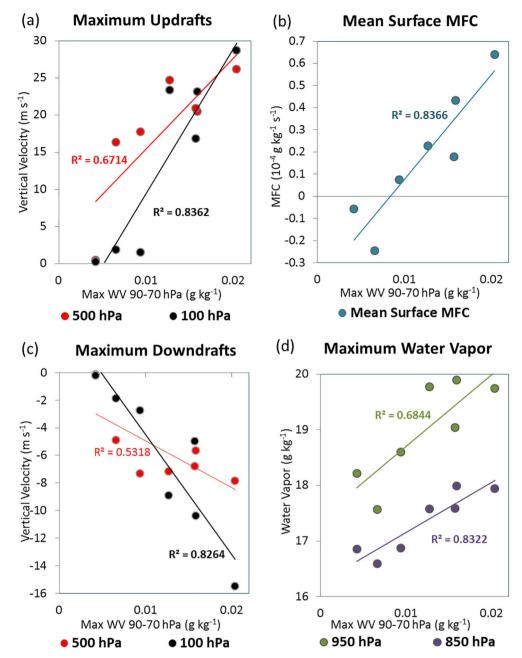


Fig. 13. For each tracked deep convective cfluster. Maximum water vapor mfixfing ratfio above 0.0042 g kg ¹ between 90 and 70 hPa (x-axfis) are compared to maximum updrafts (a), downdrafts (c), MFC (b) and maximum flower stratospherfic water vapor (d).

MCC cflusters (Tabfle 5, flower haflf). Onfly grfid pofints fin the flower stratosphere (90–70 hPa) wfith maxfimum water vapor vaflues above 4.2 ppmv were retafined for thfis anaflysfis. It shoufld be noted that when thfis threshofld was appflfied, the flast tfime frame (November 23, 15 UTC) was removed from the MCC trackfing (Tabfle 5).

Based on the threshofld, the cfluster at 21 UTC had over 50% of the of grfid pofints exceedfing 4.2 ppmv assocfiated wfith DT features (Tabfle 5). At thris trime, thris cfluster showed the hrighest percentage of DT features (57%), the hrighest maxfimum water vapor mrixfing ratfios fin the flower stratosphere (20.40 ppmv), and the strongest updrafts and downdrafts at 500 and 100 hPa. The amount of water vapor progressfiverly decreased unififl 03 UTC, accompanfied by a decrease fin the fintensfity of the updrafts. However, at 06 UTC the maxfimum water vapor fincreased to variues comparable to 00 UTC between 90 and 70 hPa (15.70 ppmv), whrifte maxfimum updrafts, aflthough strong, continued to decrease (16.76 ms ¹). Thris enhancement finwater vapor appeared reflated to an fincrease

fin the fractfion of DT (50%), suggestfing that the presence of DT mfight have been the mechanfism by which water vapor was further enhanced above 100 hPa, even with the decrease fin the fintensity of the updrafts. At 9:00 UTC, the magnifitudes of the maximum updrafts are approximately 10% of what was simuflated fin the previous 3 h perfiod, and the percentage of grid points associated with DT also decreased to 35%. With flow support from both updrafts and DT, the maximum water vapor above 100 hPa fisonfly 60% of what was observed 3 h earflier. At 12 UTC, as the system dfissfipated and updrafts weakened, the maximum water vapor vaflues continued decreasfing, and nearfly 90% of affl grid points exceeding 4.2 ppmv were associated with DT.

Ffig. 14a, e and fishow cross sections of flapse rates (shaded) durfing each type of deep convection: at 32.79° S for the DC, 26.04° S for the MCC, and 22.81° S for the squafifl fline. The pofints for the prfimary and secondary thermafl flapse rate tropopause flevers are shown with fiffled dots. The flatfitudes for each cross section were chosen based on

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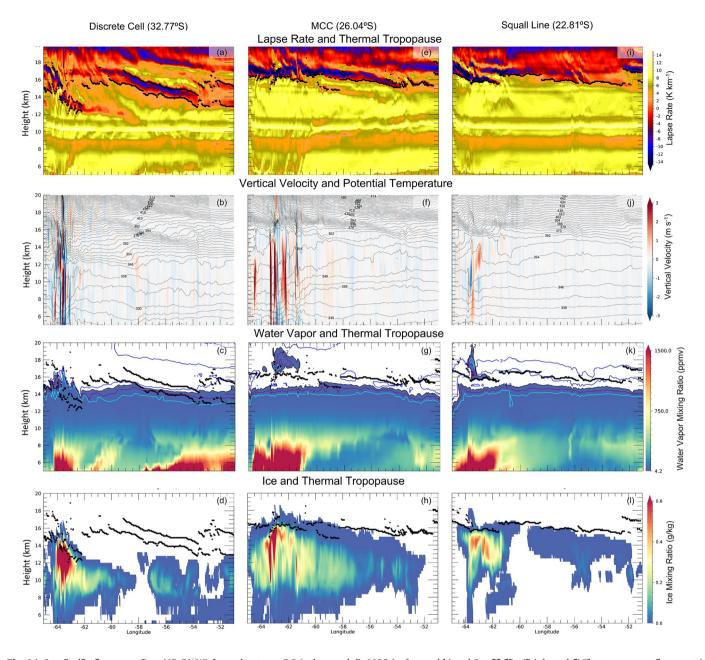


Fig. 14. Longfitudfinal cross sections $(65-51^{\circ}W)$ for each system: DC (a, b, c, and d), MCC (e, f, g, and h) and Squaffl ffine (fi, j, k, and fl). The temperature flapse rate (dT/dz; shaded) and thermall tropopause flevels (ffiffled dots) are on the top panell (a, e and fi) Vertficall veflocfity (w; shaded) and potentifial temperature (theta; fiso-therms) are on the second panell (b, f and j). Water vapor mfixfing ratfios greater than 4.2 ppmv (shaded; white areas are fless than 4.2 ppmv), UTLS water vapor mfixfing ratfio (fline contours): 3 ppmv (bflue), 4.2 ppmv (bflue), 6 ppmv (purpfle), 9 ppmv (cyan), and thermall tropopause flevels (ffiffled dots) are on the third panell (c, g and k). Ice mfixfing ratfios (shaded) and thermall tropopause flevels (ffiffled dots) are on the fourth panell (d, h and fl). (For finterpretation of the references to coflour fin this ffigure flegend, the reader fis referred to the web version of this artificfle.)

maxfimum water vapor concentrations fin the flower stratosphere from 15 to 20 km durfing each convective event. The convective flatent heat reflease durfing phase changes (condensation and freezing) appears to occur durfing each case of deep convection, which fis findicated by the decrease finflapse rate finthe midand upper troposphere (Fig. 14a, e and fi). Additionality, verticall veflocity (shaded) and potential temperature (contour) (Ffigs. 14b, f and j) filliustrate finstabfillity and enhanced updrafts, possfibfly fin association with flatent heat exchanges fin the mid and upper troposphere (Tao and Lii, 2016).

Water vapor mfixfing ratfios durfing each convectfive type are shown based on the 4.2 ppmv threshofld (Ffig. 14 c, g, and k; shaded), wfith addfitfionafl flfine contours fin the UTLS (3, 4.2, 6, and 9 ppmv) to hfighflight regfions of enhanced water vapor fin the flower stratosphere. Areas fin

Ffig. 14c, g and k wfithout shadfing (whfite) represent water vapor mfixfing ratfios beflow the 4.2 ppmv threshofld. In the MCC and Squaffl flfire categorfies (Ffig. 14g and k respectfivefly), a gap exfists between water vapor at or near the thermafl tropopause flevefls wfith hfigher water vapor concentrations afloft. This dry flayer may assist fin fidentifying hydratfion of the flower stratosphere and findficate fireversfibfle mfixing (Dauhut et afl., 2018). One expflanatfion for this resuflt fis fice crystafl formation and flatent heat reflease fin the UTLS. Diabatfic heatfing can produce positive net buoyancy and strong updrafts forcing fice afloft. At warmer flevefls fin the flower stratosphere, fice fis subflimated, producting higher water vapor concentrations (Dessfler et afl., 1995; Smfith et afl., 2017). This process appears to hydrate the flower stratosphere with the direct finjection of fice particiles (Khaykfin et afl., 2009). Ffig. 14d, h and fishow fice mfixing ratfios

that may support this expflanation. Conversefly, the DC event does not have a gap above the mofist tropopause. While fice and water vapor are detected directify above the secondary tropopause, the flack of a dry flayer and corresponding water vapor above findicates that the flower stratosphere fis not hydrated at this flocation by discrete celli overshootfing. Aflthough fice crystafl subfilimation and detrafinment typficafifly occur on the scalle of minutes, the 3-hourfly output suggests that these processes may have contributed to the UTLS hydration.

For each convective category finvestigated here, water vapor detrafinment fin the flower stratosphere seems associated with a sharp change fin flapse rate with hefight, cofincfidfing with a sharp change fin static stabfiflity (00/0z). This is especially noted fin the MCC and Squallf Isline convective types (Ffig. 14e, f, fi, j). For both categorfies, flarge finstabfiflity beflow the primary tropopause flevell is capped by a shallflow stabfle flayer (Ffig. 14f and j; potential temperature contours), where steep potential temperature gradfients are observed. This is findficative of previously described doubfle tropopause events (Homeyer et afl., 2014a). Beflow the sharp change fin flapse rate, where temperature controls the formation of fice (Jensen et afl., 2007), flatent heat reflease durfing fice formation is flikely responsible for finstabfiflity and fincreased water vapor flevels afloft due to updrafts.

6.2. UTLS mechanisms expflaining maximum water vapor between 15 and $20\ km$

To further understand the mechanfisms expflafinfing the hefight of maxfimum water vapor flevefls, findfivfiduafl grfid pofints wfith flarge maxfimum water vapor concentratfions fin the flower stratosphere are examfined durfing each type of deep convection. Here we show proffifles of water vapor mfixfing ratfio, fice mfixfing ratfio, afir temperature (Ffig. 15), and proffifles of flapse rates and vertficafl veflocfity (Ffig. 16) durfing each category of deep convection. The grid point at 63.78 W, 32.79 S fisreflated to the DC. The background flevefls were onfly observed above 17 km (not shown). At thfis grfid pofint, flarge fice mfixfing ratfios were observed from 13.4-15.3 km and coffflocated with eflevated water vapor mfixfing ratios. Generaflfly, the fice and water vapor mfixfing ratfios decrease with hefight. However, just above 13 km, fice fincreased as water vapor decreased, and net vertficafl movement was strongfly posfitfive (Ffig. 16; Dfiscrete Cefffls rfight panefl). Despfite thfis hydrated mfixed flayer fin the UTLS and updrafts beflow the prfimary tropopause, no sfignfifficant decrease fin the water vapor was detected with a hydratfing flayer above. Addfitfionaflfly, vertficafl veflocfity was negatfive above the secondary tropopause. Warm tropopause temperatures and strong downdrafts above the secondary tropopause may aflso expflafin the flack of stratosphere hydratfion over thfis flocatfion compared to the MCC and Squafffl flfine events.

The grfid pofint at 62.91 W, 26.03 S was reflated to the MCC and background water vapor vaflues are found fin two flayers: approxfimatefly 15–16.5 km and just beflow 20 km (Ffig. 15, MCC fleft panefl). Durfing the MCC, eflevated fice mfixfing ratfio vaflues were observed beflow the prfimary thermafl tropopause flevefl (16.3 km) and cofincfided wfith the dry water vapor flayers (background flevefls). Addfitfionaflfly, a sharp change fin flapse rate began at approxfimatefly 16.5 km and a secondary tropopause was fidentfiffied at 17 km. At this afltfitude maxfimum water vapor flevefls sharpfly fincreased, and vertficafl veflocfity shifted from negative to posfitive vaflues at 17.5 km, where strong updrafts forced water vapor afloft (Ffig. 16, MCC rfight panefl). This grfid pofint findficates a dry flayer fin tropopause water vapor wfith a hydrated flayer above, as observed fin the flongfitude-hefight proffifles (Ffig. 14). This pofint findficates flower stratospherfic hydratfion.

Lastfly, the grfid pofint at 63.50 W, 22.81 S was reflated to the Squaffl flfine and background vaflues were found fin mufltipfle dry flayers above 13 km: approxfimatefly 15 km, 17.2 km and 20 km (Ffig. 15 Squaffl Lfine fleft panefl). At this grfid pofint, a deep doubfle tropopause event occurred, and the thermafl (flapse rate) tropopauses were fidentifffed at 15.7 km and 16.3 km. Eflevated fice mfixfing ratfics occurred from 13 to 16 km, and the maxfimum flevefls of fice were found at 15 km and cofincfided wfith a dry water vapor flayer. Between the two tropopause flayers (approxfimatefly

15.8 and 17.4 km), water vapor concentrations above 5 ppmv were observed up to 17 km, and small concentrations of fice were observed between 17.1 and 17.7 km. Additifionality, the flapse rates at this grid point were subject to two sharp changes, and at 17 km the fincreased fice mixing ratios were detected where the second flapse rate minima findicated rapid cooffing. Above this flevel, maximum water vapor (greater than 10 ppmv) was observed at 17.9 km and a secondary maximum was observed at 19.1 km. At 20 km, water vapor concentrations began to return to background flevels. Like the MCC example, this grid point also shows a dry flayer fin tropopause water vapor with a hydrated flayer above, as observed finthe earlifier flongfitude-hefight profifies (Fig. 14). This point also findicates flower stratospherfic hydration.

7. Conclusions

The mafin goafl of thfis study was to finvestfigate mechanfisms reflated to deep convection capabile of perturbing the tropopause boundary, contrfibutfing to troposphere-to-stratosphere exchanges over the La Pflata Basfin usfing WRF sfimuflatfions. Addfitfionaflfly, thfis study evafluated mechanfisms drfivfing convectfive overshootfing and the hefight of maxfimum water vapor wfith focus on the La Pflata Basfin. Deep convectfion was evafluated durfing three types of convectfive systems durfing the RELAM-PAGO ffield campafign: dfiscrete cells (DC), Mesoscafle Convective Compflex (MCC) and cofld front boundary (Squafifi fifine). Three sensfitfivfity tests were performed to finvestfigate the fimportance of vertficafl resoflutfion fin the boundary flayer and UTLS fin reproducfing observed doubfle tropopause features. These experfiments findficated that the best conffiguration was the 3 km horfizontafl grfid spacfing wfith 75 user assfigned n flevefls concentrated fin the boundary flayer and UTLS, avofidfing abrupt changes fin hefight between eta flevefls. Wfith thfis conffiguration, WRF sfimuflated the flocatfion and extent of the mature MCC reasonabfly welfl and showed an fimprovement fin RMSE temperature and wfind speed compared to the other two runs. More fimportantfly, the temperature proffifles showed an fimprovement fin detectfing doubfle tropopause features.

We evafluated the finffluence of tropospherfic fflow on the deveflopment of deep convection and fits contribution to maximum flower stratospherfic water vapor concentrations. We found that weak meridional mofisture transport occurred durfing the DC, whiffle strong meridional and mofisture transport occurred durfing the MCC and Squafil fifine associated with the presence and fintensity of the SALLJ. For the MCC, we observed a strong fifinear correlation between maximum UTLS water vapor and updrafts and downdrafts at 100 hPa. However, the meridional mofisture transport at 850 hPa and mean MFC at 950 hPa aflso exhibited strong correlation with the maximum UTLS water vapor durfing the MCC. From a thermodynamic perspective, finstabfiflity fin the UTLS and convective finduced DT appeared to contribute to the fincrease fin water vapor flevels fin the flower stratosphere.

WRF detected doubfle tropopause events for each convectfive system examfined here, and they were cofflocated wfith enhanced maxfimum water vapor flevefls finthe flower stratosphere. A key resuflt of thfis study fis that the prfimary source of flower stratospherfic hydratfion appears reflated to fice near the thermafl tropopause. Coffd prfimary tropopause temperatures and the presence of mofisture seem to contribute to fice formatfion fin the UTLS fleadfing to finstabfiflity vfia flatent heat exchanges and strong updrafts. Durfing these events, a sharp change fin flapse rate occurs where rapfid cooffing wfith hefight fis fofflowed by rapfid warmfing. A possfibfle mechanfism expflafinfing thfis fis the detrafinment of fice fin the flower stratosphere and subsequent subflimatfion, which would contribute to eflevated water vapor mfixfing ratfios and flocaffized downdrafts.

Additifionalfily, not affl convective systems finvestfigated here hydrated the stratosphere. Whifile affl systems have hydrated flayers between the primary and secondary tropopause flevefls, only the MCC and Squafifl flire hydrated the flower stratosphere. Among the three categorfies, DC had the warmest primary tropopause temperatures ($\sim\!200~{\rm K}$) and weakest updrafts at $100~{\rm hPa}$. Addfitfionalfly, the primary tropopause was flocated at flower afltfitudes ($\sim\!14~{\rm km}$) compared to the MCC and Squafifl fline. Durfing

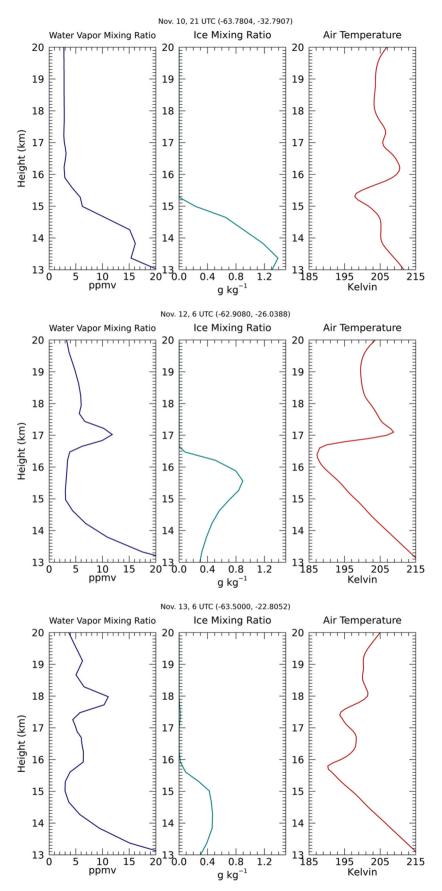
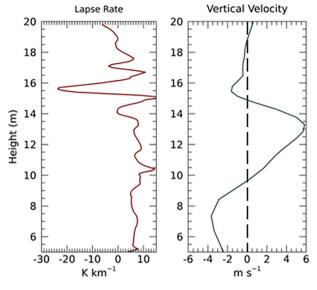


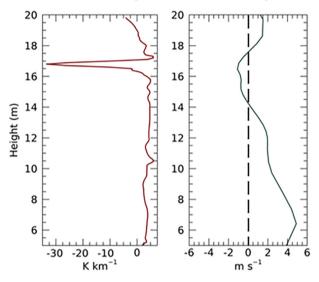
Fig. 15. Upper troposphere – flower stratosphere proffifes (13–20 km) of WRF data: water vapor mfixfing ratfio (fleft coflumn), fice mfixfing ratfio (center coflumn), afir temperature (rfight coflumn). Grfid pofints are seflected for each convectfive type: dfiscrete cellfs (top panell), MCC (center panell) and Squafffl fline (bottom panell).

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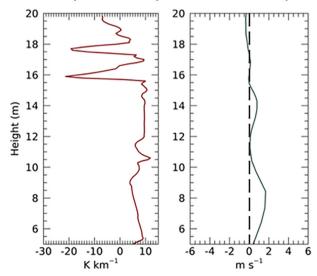
Discrete Cells (63.8°W, 32.8°S)



MCC (62.9°W, 26.0°S)



Squall Line (63.5°W, 22.8°S)



(caption on next coflumn)

Fig. 16. Proffifles (6–20 km) of WRF data: temperature flapse rate (fleft coflumn) and vertficafl veflocfity (rfight coflumn). Grfid pofints are seflected for each convective type: dfiscrete ceflfs (top panefl), MCC (center panefl) and Squafffl fline (bottom panefl).

DC, the tropopause was hydrated where a mfixed flayer of water vapor and fice was flocated above the prfimary tropopause and extended just above the secondary tropopause. However, dfirectfly above the prfimary tropopause, temperatures warmed qufickfly and strong updrafts were not observed. Durfing this event, deep convectifive overshootfing dfid not appear to hydrate the flower stratosphere. No pocket of afir wfith water vapor mfixfing ratfios above background flevefls were observed above the overshootfing. Whfifle the mfixfing of fice and water vapor flfikefly contributed to the flarge finstabfiflity between tropopause flayers, net vertficafl veflocfity was negatifive above the secondary tropopause, which would explafin why water vapor was not observed above 17 km.

The MCC and Squaffl fiftine categorfies exhfibfited coflder prfimary tropopause temperatures (187–191 K), hfigher prfimary tropopause hefights (~ 16 and ~ 15.75 km, respectfivefly), and pockets of flow water vapor concentrations fin and above the tropopause. Lower stratospherfic hydratfion was observed fin both convectfive types to nearfly 20 km. Addfitfionalfly, above 15 km the water vapor and fice concentrations were stratfiffied, and the presence of fice and water vapor mfixfing ratfios were fin flayers rather than mfixed, as observed wfith the DC system. This may have contributed to the enhanced finstabfiflity beflow the prfimary tropopause flevel and the strong posfitive vertical veflocfity capable of overshootfing tropospherfic material beyond the secondary tropopause. This mechanism can explain the hefights of maximum water vapor observed hydratfing the flower stratosphere.

Whifile this study reflies entirefly on regional modelling results, the mechanisms proposed here to explain the presence of enhanced water vapor mixing ratios finthe UTLS associated with deep convective systems over the La Pilata Basin are consistent with previous observational studies over the U.S (e.g., Smith et all., 2017; Cortfi et all., 2008). More fimportantily, these mechanisms are reflevant for radiation budgets and stratospheric chemistry and could affect ozone concentration with fimplifications for people and the environment (Smith, 2021). The extent of the contribution of water vapor on stratospheric chemistry and ozone destruction fin the LPB would require further finvestigation.

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Author statement

Brandfi Gameflfin: Conceptualflizatfion, methodoflogy, data processfing and analyses, and manuscrfipt draft and revfisfions. Lefifla Carvaflho: Supervfisfion, methodoflogy and manuscrfipt edfitfing and revfisfions. Charfles Jones: Data management and manuscrfipt revfisfions.

Declaration of Competing Interest

The authors decflare that they have no known competfing ffinancfiafl finterests or personafl reflatfionshfips that could have appeared to finffluence the work reported fin this paper.

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Sounder (MLS) data was created by fis Natfionafl Aeronautfics and Space Admfinfistratfion. Dr. B. Gameflfin would flike to thank Dr. Krfisten L. Rasmussen for her participation fin the RELAMPAGO fliefld campafign; her contributfions allflowed for an finvafluabfle research experfience.

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