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# DART: improvement of thermal infrared radiative transfer

# 2 modelling for simulating top of atmosphere radiance

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#### Abstract

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13 Land surface temperature (LST) is increasingly needed for studying the functioning of the 14 Earth's surface at local to global scale. Radiative transfer (RT) models that simulate top of 15 atmosphere (TOA) radiance are essential tools to derive accurate LST from thermal infrared 16 (TIR) signals of Earth observation (EO) satellites. DART (Discrete Anisotropic Radiative 17 Transfer) is one of the most accurate and comprehensive three-dimensional models that 18 simulate RT in the Earth-atmosphere system. Up to version 5.7.3, the mean absolute error 19 (MAE) of DART atmospheric TIR radiance of six standard atmospheres (USSTD76, 20 TROPICAL, MIDDLATSUM, MIDDLATWIN, SUBARCSUM, SUBARCWIN) over 3.5 µm 21 - 20 µm was 3.1 K compared to the reference atmospheric RT model MODTRAN, which is 22 much larger than the 1 K accuracy needed by most LST applications. Also, the radiance error 23 reached 2.6 K for some TIR bands whereas the noise equivalent differential temperature (NeDT) of satellite TIR sensor is usually less than 0.4 K. Recently, the DART atmospheric RT modelling was greatly improved by (1) introducing the equivalent absorption cross-section of five most absorbing gases (H<sub>2</sub>O, CO<sub>2</sub>, O<sub>3</sub>, CH<sub>4</sub>, N<sub>2</sub>O), and (2) implementing a double-layer thermal emission method. The MAE of DART atmospheric TIR radiance of six standard atmospheres and actual atmospheres over France and the Mediterranean Sea is now better than 1.0 K. The band radiance error is less than 0.2 K in the EO satellite TIR bands. DART is still accurate if the temperature profiles of standard atmospheres are offset by less than 6 K and if the viewing zenith angle is less than 50°. In short, the improved DART meets the requirements of both LST applications, and present and future TIR EO satellite missions. It is already available to scientists (https://dart.omp.eu).

- Keywords: DART, radiative transfer, atmosphere, thermal infrared, absorption cross-section,
- 36 MODTRAN

## 1. Introduction

Land surface temperature (LST) has a wide range of applications in different fields: evapotranspiration, soil moisture, precision agriculture, urban climate, river environments, oceanography, etc. (Dugdale, 2016; Khanal et al., 2017; Kilpatrick et al., 2015; Voogt and Oke, 2003; Wang et al., 2006; Wang and Qu, 2009). Due to its high temporal resolution, broad coverage and low cost, thermal infrared (TIR) remote sensing is an ideal tool to measure LST (Li et al., 2013). Therefore, an increasing number of space missions embark sensors with TIR bands. For example, the Trishna mission of French Space Agency (CNES) and Indian Space Research Organization (ISRO), to be launched in 2024-2025, will embark a sensor that has four TIR bands with noise equivalent differential temperature (NeDT) of 0.3 K at 300 K (Lagouarde 

et al., 2018). The sea and land surface temperature radiometer on board the European Space Agency (ESA) Sentinel 3 satellite has three TIR bands with NeDT of 0.05 K at 270 K (Donlon et al., 2012). The National Aeronautics and Space Administration (NASA) Landsat 8 satellite has a TIR sensor with NeDT of 0.4 K at 300 K (Irons et al., 2012). Landsat 9 satellite, due to be launched on 2021, should embark a TIR sensor similar to the Landsat 8 TIR sensor (McCorkel et al., 2018).

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Most LST applications require accuracy less than 1 K (Sobrino et al., 2016). Although the sensibility (NeDT) of most satellite TIR sensors is less than 0.4 K, the LST derived from remotely sensed data is usually less accurate, mainly due to atmospheric conditions, topography, land surface heterogeneity, and directional effects (Bento et al., 2017; Bonafoni, 2016; Ermida et al., 2018; He et al., 2019; Price, 1983; Vermote et al., 2002). Therefore, there is a need to better link LST and observations from satellite TIR sensors. Physical models that accurately simulate TIR radiative transfer (RT) in the Earth-atmosphere system are essential tools. However, most RT models are either for the atmosphere (e.g., 4A/OP, MODTRAN, LBLRTM, RFM, ARTS) or for the Earth surfaces (e.g., Rayspread, RAPID3, FLiES, SAIL) (Berk et al., 2015; Buehler et al., 2018; Clough et al., 2005; Huang, 2018; Kobayashi and Iwabuchi, 2008; Scott, 1974; Verhoef, 1984; Vincent and Dudhia, 2017; Widlowski et al., 2006). DART (Discrete Anisotropic Radiative Transfer) is one of the few models that simulate RT in the Earth-atmosphere system. Its Earth surface RT modelling accuracy in the short and long waves was already verified in the four phases of the RAdiative transfer Model Intercomparison (RAMI) project (Widlowski et al., 2015, 2013, 2007) and in experiments (Guillevic et al., 2003, 2013). Its atmospheric short wave RT modelling was validated with the reference atmospheric RT model MODTRAN-5 (Gastellu-Etchegorry et al., 2017; Grau and Gastellu-Etchegorry, 2013).

However, as presented below, its atmospheric RT modelling in the TIR region did not meet the requirements of LST applications and TIR Earth observation (EO) satellite missions.

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DART simulates atmosphere in three altitude regions: (1) the bottom atmosphere inside the Earth scene voxel matrix, (2) the mid-atmosphere made of voxels of any size, and (3) the high atmosphere made of layers. Voxels in the mid-atmosphere allows DART to simulate the spatial heterogeneity of the atmosphere backscattering. Any atmosphere layer is homogeneously filled with gasses, aerosols and/or clouds that have specific physical (i.e., temperature, pressure, density) and spectral (i.e., absorption/scattering extinction coefficient, scattering phase function) properties. The atmospheric RT modelling relies on the spectral application of Beer's law and band mean optical properties (Gastellu-Etchegorry et al., 2004). The extinction coefficient at each layer is calculated so that the use of Beer's law gives the same vertical atmospheric transmittance as MODTRAN, assuming that the cross-section of the gases is independent of pressure and temperature. Although initial methodology simulates accurate atmospheric radiance in short waves, the TIR radiance could differ significantly from MODTRAN. For example, in [3.5  $\mu$ m - 20  $\mu$ m] region, its mean absolute error (MAE) of top of atmosphere (TOA) atmospheric TIR brightness temperature (BT) of the USSTD76 atmosphere was 3.1 K, which is much larger than LST application requirements. This is due to three approximations: (1) gas absorption cross-section is independent of pressure and temperature; (2) gas absorption transmittance is computed with Beer's law and band mean optical properties; (3) the method that computes layer thermal emission is only suited to optically thin atmosphere.

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Actually, the gas absorption cross-section varies with pressure and temperature due to the Doppler and Lorentz broadening. Many atmospheric RT models, including MODTRAN, compute the pressure- and temperature-dependent gas absorption cross-section lines based on

the high resolution (spectral resolution up to 0.001 cm<sup>-1</sup>) spectroscopic databases, such as HITRAN and GEISA (Jacquinet-Husson et al., 2016; Rothman et al., 2009). These models compute the absorption transmittance with either the exact gas absorption cross-section lines (line-by-line models like 4A/OP) or the statistically determined gas absorption cross-section lines (band models like MODTRAN). Therefore, their absorption transmittance is usually more accurate than the absorption transmittance calculated with Beer's law and band mean absorption cross-sections. In addition, the thermal emission of an atmosphere layer computed with the layer mean temperature is incorrect if the layer is optically thick. MODTRAN improved it by computing the layer thermal emission with the "linear-in-optical depth" method (Clough et al., 1992).

This paper presents two major improvements of DART TIR RT modelling in order to meet the requirements of LST applications and TIR EO satellite missions: (1) introduction of the pressure- and temperature-dependent equivalent absorption cross-section of five most absorbing gases (H<sub>2</sub>O, CO<sub>2</sub>, O<sub>3</sub>, CH<sub>4</sub>, N<sub>2</sub>O); (2) implementation of an efficient double-layer thermal emission method that is adapted to most atmospheric conditions. Limits of these two improvements are also discussed. Then, the improved DART is compared with MODTRAN-5 using standard atmosphere profiles and the actual atmosphere profiles from ECMWF reanalysis dataset.

#### 2. DART model

DART (https://dart.omp.eu) has been developed at CESBIO since 1992 (Gastellu-Etchegorry et al., 2017, 1996). It is one of the most accurate and comprehensive 3D RT models for the remote sensing community. It simulates the radiative budget, bi-directional reflectance factor

(BRF) and images at any altitude and along any viewing direction for 3D natural and urban scenes, with topography and atmosphere (Figure 1), from visible to thermal infrared region. For that, it uses an iterative discrete ordinate method (DOM) that tracks radiation fluxes along a finite number of discrete directions. It also simulates terrestrial and aero-spatial LiDAR signal (point cloud, waveform, photon counting) with an approach that combines Monte Carlo method and DOM.

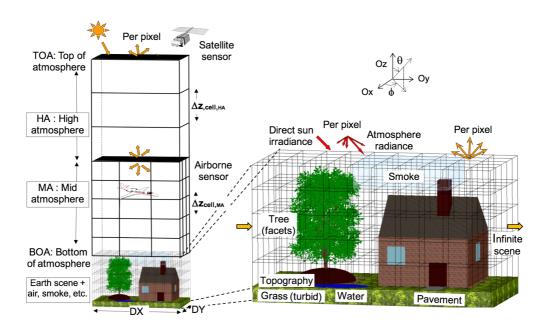


Figure 1. DART 3D mock-up and voxel matrix. Atmosphere is separated in three altitude regions: high atmosphere (HA) made of layers, mid-atmosphere (MA) made of voxels of any size, and bottom atmosphere (BA) in the Earth scene. Earth scene elements are made of facets (triangles), and/or fluid and turbid vegetation voxels. The voxel matrix is introduced to optimize ray tracing.

# 2.1 DART atmosphere profiles

DART simulates the atmosphere as three superimposed volumes: (1) bottom atmosphere (BA) inside the Earth scene voxel matrix, (2) mid-atmosphere (MA) made of voxels, and (3) high 6

atmosphere (HA) made of layers (Figure 1). The geometry of MA and HA (i.e., number of layers, layer thickness, voxel size) is either user-defined or analytically computed. The geometry of BA is the same as the Earth scene. The DART atmosphere SQL database stores vertical profiles of atmospheric constituents (i.e., temperature  $T_{DB}(z)$ , pressure  $P_{DB}(z)$ , number density  $N_{m_i,DB}(z)$  per gas  $m_i$ , relative density  $\rho_{m,DB}^s(z)$  of scattering gases to air at standard temperature and pressure and aerosol extinction coefficient profile  $\alpha_{p,DB}^e(z)$  at 550 nm). These profiles are stored at 36 altitude levels (0 to 25 km with 1 km interval, 30 to 60 km with 5 km interval and 3 levels at 70 km, 80 km and 100 km) for: - six standard atmospheres (Anderson et al., 1986): (1) TROPICAL: Tropical (15°N annual average), (2) MIDLATSUM: Mid-Latitude Summer (45°N July), (3) MIDLATWIN: Mid-Latitude Winter (45°N January), (4) SUBARCSUM: Sub-Arctic Summer (60°N July), (5)

SUBARCWIN: Sub-Arctic Winter (60°N January), and (6) USSTD76: US Standard 1976.

- five aerosol models (Shettle and Fenn, 1979): (1) Rural, (2) Urban, (3) Maritime, (4) Tropospheric and (5) Fog.

The DART atmosphere SQL database also stores the spectral optical properties of atmospheric constituents (i.e., gas: vertical absorption transmittance  $t^a_{m_i,DB}(\lambda)$  per gas  $m_i$ , vertical scattering transmittance  $t^s_{m,DB}(\lambda)$ ; aerosol: vertical optical depth  $\tau_{p,DB}(\lambda)$ , single scattering albedo  $\omega_{p,DB}(\lambda)$ , asymmetry factors of double Henyey-Greenstein phase function) from 10 to 40000 cm<sup>-1</sup> with a spectral resolution of 1 cm<sup>-1</sup>. They were derived from MODTRAN simulations and LOWTRAN source code for the six standard atmospheres and for the five aerosol models per standard atmosphere. The optical properties and vertical profiles of gases and aerosols derived from reanalysis datasets (e.g., ECMWF reanalysis: https://www.ecmwf.int) and measurements (e.g., Aeronet: <a href="https://aeronet.gsfc.nasa.gov">https://aeronet.gsfc.nasa.gov</a>) can also be imported into the DART atmosphere database.

The atmosphere properties at any altitude z are interpolated by the multi-quadric RBF (Radial Basis Function) (Press et al., 2007) using vertical profiles and optical properties in the SQL database. The band (central wavelength  $\lambda$ , bandwidth  $\Delta\lambda$ ) mean optical properties (*i.e.*, vertical absorption transmittance  $t_{m_i}^a(\lambda)$  of each gas  $m_i$ , gas vertical scattering transmittance  $t_m^s(\lambda)$ , aerosol vertical optical depth  $\tau_p(\lambda)$ ) are computed (trapezoidal integration) using the database spectral vertical transmittance  $t_{m_i,DB}^a(\lambda')$ ,  $t_{m,DB}^s(\lambda')$  and optical depth  $\tau_{p,DB}(\lambda')$  at 1 cm<sup>-1</sup> spectral resolution in the spectral bin  $\Delta\lambda$ :

$$t_{m_{i}}^{a}(\lambda) = \frac{\int_{\lambda-\Delta\lambda/2}^{\lambda+\Delta\lambda/2} t_{m_{i},DB}^{a}(\lambda') d\lambda'}{\Delta\lambda}, \ t_{m}^{s}(\lambda) = \frac{\int_{\lambda-\Delta\lambda/2}^{\lambda+\Delta\lambda/2} t_{m,DB}^{s}(\lambda') d\lambda'}{\Delta\lambda}$$

$$\tau_{p}(\lambda) = \frac{\int_{\lambda-\Delta\lambda/2}^{\lambda+\Delta\lambda/2} \tau_{p,DB}(\lambda') d\lambda'}{\Delta\lambda}$$
(1)

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In DART flux tracking mode, the extinction coefficient  $\alpha$  (i.e., total  $\alpha^e$ , absorption  $\alpha^a$  and scattering  $\alpha^s$  extinction coefficient) are constant values per layer j such that their use with Beer's law gives the band vertical transmittance and optical depth computed in Eq. (1).

$$\alpha_{j,m_{i}}^{a}(\lambda) = \frac{-\ln\left(t_{m_{i}}^{a}(\lambda)\right)}{z_{j} - z_{j-1}} \cdot \frac{\int_{z_{j-1}}^{z_{j}} \sigma_{m_{i}}^{a}(\lambda) \cdot N_{m_{i},DB}(z)dz}{\int_{0}^{\infty} \sigma_{m_{i}}^{a}(\lambda) \cdot N_{m_{i},DB}(z)dz}$$

$$\alpha_{j,m}^{s}(\lambda) = \frac{-\ln\left(t_{m}^{s}(\lambda)\right)}{z_{j} - z_{j-1}} \cdot \frac{\int_{z_{j-1}}^{z_{j}} \sigma_{m}^{s}(\lambda) \cdot N_{m}^{s}(z)dz}{\int_{0}^{\infty} \sigma_{m}^{s}(\lambda) \cdot N_{m}^{s}(z)dz} = \frac{-\ln\left(t_{m}^{s}(\lambda)\right)}{z_{j} - z_{j-1}} \cdot \frac{\int_{z_{j-1}}^{z_{j}} \rho_{m,DB}^{s}(z)dz}{\int_{0}^{\infty} \rho_{m,DB}^{s}(z)dz}$$

$$\alpha_{j,p}^{e}(\lambda) = \frac{\tau_{p,DB}(\lambda)}{z_{j} - z_{j-1}} \cdot \frac{\int_{z_{j-1}}^{z_{j}} \alpha_{p,DB}^{e}(z)dz}{\int_{0}^{\infty} \alpha_{p,DB}^{e}(z)dz}$$
(2)

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The Newton-Cotes integration method is used in Eq. (2) with 10 interpolated equal-distance values per layer (Abramowitz and Stegun, 1948) assuming that the absorption cross-section 8

 $\sigma_{m_i}^a(\lambda)$  of gas  $m_i$  only depends on wavelength. The gas scattering cross-section  $\sigma_m^s(\lambda)$  only depends on wavelength and gas composition (Bodhaine et al., 1999). Therefore,  $\sigma_m^s(\lambda) \cdot N_m^s(z)$ , with  $N_m^s(z)$  being the number density of scattering gases at altitude z, is proportional to the relative density of scattering gases  $\rho_{m,DB}^s(z)$ .

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Then, the total gas extinction coefficient  $\alpha_{j,m}^e(\lambda)$ , aerosol absorption  $\alpha_{j,p}^a(\lambda)$  and scattering  $\alpha_{j,p}^s(\lambda)$  extinction coefficient and total extinction coefficient  $\alpha_j^e(\lambda)$  are computed per layer:

$$\alpha_{j,m}^{e}(\lambda) = \alpha_{j,m}^{a}(\lambda) + \alpha_{j,m}^{s}(\lambda), \alpha_{j,m}^{a}(\lambda) = \sum_{m_{i}} \alpha_{j,m_{i}}^{a}(\lambda)$$

$$\alpha_{j,p}^{a}(\lambda) = \alpha_{j,p}^{e}(\lambda) \cdot \left(1 - \omega_{p,DB}(\lambda)\right), \alpha_{j,p}^{s}(\lambda) = \alpha_{j,p}^{e}(\lambda) \cdot \omega_{p,DB}(\lambda)$$

$$\alpha_{i}^{e}(\lambda) = \alpha_{i,m}^{e}(\lambda) + \alpha_{i,p}^{e}(\lambda)$$

$$(3)$$

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188 As explained in section 4, in order to improve the modelling of thermal emission, we adapted 189 the continuous optical depth profiles per atmosphere layer computed in the DART LiDAR mode (Gastellu-Etchegorry et al., 2015). Hence,  $\alpha_j^e(\lambda, h)$  and  $\tau_j(\lambda, h) = \int_0^{\Delta z_j} \alpha_j^e(\lambda, h) dh$  are 190 atmosphere 191 continuous functions layer defined per as  $\tau_i(\lambda, h) = A_i(\lambda) \cdot h^3 + B_i(\lambda) \cdot h^2 + C_i(\lambda) \cdot h + D_i(\lambda)$  and  $\alpha_i^e(\lambda, h) = -3A_i(\lambda) \cdot h^2 - 2B_i(\lambda) \cdot h - C_i(\lambda)$ , 192 where h is the relative altitude in layer j, with h=0 at the bottom of layer j and  $h=\Delta z_i$  at the top 193 of layer j. The verification of the four equalities  $\tau(\lambda, 0) = \Delta \tau_j(\lambda)$ ,  $\tau(\lambda, \Delta z_j) = 0$ , 194  $\alpha_j^e(\lambda, 0) = \alpha_{z_{j-1}}^e(\lambda), \ \alpha_j^e(\lambda, \Delta z_j) = \alpha_{z_j}^e(\lambda)$  derives the coefficients  $A_j(\lambda), B_j(\lambda), C_j(\lambda)$  and  $D_j(\lambda)$ 195 196 (Eq. (4)).

$$A_{j}(\lambda) = \frac{2\Delta\tau_{j}(\lambda) - \left(\alpha_{z_{j-1}}^{e}(\lambda) + \alpha_{z_{j}}^{e}(\lambda)\right)\Delta z_{j}}{\Delta z_{j}^{3}}, B_{j}(\lambda) = \frac{-3A_{j}(\lambda)\Delta z_{j}^{2} + \alpha_{z_{j-1}}^{e}(\lambda) - \alpha_{z_{j}}^{e}(\lambda)}{2\Delta z_{j}}$$
(4)

$$C_j(\lambda) = -\alpha_{z_{j-1}}^e(\lambda), D_j(\lambda) = \Delta \tau_j(\lambda)$$

layer 
$$j$$

$$\Delta z_{j}$$

$$h = \Delta z_{j}, \tau = 0, \alpha = \alpha_{z_{j}}^{e}$$

$$h = 0, \tau = \Delta \tau_{j}, \alpha = \alpha_{z_{j-1}}^{e}$$

Figure 2. DART horizontally homogeneous atmosphere layer with layer thickness  $\Delta z_j$ . The upper and lower boundary parameters are marked.

# 2.2 Layer thermal emission

Thermal emitted vector source (Eq. (5)) of a DART atmosphere layer j (horizontal surface  $\Delta S$ , thickness  $\Delta z_j$ ) per direction vector  $\Omega(\Delta\Omega)$  (zenith angle  $\theta$ , azimuth angle  $\varphi$ ) is computed using layer mean temperature  $T_j$  and two optical properties: single scattering albedo  $\omega_j(\lambda) = \frac{\alpha_j^s(\lambda)}{\alpha_j^e(\lambda)}$  and extinction coefficient  $\alpha_j^e(\lambda) = \alpha_j^a(\lambda) + \alpha_j^s(\lambda)$ , with  $\alpha_j^a(\lambda) = \alpha_{j,m}^a(\lambda) + \alpha_{j,p}^a(\lambda)$  the total absorption extinction coefficient and  $\alpha_j^s(\lambda) = \alpha_{j,m}^s(\lambda) + \alpha_{j,p}^s(\lambda)$  the total scattering extinction coefficient.

$$W_{j}(\Omega,\lambda) = \int_{0}^{\Delta z_{j}} L_{B}(T_{j},\lambda) \cdot \alpha_{j}^{a}(\lambda) \cdot \Delta S \cdot \Delta \Omega \cdot e^{-\int_{z}^{\Delta z_{j}} \alpha_{j}^{e}(\lambda) \frac{dz}{\mu}} dz$$

$$= \left(1 - \omega_{j}(\lambda)\right) \cdot L_{B}(T_{j},\lambda) \cdot \left[1 - e^{-\frac{\Delta \tau_{j}}{\mu}}\right] \cdot \mu \cdot \Delta S \cdot \Delta \Omega$$
(5)

where  $L_B(T_j, \lambda)$  (unit:  $W/m^2/sr/\mu m$ ) is the spectrally averaged Planck function at layer mean temperature  $T_i$ .  $\Delta \tau_i$  is the optical depth of the atmosphere layer j.  $\mu = \cos(\theta)$ .

#### 2.3 RT in the Earth-atmosphere system

RT modelling in the Earth-atmosphere system involves five major steps (Figure 3): (1) Sun illumination and atmosphere thermal emission; (2) Earth surface RT; (3) Earth-atmosphere radiative coupling and atmosphere backscattering; (4) Earth surface RT of the backscattered radiation; (5) Transfer of bottom of atmosphere (BOA) radiation to any altitude, including TOA (Grau and Gastellu-Etchegorry, 2013).

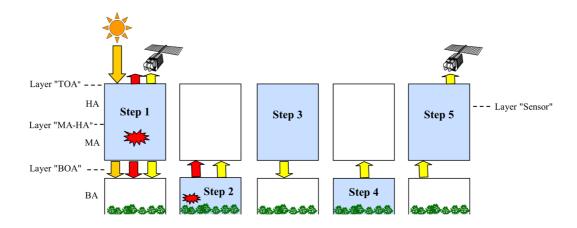


Figure 3. Major steps for modelling the RT in the Earth-atmosphere system. Red colour indicates thermal emission (steps 1 and 2), orange colour indicates solar incident radiation, and yellow colour indicates thermal and/or solar radiation that is scattered.

#### 3. Initial DART atmospheric RT modelling accuracy

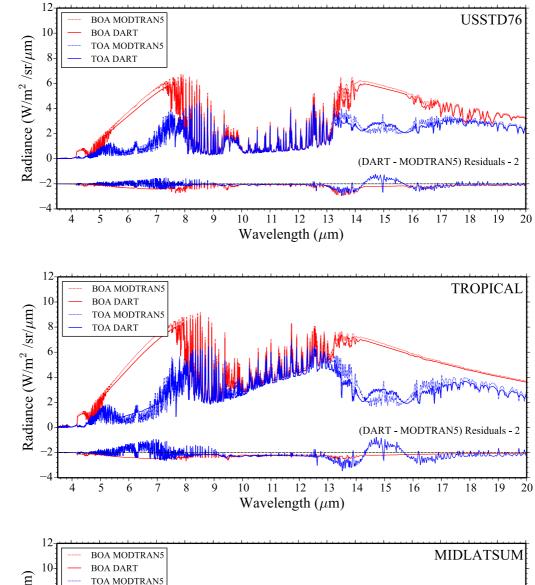
DART atmospheric RT modelling accuracy was assessed using MODTRAN-5 since it is one of the most accurate atmospheric RT models, with transmittance accuracy  $\pm 0.005$ , radiance accuracy  $\pm 2\%$  and thermal brightness temperature (BT) accuracy better than 1 K (Berk et al., 2008, 2005, 1987). In the short waves (*i.e.*, [0.4  $\mu$ m, 3.0  $\mu$ m]), with ground albedo 0.5, TOA nadir reflectance absolute difference between DART and MODTRAN-5 was less than 0.004,

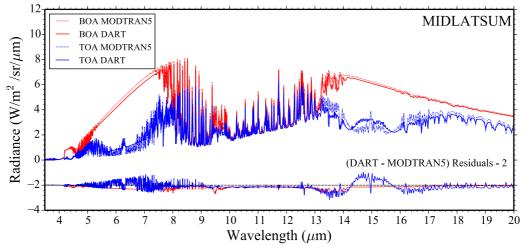
which meets MODTRAN-5 accuracy (Gastellu-Etchegorry et al., 2017; Grau and Gastellu-Etchegorry, 2013). Here, the comparison is extended to TIR region from 3.5  $\mu$ m to 20  $\mu$ m, using DART version 5.7.3, hereafter called "initial DART". To analyse pure gas atmosphere emission, MODTRAN-5 and DART were run with thermal emission mode, no aerosol, the Earth skin temperature is 0 K, surface albedo is 0, and the atmosphere layer depth is equal to 1 km from 0 to 25 km, and 5 km from 30 km to 100 km. Figure 4 shows DART and MODTRAN-5 TOA and BOA TIR radiance spectra and the residuals, for four standard atmospheres (USSTD76, TROPICAL, MIDLATSUM, SUBARCWIN). The mean absolute error (MAE) and mean absolute relative error (MARE) instead of the root-mean-square-error (RMSE) are used to quantify DART and MODTRAN-5 differences since they bring a more unambiguous information (Willmott and Matsuura, 2005). For a variable X(q) (e.g., BT, radiance) at band q and Q spectral bands:

$$MAE = \frac{1}{Q} \cdot \sum_{q=1}^{Q} |X_{DART}(q) - X_{MODTRAN5}(q)|$$

$$MARE = \frac{1}{Q} \cdot \sum_{q=1}^{Q} \frac{|X_{DART}(q) - X_{MODTRAN5}(q)|}{X_{MODTRAN5}(q)} \cdot 100 \%$$
(6)

Note that the error defined in Eq. (6) is relative to MODTRAN, one should take into account the accuracy of MODTRAN in practical application.





c)

a)

b)

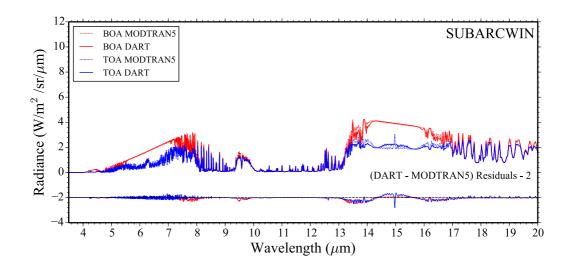


Figure 4. Initial DART and MODTRAN-5 TOA / BOA TIR radiance in [3.5  $\mu$ m, 20  $\mu$ m] region for USSTD76 (a), TROPICAL (b), MIDLATSUM (c) and SUBARCWIN (d) atmospheres. 1 cm<sup>-1</sup> spectral resolution. DART and MODTRAN-5 configurations are detailed in section 3.

Table 1 summarizes the "Initial DART - MODTRAN-5" MAEs for BT and MAREs for radiance, for six standard atmospheres. For most standard atmospheres, BT MAEs are larger than 2.0 K and 1.5 K for TOA and BOA radiance spectra, respectively. The maximal BT MAE

occur for the TROPICAL atmosphere at TOA level with Max (BT MAE) = 4.7 K.

Table 1. TOA and BOA BT MAE and radiance MARE of initial DART in [3.5  $\mu$ m, 20  $\mu$ m] region for six standard atmospheres. MODTRAN-5 results are the reference.

Atmosphere	BT I	MAE	Radiance	Radiance MARE		
	TOA (K)	BOA (K)	TOA (%)	BOA (%)		
USSTD76	3.1 K	2.7 K	12.6	8.6		
TROPICAL	4.7 K	2.4 K	18.9	6.8		
MIDLATSUM	3.8 K	2.1 K	15.0	6.1		

d)

MIDLATWIN	2.3 K	1.8 K	10.1	6.3
SUMARCSUM	2.9 K	2.3 K	11.5	7.1
SUMARCWIN	1.8 K	1.3 K	8.0	5.2
Average	3.1 K	2.1 K	12.7	6.7

DART and MODTRAN-5 TOA / BOA radiance values diverge more in absorbing spectral regions than in non-absorbing spectral regions. For example, Table 2 shows that very large BT differences, up to 7 K, occur in the four absorbing spectral regions: ABS1 ([3.5  $\mu$ m, 4.5  $\mu$ m]), ABS2 ([6  $\mu$ m, 7  $\mu$ m]), ABS3 ([9  $\mu$ m, 10  $\mu$ m]) and ABS4 ([14  $\mu$ m, 16  $\mu$ m]) for the USSTD76 atmosphere.

Table 2. TOA and BOA BT MAE and radiance MARE of initial DART in four TIR absorbing bands (ABS1, ABS2, ABS3, ABS4) for the USSTD76 atmosphere. MODTRAN-5 results are the reference.

Absorption	Central	Central BT MAE Bandwidth		Radiance	e MARE	
band	wavelength	Bandwidui	TOA (K)	BOA (K)	TOA (%)	BOA (%)
ABS1	4.0 μm	1.0 μm	2.0 K	1.7 K	12.7	8.3
ABS2	6.5 μm	$1.0~\mu\mathrm{m}$	5.4 K	3.0 K	25.1	7.9
ABS3	9.5 μm	$1.0~\mu\mathrm{m}$	2.2 K	3.5 K	7.7	11.0
ABS4	15.0 μm	2.0 μm	7.0 K	3.4 K	13.8	4.0

DART accuracy was also analysed in relation to three EO satellite missions (Trishna, Sentinel 3, Landsat 8). Table 3 shows the BT difference (DIFF) of their TIR bands, for the USSTD76 15

atmosphere. Band BTs are computed by inverting Planck function using band mean radiance and band central wavelength. The resulting DART BT DIFFs greatly exceed the satellite sensor sensitivity (Table 3) and also the accuracy usually required for LST applications (*i.e.*, 1 K).

Three already mentioned DART approximations can explain these large differences: (1) Neglect of gas absorption cross-section dependence on pressure and temperature. Indeed, due to the Doppler and Lorentz broadening, absorption cross-sections vary with pressure and temperature, and consequently with altitude; (2) Transmittance computation with Beer's law and band mean optical properties. Indeed, Beer's law is less correct if the absorption cross-section varies strongly within the spectral bin; (3) Computation of layer thermal emission with the layer mean temperature  $T_j$ , which is only suited for optically thin layers. Therefore, with the objective that DART accuracy meets the requirements of TIR EO satellite missions and LST applications while using Beer's law, two major modelling improvements have been made: (1) account of the vertical variation of gas absorption cross-section, and (2) accurate computation of thermal emission per layer.

Table 3. TOA BT DIFF of initial DART in the TIR bands of three EO satellite missions for the USSTD76 atmosphere. MODTRAN-5 results are the reference.

Satellite	Launch date	Organization	Central wavelength	Bandwidth	Sensitivity (NeDT)	DIFF
Trishna	Foreseen	CNES+ISRO	8.6 μm	0.35 μm	0.3 K@300 K	0.65 K
	2024-2025		9.1 μm	0.35 μm	0.3 K@300 K	1.57 K
			10.3 μm	$1.0~\mu\mathrm{m}$	0.3 K@300 K	2.60 K

		11.5 μm	$1.0~\mu\mathrm{m}$	0.3 K@300 K	1.50 K
2013	NASA	10.9 μm	0.6 μm	0.4 K@300 K	1.97 K
		12.0 μm	$1.0~\mu\mathrm{m}$	0.4 K@300 K	1.73 K
2016	ESA	$3.74~\mu\mathrm{m}$	$0.38~\mu\mathrm{m}$	0.08 K@270 K	0.10 K
		10.95 μm	$0.9~\mu\mathrm{m}$	0.05 K@270 K	1.88 K
		12.0 μm	$1.0~\mu\mathrm{m}$	0.05 K@270 K	1.73 K
			2013 NASA 10.9 μm 12.0 μm 2016 ESA 3.74 μm 10.95 μm	2013 NASA 10.9 μm 0.6 μm 12.0 μm 1.0 μm 2016 ESA 3.74 μm 0.38 μm 10.95 μm 0.9 μm	2013 NASA 10.9 μm 0.6 μm 0.4 K@300 K 12.0 μm 1.0 μm 0.4 K@300 K 2016 ESA 3.74 μm 0.38 μm 0.08 K@270 K 10.95 μm 0.9 μm 0.05 K@270 K

#### 4. Improvement to TIR RT modelling

# 4.1 Equivalent absorption cross-section database

## 4.1.1 Equivalent absorption cross-section

As stated above, the initial DART neglects the dependence of gas absorption cross-sections with pressure and temperature. We improved this situation by introducing vertical profiles of equivalent absorption cross-section  $\sigma_{m_i}^a(\lambda, z, \Delta L)$  (Eq. (7)) for five most absorbing gases (H<sub>2</sub>O, CO<sub>2</sub>, O<sub>3</sub>, CH<sub>4</sub>, N<sub>2</sub>O).  $\sigma_{m_i}^a$  is the exact band mean absorption cross-section if Beer's law is obeyed.

$$\sigma_{m_i}^a(\lambda, z, \Delta L) = \frac{-\ln\left(t_{m_i}^a(\lambda, z, \Delta L)\right)}{N_{m_i}(z) \cdot \Delta L}$$
(7)

with  $t_{m_i}^a(\lambda, z, \Delta L)$  the path absorption transmittance of gas  $m_i$  at altitude z, at wavelength  $\lambda$ , along path segment  $\Delta L$ .  $N_{m_i}(z)$  is the number density of gas  $m_i$  at altitude z.

To compute  $\sigma_{m_i}^a(\lambda, z, \Delta L)$  (Eq. (7)), MODTRAN 1 cm<sup>-1</sup> resolution absorption transmittances  $t_{m_i}^a(\lambda, z, \Delta L)$  were simulated per gas  $m_i$  (H<sub>2</sub>O, CO<sub>2</sub>, O<sub>3</sub>, CH<sub>4</sub>, N<sub>2</sub>O) for identical horizontal paths  $\Delta L$  at 36 altitudes z: 26 altitudes from 0 km up to 25 km with a step of 1 km, 7 altitudes from 25 km up to 60 km with a step of 5 km, and 3 altitudes at 70 km, 80 km and 100 km. The gas number density  $N_{m_i}(z)$  is derived from MODTRAN tape6 file (Berk et al., 2008).

Figure 5.a and Figure 5.c show the CO<sub>2</sub> vertical profiles of  $\sigma_{m_i}^a(\lambda, z, \Delta L)$  from 0 km altitude up to 25 km for 13.4  $\mu$ m and up to 15 km for 13.1  $\mu$ m, with  $\Delta L = 1$  km, 2 km, 5 km and 10 km.  $\sigma_{m_i}^a(\lambda, z, \Delta L)$  profiles depend on  $\Delta L$  if Beer's law is not obeyed (Figure 5.a) and do not depend on  $\Delta L$  if Beer's law is obeyed (Figure 5.c). Figure 5.b, d shows that the relative vertical distribution of equivalent absorption cross-section  $\sigma_{m_i}^{a(*)}(\lambda, z, \Delta L) = \frac{\sigma_{m_i}^a(\lambda, z, \Delta L)}{\sigma_{m_i}^a(\lambda, 0, \Delta L)}$  (profiles scaled by  $\sigma_{m_i}^a(\lambda, 0, \Delta L)$  at z = 0) is almost independent of  $\Delta L$ , even if Beer's law is not obeyed, with slightly variations depending on the absorption feature, temperature and pressure. It explains that DART TIR radiance computed with  $\sigma_{m_i}^a(\lambda, z, \Delta L)$  only slightly varies with  $\Delta L$ . Results in section 5 show that the optimal  $\Delta L$  is 7 km. Hereafter,  $\sigma_{m_i}^a(\lambda, z)$  stands for  $\sigma_{m_i}^a(\lambda, z, \Delta L) = 7$  km).

Note that  $\sigma_{m_i}^a(\lambda, z)$  is underestimated if the minus logarithm of total transmittance reaches the limit 100 in MODTRAN (*i.e.*, extreme absorbing bands). It can occur at low altitude. Then, the low atmosphere tends to behave as a black body, and the vertical distribution of absorption extinction coefficient within the low atmosphere has little impact on TIR radiance.

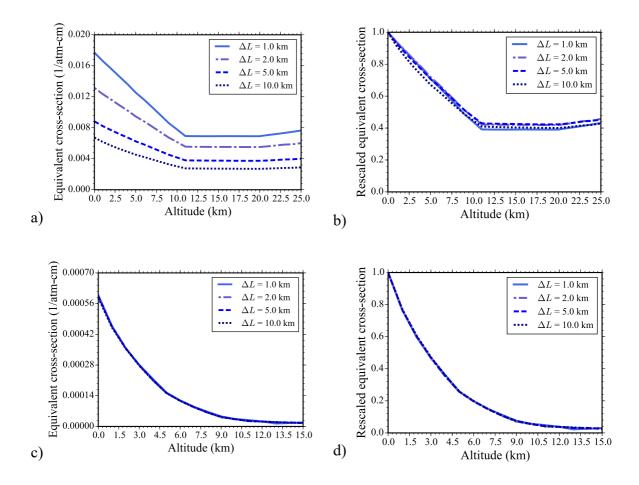


Figure 5. CO<sub>2</sub> equivalent absorption cross-section  $\sigma_{m_i}^a(\lambda,z,\Delta L)$  (a, c) and rescaled equivalent absorption cross-section  $\sigma_{m_i}^{a(*)}(\lambda,z,\Delta L)$  (b, d) at 13.4  $\mu$ m (a, b) and 13.1  $\mu$ m (c, d), in 1 cm<sup>-1</sup> spectral bin, for 4 identical horizontal paths ( $\Delta L = 1$  km, 2 km, 5 km, 10 km) at altitudes up to 25 km for 13.4  $\mu$ m and up to 15 km for 13.1  $\mu$ m, in the USSTD76 atmosphere.

4.1.2 Creation of SQL database

The equivalent absorption cross-section profiles  $\sigma_{m_i}^a(\lambda,z)$  were computed per gas  $m_i$  for the six standard atmospheres, from 10 to 3500 cm<sup>-1</sup> at 1 cm<sup>-1</sup> spectral resolution. To ease data access and management, they were stored in a SQL database per spectral band, per gas  $m_i$  and per standard atmosphere. Three criteria were used to select the spectral bands of interest: (1) wavelength larger than 3  $\mu$ m; (2) absorbing gases; (3) absorbing spectral regions.

The spectral region over 3  $\mu$ m is chosen because the vertical variation of absorption cross-section impacts much more the TIR region than short waves. Also, since non-absorbing gases have a negligible impact on the TOA / BOA radiance,  $\sigma_{m_i}^a(\lambda,z)$  is stored only for the five most absorbing gases (H<sub>2</sub>O, CO<sub>2</sub>, O<sub>3</sub>, CH<sub>4</sub>, N<sub>2</sub>O) and for the absorbing spectral regions of these gases. This trade-off allows one to get accurate TIR RT modelling without increasing too much the DART code complexity and computer time. In non-absorbing bands, MODTRAN absorption transmittance  $t_{m_i}^a(\lambda,z)$  of gas  $m_i$  at any altitude z along the horizontal path is very close to 1 (e.g., 0.99995), which implies that the computed equivalent absorption cross-section is either zero or inaccurate. Therefore, we selected absorbing regions per gas  $m_i$ . For that, a specific altitude  $Z_{m_i}^*$  is defined per gas  $m_i$  such that under this altitude over 98% of gas  $m_i$  is present.  $Z_{\rm H_2O}^*$  is 8 km,  $Z_{\rm CO_2}^*$  is 25 km,  $Z_{\rm O_3}^*$  is 40 km,  $Z_{\rm CH_4}^*$  and  $Z_{\rm N_2O}^*$  are both 23 km. If the sum of equivalent optical depth -  $\ln \left(t_{m_i}^a(\lambda,z)\right)$  for altitude  $z > Z_{m_i}^*$  is not negligible (Eq. (8)), the spectral band is considered as an absorbing band for gas  $m_i$ , and the  $\sigma_{m_i}^a(\lambda,z)$  profile is stored.

$$\sum_{z>Z_{m_i}^*} -\ln\left(t_{m_i}^a(\lambda, z)\right) > \varepsilon \tag{8}$$

where the threshold  $\varepsilon$  corresponds to MODTRAN precision. Any line-of-sight with equivalent optical depth -  $\ln\left(t_{m_i}^a(\lambda,z)\right)$  smaller than  $\varepsilon$  is considered as transparent.

#### 4.1.3 Improved absorption extinction coefficient profile

Eq. (9) indicates how the initial gas absorption extinction coefficient Eq. (2) was improved using the pressure- and temperature-dependent equivalent absorption cross-section.

$$\alpha_{j,m_{i}}^{a}(\lambda) = \begin{cases} \frac{-\ln\left(t_{m_{i}}^{a}(\lambda)\right)}{z_{j} - z_{j-1}} \cdot \frac{\int_{z_{j-1}}^{z_{j}} \sigma_{m_{i}}^{a}(\lambda, z) \cdot N_{m_{i},DB}(z)dz}{\int_{0}^{\infty} \sigma_{m_{i}}^{a}(\lambda, z) \cdot N_{m_{i},DB}(z)dz}, m_{i} = H_{2}O, CO_{2}, O_{3}, CH_{3}, N_{2}O\\ \frac{-\ln\left(t_{m_{i}}^{a}(\lambda)\right)}{z_{j} - z_{j-1}} \cdot \frac{\int_{z_{j-1}}^{z_{j}} \sigma_{m_{i}}^{a}(\lambda) \cdot N_{m_{i},DB}(z)dz}{\int_{0}^{\infty} \sigma_{m_{i}}^{a}(\lambda) \cdot N_{m_{i},DB}(z)dz}, m_{i} \neq H_{2}O, CO_{2}, O_{3}, CH_{3}, N_{2}O \end{cases}$$

$$(9)$$

Figure 6 shows vertical profiles of the new absorption extinction coefficients in the USSTD76 atmosphere at four spectral bands. Compared to the initial absorption extinction coefficients, they tend to be larger at lower altitudes and smaller at higher altitudes. This is consistent with the stronger absorption behaviour of bottom atmosphere.  $O_3$  absorption explains the local maximum ( $\approx 20$  km) of the initial and new absorption extinction coefficients at  $10 \, \mu m$ .

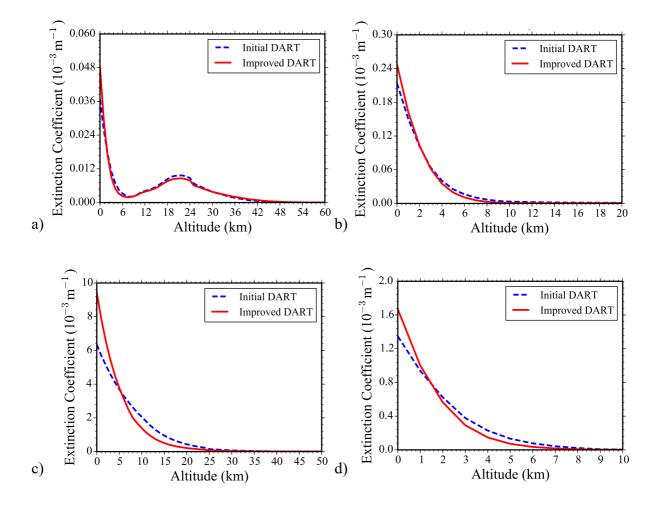


Figure 6. Profiles of DART initial and improved absorption extinction coefficients in the USSTD76 atmosphere. a)  $10.0 \,\mu\text{m}$ . b)  $13.0 \,\mu\text{m}$ . c)  $15.4 \,\mu\text{m}$ . d)  $19.6 \,\mu\text{m}$ . Spectral bin is  $1 \,\text{cm}^{-1}$ .

#### 4.2 Layer thermal emission

## 4.2.1 A double-layer method

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- 371 The initial thermal emission method (Eq. (5)) is less correct for optically thick atmosphere layer
- 372 (i.e.,  $\Delta \tau_i \gg 1$ ). For example, if lower boundary temperature is larger than layer mean
- temperature and if  $\Delta \tau_i \gg 1$ , Eq. (5) tends to underestimate downward thermal vector sources
- 374  $W_i^{\downarrow}(\Omega, \lambda)$ . Hence, a double-layer method was first designed (Eq. (10)): half a layer emits with
- Planck function  $L_B(T_x, \lambda)$ , and the other half emits with Planck function  $L_B(T_y, \lambda)$ .

$$W_{j}^{\uparrow}(\Omega,\lambda) = \left(1 - \omega_{j}(\lambda)\right) \cdot \left[L_{B}(T_{x},\lambda)e^{-\frac{\Delta\tau_{j}}{2\mu}} + L_{B}(T_{y},\lambda)\right] \left[1 - e^{-\frac{\Delta\tau_{j}}{2\mu}}\right] \cdot \mu \cdot \Delta S \cdot \Delta \Omega$$

$$W_{j}^{\downarrow}(\Omega,\lambda) = \left(1 - \omega_{j}(\lambda)\right) \cdot \left[L_{B}(T_{x},\lambda) + L_{B}(T_{y},\lambda)e^{-\frac{\Delta\tau_{j}}{2\mu}}\right] \left[1 - e^{-\frac{\Delta\tau_{j}}{2\mu}}\right] \cdot \mu \cdot \Delta S \cdot \Delta \Omega$$

$$(10)$$

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- In order to get  $T_x$  and  $T_y$ , four equations associated to schematic configurations must be verified:
- 378 1) Blackbody ( $\Delta \tau_j \gg 1$  and  $\omega_j(\lambda) \approx 0$ )

$$W_{j}^{\uparrow}(\Omega,\lambda) = L_{B}(T_{j}^{U},\lambda) \cdot \mu \cdot \Delta S \cdot \Delta \Omega$$

$$W_{j}^{\downarrow}(\Omega,\lambda) = L_{B}(T_{j}^{L},\lambda) \cdot \mu \cdot \Delta S \cdot \Delta \Omega$$
(11)

- with  $T_j^U$  and  $T_j^L$  respectively the upper and lower boundary temperature of layer j.
- 381 2) Isothermal  $(T_x = T_y = T_j)$

$$W_j^{\uparrow}(\Omega,\lambda) = \left(1 - \omega_j(\lambda)\right) \cdot L_B(T_j,\lambda) \cdot \left[1 - e^{-\frac{\Delta \tau_j}{\mu}}\right] \cdot \mu \cdot \Delta S \cdot \Delta \Omega \tag{12}$$

$$W_j^{\downarrow}(\Omega,\lambda) = \left(1 - \omega_j(\lambda)\right) \cdot L_B(T_j,\lambda) \cdot \left[1 - e^{-\frac{\Delta \tau_j}{\mu}}\right] \cdot \mu \cdot \Delta S \cdot \Delta \Omega$$

Eq. (11) and (12) lead to  $T_x = T_j^L$  and  $T_y = T_j^U$ . The resulting upward and downward vector sources are:

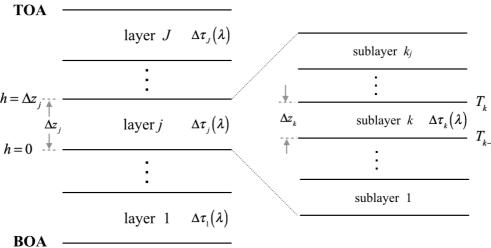
$$W_{j}^{\uparrow}(\Omega,\lambda) = \left(1 - \omega_{j}(\lambda)\right) \cdot \left[L_{B}(T_{j}^{L},\lambda)e^{-\frac{\Delta\tau_{j}}{2\mu}} + L_{B}(T_{j}^{U},\lambda)\right] \left[1 - e^{-\frac{\Delta\tau_{j}}{2\mu}}\right] \cdot \mu \cdot \Delta S \cdot \Delta \Omega$$

$$W_{j}^{\downarrow}(\Omega,\lambda) = \left(1 - \omega_{j}(\lambda)\right) \cdot \left[L_{B}(T_{j}^{L},\lambda) + L_{B}(T_{j}^{U},\lambda)e^{-\frac{\Delta\tau_{j}}{2\mu}}\right] \left[1 - e^{-\frac{\Delta\tau_{j}}{2\mu}}\right] \cdot \mu \cdot \Delta S \cdot \Delta \Omega$$

$$(13)$$

## 4.2.2 Thermal emission with virtual sub-layers

Same as the "linear-in-optical depth" assumption (Clough et al., 1992), the double-layer method (Eq. (13)) is less correct if the temperature and absorption extinction coefficient gradient within a layer is large (Wiscombe, 1976). Hence, there is a need to take into account the vertical distribution of temperature and optical depth in each atmosphere layer. For that, each DART atmosphere layer j ( $j \in [1, J]$ , j = 1 for the bottom layer) is virtually divided into  $k_j$  sub-layers  $\Delta \tau_k(\lambda) = \int_{\tau_{k-1}(\lambda)}^{\tau_k(\lambda)} d\tau$  with  $k \in [1, k_j]$  (Figure 7). The optical depth of the bottom and top planes of layer j are noted  $\tau_{j-1}(\lambda)$  and  $\tau_j(\lambda)$ , respectively, with  $\tau_j(\lambda) = 0$  and  $\tau_{j-1}(\lambda) = \Delta \tau_j(\lambda)$ . The terms  $\Delta \tau_k(\lambda)$ ,  $\tau_j(\lambda)$ ,  $\tau_{j-1}(\lambda)$ ,  $\tau_k(\lambda)$  and  $\tau_{k-1}(\lambda)$  are computed using analytical expressions of layer optical depth that was already implemented in DART for LiDAR mode (i.e.,  $\tau_j(h, \lambda) = A_j(\lambda) \cdot h^3 + B_j(\lambda) \cdot h^2 + C_j(\lambda) \cdot h + D_j(\lambda)$ ). Temperature profile  $T_j(h)$  is written as a linear approximation:  $T_j(h) = T_j^L + \frac{T_j^U - T_j^L}{\Delta z_j} \cdot h$ .



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respectively.

Figure 7. DART atmosphere is made of J layers, with layer optical depth  $\Delta \tau_j$  and layer thickness  $\Delta z_j$ . Each layer j is virtually divided into  $k_j$  sub-layers, with sub-layer thickness  $\Delta z_k = \frac{\Delta z_j}{k_j}$  and sub-layer optical depth  $\Delta \tau_k$ , with upper and lower boundary temperature  $T_k$  and  $T_{k-1}$ ,

The expressions of  $W_j^{\uparrow}(\Omega, \lambda)$  and  $W_j^{\downarrow}(\Omega, \lambda)$  are computed by summing up all contributions of virtual sub-layer thermal emission using Eq. (13).

$$W_{j}^{\uparrow}(\Omega,\lambda) = \left(1 - \omega_{j}(\lambda)\right) \sum_{k=1}^{k_{j}} \left[ L_{B}(T_{k-1},\lambda) e^{-\frac{\Delta \tau_{k}}{2\mu}} + L_{B}(T_{k},\lambda) \right] \left[1 - e^{-\frac{\Delta \tau_{k}}{2\mu}}\right] e^{-\frac{\tau_{k}}{\mu}} \cdot \mu \cdot \Delta S \cdot \Delta \Omega$$

$$(14)$$

$$W_{j}^{\downarrow}(\Omega,\lambda) = \left(1 - \omega_{j}(\lambda)\right) \sum_{k=1}^{k_{j}} \left[ L_{B}(T_{k-1},\lambda) + L_{B}(T_{k},\lambda) e^{-\frac{\Delta \tau_{k}}{2\mu}} \right] \left[1 - e^{-\frac{\Delta \tau_{k}}{2\mu}}\right] e^{-\frac{(\tau_{j-1} - \tau_{k-1})}{\mu}} \cdot \mu \cdot \Delta S \cdot \Delta \Omega$$

The optimal number  $k_j$  of sub-layers in Eq. (14) was assessed by computing the upward vector sources ( $\omega_j$ =0,  $\mu$ =1,  $\Delta S$ =100 m<sup>2</sup>,  $\Delta \Omega$ =0.01 sr) of a hot (~300 K) and cold (~200 K) atmosphere layer ( $\Delta z_j$ =1 km) with small (0.2) and large (0.8) transmittance  $e^{-\Delta \tau_j}$ , for  $k_j$  from 1 to 10, from 3  $\mu$ m to 20  $\mu$ m. Bottom layer parameters are:  $T_j^L$ = $T^L$ ,  $\alpha_j^e$ (0, $\lambda$ )= $\alpha_0^e$ ,  $\tau_j$ (0, $\lambda$ )= $\Delta \tau_j$ ; upper layer parameters are:  $T_j^U$ = $T^U$ ,  $\alpha_j^e$ ( $\Delta z_l$ ,  $\lambda$ )= $\alpha_0^e$ · $e^{-\frac{\Delta z_j}{H}}$ ,  $\tau_j$ ( $\Delta z_j$ ,  $\lambda$ )=0, with H=8.4 km the usual scale

height of major gases. Sub-layer boundary temperature and optical depth are computed as described at the beginning of this section. Here, the reference is the vector source  $W_{\text{ref}}^{\uparrow}(\Omega, \lambda)$  computed with  $k_j = 1000$ . Figure 8 shows that MARE for  $k_j = 1$  can reach 7% and that  $k_j = 5$  gives accurate source vectors for most atmospheric conditions. Note that for atmospheric conditions less extreme than these in this test, the double-layer method usually gives better results.



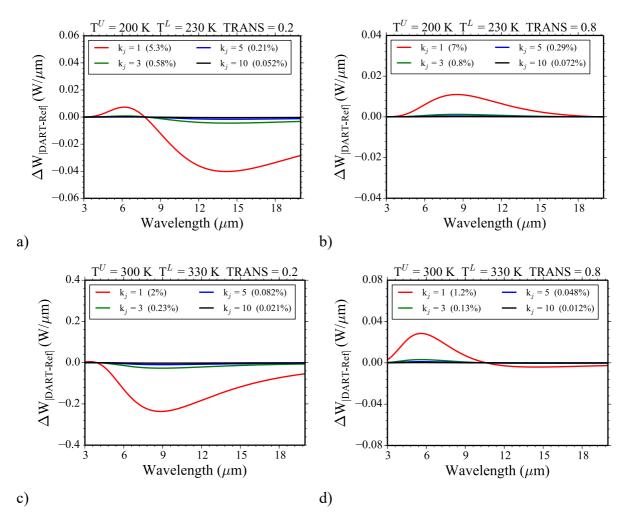


Figure 8. Difference of DART double-layer upward vector source compared with the reference, for various numbers of sub-layers.  $T^U$  and  $T^L$  are respectively the upper and lower boundary temperatures. TRANS represents the layer transmittance. MARE is marked in the legend.

#### 5. Results and discussion

#### 5.1 Results

The combined introduction of the equivalent absorption cross-section and double-layer thermal emission method greatly improves the accuracy of DART TIR radiance as illustrated below.

# 5.1.1 Optimal path length $\Delta L$

Section 4 stresses that the path length  $\Delta L$  used to compute the equivalent absorption cross-section can slightly impact the TIR radiance. Therefore, we investigated 10 equivalent absorption cross-section databases with  $\Delta L$  from 1 km to 10 km, with 1 km interval, in order to determine the optimal  $\Delta L$ . TOA and BOA radiance spectra over [3.5  $\mu$ m, 20  $\mu$ m] were simulated with these databases for the six standard atmospheres. Table 4 shows the corresponding average MAE of TOA and BOA BT of six standard atmospheres for the equivalent absorption cross-section databases with  $\Delta L$  from 4 km to 9 km. We chose  $\Delta L$ =7 km since it gives the best results compared to MODTRAN-5. Note that  $\Delta L$  = 6 km, 8 km, and 9 km can also give good results with average BT MAE less than 0.7 K. Hereafter, all the DART simulations use the " $\Delta L$ =7 km" absorption cross-section database.

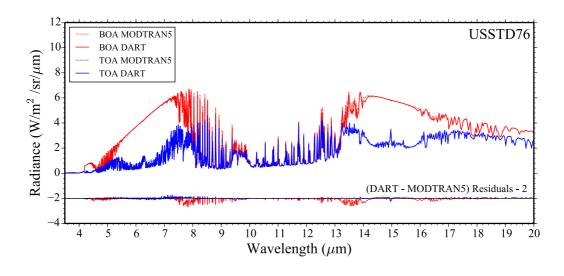
Table 4. Average MAE of TOA and BOA BT over [3.5  $\mu$ m, 20  $\mu$ m] region of six standard atmospheres, with path lengths  $\Delta L$  from 4 km to 9 km. MODTRAN-5 results are the reference.

$\Delta L$	4 km	5 km	6 km	7 km	8 km	9 km
AVG BT	0.7489	0.7157	0.6828	0.6728	0.6731	0.6805
MAE (K)	0.7 105	0.7157	0.0020	0.0720	0.0751	0.0003

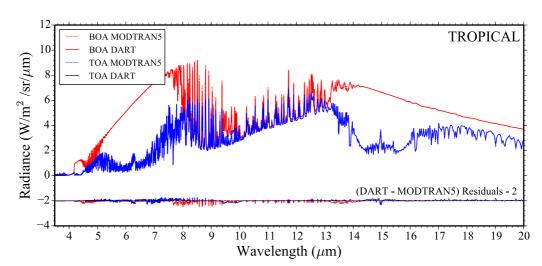
#### 5.1.2 Improved TOA and BOA thermal radiance

Figure 9 shows the DART and MODTRAN-5 TIR radiance spectra of the USSTD76, MIDDLATSUM, TROPICAL and SUBARCWIN atmospheres, with the same configurations as in Figure 4. Table 5 gives the MAE of TIR BT and MARE of TIR radiance of the improved DART and MODTRAN-5 for the six standard atmospheres over [3.5  $\mu$ m, 20  $\mu$ m]. Compared to initial results in section 3, the average TIR radiance MARE of the six standard atmospheres is reduced from 12.7% to 3.0% at TOA level, and from 6.7% to 2.3% at BOA level. Similarly, the average BT MAE is reduced from 3.1 K to 0.71 K at TOA level and from 2.1 K to 0.64 K at BOA level. Table 6 indicates that the largest improvements occur in TIR absorbing regions (*e.g.*, 3.5 - 4.5  $\mu$ m, 6-7  $\mu$ m, 9-10  $\mu$ m, 14-16  $\mu$ m). For example, with the USSTD76 atmosphere, the BT MAE in [14  $\mu$ m, 16  $\mu$ m] region is reduced from 7.0 K to 0.9 K at TOA level and from 3.4 K to 0.7 K at BOA level.

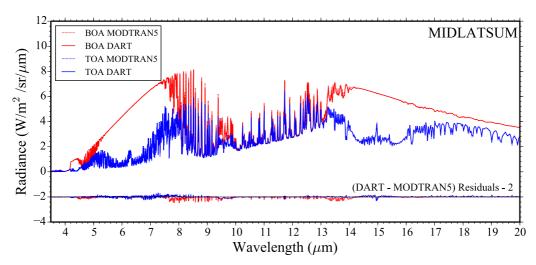
The BT DIFF "improved DART vs. MODTRAN-5" for the TIR bands of the aforementioned EO satellite missions (Table 7) stresses that current DART accuracy meets the sensitivity of these three satellite missions. For example, for the 12  $\mu$ m band of Landsat 8, the DIFF is reduced from 1.73 K to 0.025 K, which is much smaller than the sensor sensitivity (0.4 K at 300 K).



a)



b)



c)

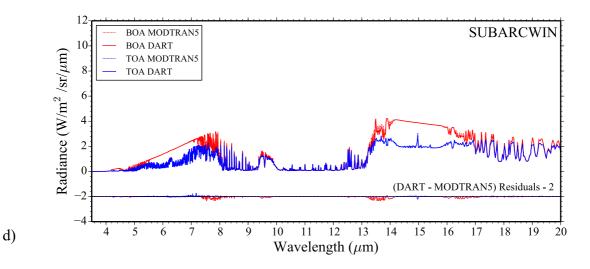


Figure 9. Improved DART and MODTRAN-5 TOA / BOA TIR radiance in [3.5  $\mu$ m, 20  $\mu$ m] region for USSTD76 (a), TROPICAL (b), MIDLATSUM (c) and SUBARCWIN (d) atmospheres. 1 cm<sup>-1</sup> spectral resolution. DART and MODTRAN-5 configurations are detailed in section 3.

Table 5. TOA and BOA BT MAE and radiance MARE of improved DART in [3.5  $\mu$ m, 20  $\mu$ m] region for six atmospheres. MODTRAN-5 results are the reference.

Atmosphere	TOA MAE	BOA MAE	TOA MARE	BOA MARE
USSTD76	0.68K	0.83K	3.0%	2.8%
TROPICAL	0.97K	0.58K	3.8%	2.0%
MIDLATSUM	0.88K	0.57K	3.5%	2.0%
MIDLATWIN	0.55K	0.63K	2.5%	2.3%
SUMARCSUM	0.75K	0.66K	3.1%	2.3%
SUMARCWIN	0.44K	0.54K	2.2%	2.2%
AVERAGE	0.71K	0.64K	3.0%	2.3%

Table 6. TOA and BOA BT MAE and radiance MARE of improved DART in three TIR absorbing bands for the USSTD76 atmosphere. MODTRAN-5 results are the reference.

Absorption	Central	D 1 114	TOLINA	DO A MAE	TO A MARE	DOL MARE
bands	wavelength	Bandwidth	TOA MAE	BOA MAE	TOA MARE	BOA MARE
ABS1	4.0 μm	1.0 μm	0.7 K	0.7 K	4.0%	3.5%
ABS2	6.5 μm	$1.0~\mu\mathrm{m}$	1.4 K	0.1 K	5.5%	0.3%
ABS3	9.5 μm	$1.0~\mu\mathrm{m}$	0.6 K	1.0 K	1.8%	2.9%
ABS4	15.0 μm	$2.0~\mu\mathrm{m}$	0.9 K	0.7 K	1.7%	0.9%

Table 7. TOA BT DIFF improved DART in the TIR bands of three EO satellite missions for the USSTD76 atmosphere. MODTRAN-5 results are the reference.

Satellite	Launch date	Organization	Central	Dandyvidth	Sensitivity Bandwidth	
Saterine	Launch date	Organization	wavelength	Dandwidin	(NeDT)	DIFF
Trishna	foreseen	CNES+ISRO	8.6 μm	0.35 μm	0.3 K@300 K	0.153 K
	2024-2025		9.1 μm	$0.35~\mu\mathrm{m}$	0.3 K@300 K	0.049 K
			10.3 μm	1.0 μm	0.3 K@300 K	0.197 K
			11.5 μm	1.0 μm	0.3 K@300 K	0.005 K
Landsat 8	2013	NASA	10.9 μm	$0.6~\mu\mathrm{m}$	0.4 K@300 K	0.009 K
			$12.0~\mu\mathrm{m}$	1.0 μm	0.4 K@300 K	0.025 K
Sentinel 3	2016	ESA	$3.74~\mu\mathrm{m}$	$0.38~\mu\mathrm{m}$	0.08 K@270 K	0.022 K
			$10.95 \ \mu {\rm m}$	0.9 μm	0.05 K@270 K	0.011 K
			12.0 μm	$1.0~\mu\mathrm{m}$	0.05 K@270 K	0.025 K

The accuracy of the improved DART was successfully tested for oblique viewing directions. Table 8 summarizes the MAE of TOA and BOA BT for viewing directions with  $\theta$  from 0° to 60°. Figure 10 shows TOA / BOA TIR radiance spectra for viewing zenith angles  $\theta$ =30° and  $\theta$ =60°, for the USSTD76 atmosphere. Along viewing zenith angle  $\theta$ =30°, the BT MAE is 0.74 K at TOA level and 0.70 K at BOA level, along viewing zenith angle  $\theta$ =60°, the BT MAE is 1.36 K at TOA level and 0.52 K at BOA level.

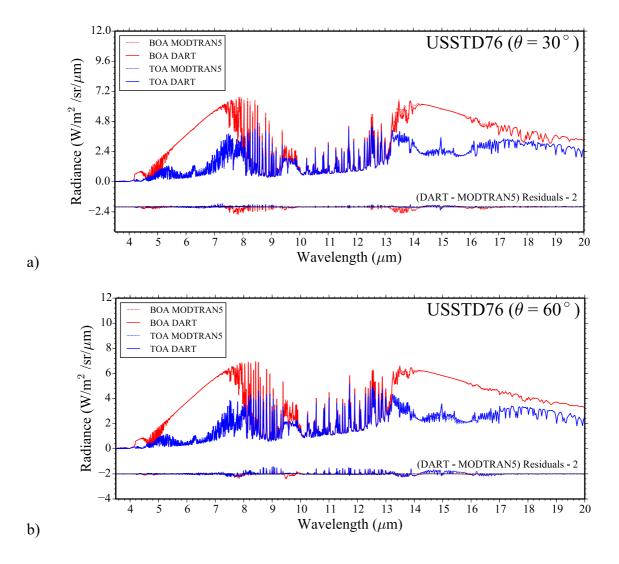


Figure 10. Improved DART and MODTRAN-5 TOA / BOA TIR radiance in [3.5  $\mu$ m, 20  $\mu$ m] region for the USSTD76 atmosphere. Viewing zenith angle  $\theta = 30^{\circ}$  (a) and  $\theta = 60^{\circ}$  (b).

Table 8. Average MAE of TOA and BOA BT of the USSTD76 atmosphere over [3.5  $\mu$ m, 20  $\mu$ m] region, with viewing directions  $\theta$  from 0° to 60°. MODTRAN-5 results are the reference.

θ	0°	10°	20°	30°	40°	50°	60°
TOA BT  MAE (K)	0.68	0.71	0.71	0.74	0.82	1.0	1.36
BOA BT MAE (K)	0.83	0.83	0.78	0.70	0.60	0.53	0.52

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#### 5.2 Validation

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DART improvement was validated by comparing DART and MODTRAN-5 simulations with atmosphere profiles from ECMWF (European Centre for Medium-range Weather Forecasts) reanalysis dataset: ERA-Interim (https://apps.ecmwf.int/datasets/). These profiles include the pressure, temperature, specific humidity (mass of water vapour per kilogram of moist air, nearly equal to mass mixing ratio within a few percent) and O<sub>3</sub> mass mixing ratio (mass of ozone per kilogram of dry air) at 60 **ECMWF** model levels (https://www.ecmwf.int/en/forecasts/documentation-and-support/60-model-levels) as well as the surface albedo, skin temperature over France (49 ° N, -1 ° W, 44 ° S, 7 ° E) and the Mediterranean Sea (37°N,12°W, 34°S, 26°E) from 01/06/2018 to 31/08/2018. These data were averaged over time and space and the vertical profiles were interpolated into 37 altitude levels (1 km interval from 0 to 25 km, and 5 km interval from 30 to 80 km) that are configured in both DART and MODTRAN-5. The number density profile  $N_{m_i}(z)$  of other gases (N<sub>2</sub>, CO<sub>2</sub>, CO, CH<sub>4</sub>, N<sub>2</sub>O, O<sub>2</sub>, NH<sub>3</sub>, NO, NO<sub>2</sub>, SO<sub>2</sub>, HNO<sub>3</sub>, CFC<sub>12</sub>, CFC<sub>13</sub>, CFC<sub>14</sub>, CFC<sub>22</sub>, CFC<sub>113</sub>, CFC<sub>114</sub>, CFC<sub>115</sub>, CLONO<sub>2</sub>, HNO<sub>4</sub>, CHCL<sub>2</sub>F, CCL<sub>4</sub>, N<sub>2</sub>O<sub>5</sub>) and the relative density profile  $\rho_m^s(z)$  of scattering gases are adjusted by MODTRAN-5 based on the MIDLATSUM atmosphere and the actual pressure and temperature profile from ERA-Interim dataset.

Figure 11.a shows the pressure, temperature, H<sub>2</sub>O, O<sub>3</sub> and CO<sub>2</sub> number density profiles for three summer atmospheres in the mid-latitude region: France, Mediterranean Sea, and the standard MIDLATSUM atmosphere. Figure 11.b shows the corresponding maximum difference values of profiles per altitude level. Temperature varies up to 10 K at around 11 km, water vapour mass varies up to 38% at the Earth surface and O<sub>3</sub> mass varies up to 40% at around 16 km. The averaged continental surface albedo and skin temperature of France are 0.132 and 292 K, respectively. For the Mediterranean Sea, they are 0.07 and 296 K, respectively.

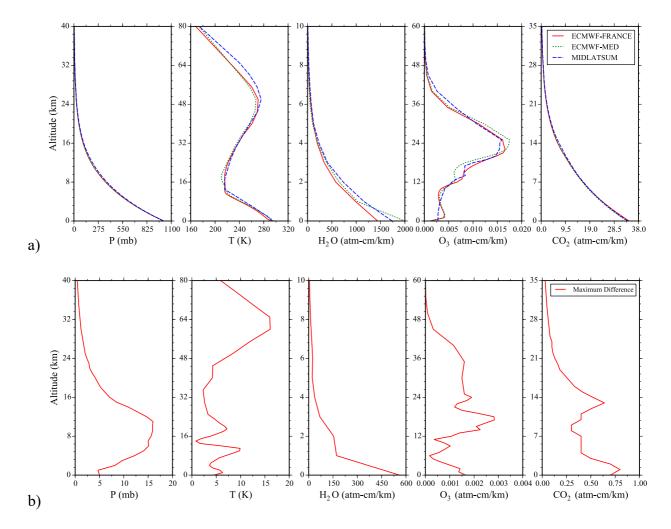


Figure 11. a) Vertical profiles of pressure (mb), temperature (K), and H<sub>2</sub>O, O<sub>3</sub> and CO<sub>2</sub> number densities (atm-cm/km) for three summer atmospheres: France, Mediterranean Sea and MIDLATSUM atmosphere. b) Maximum difference of vertical profiles.

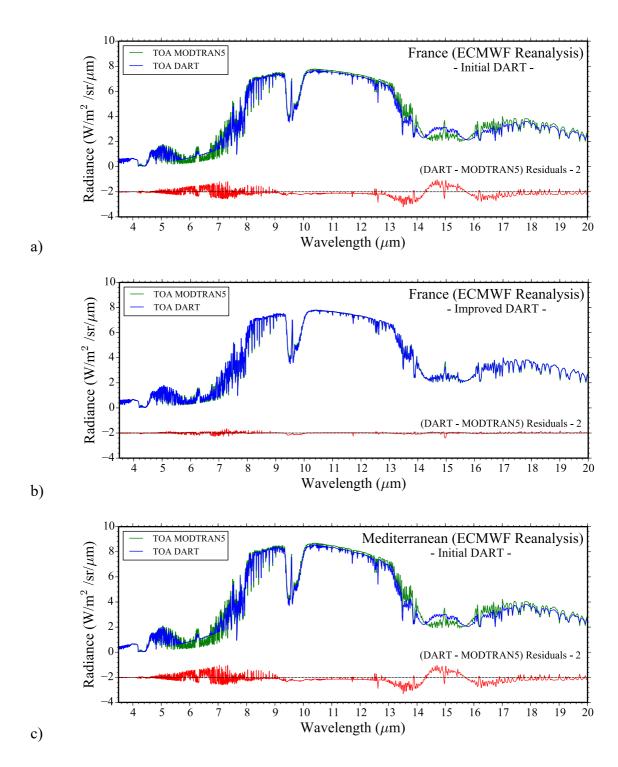
DART and MODTRAN-5 were run in full radiance mode (simulation with solar radiation and thermal emission), with the same sun viewing angle ( $\theta_{\text{sun}} = 30^{\circ}$ ,  $\varphi_{\text{sun}} = 225^{\circ}$ ), surface parameters, discrete altitude levels, pressure, temperature profiles and gas number density profiles. Eq. (15) indicates how the gas optical depth was adjusted in DART using the user-defined density profiles  $N_{m_i}(z)$  and  $\rho_m^s(z)$ .

$$\tau_{m_{i}}^{a}(\lambda) = \begin{cases}
-\ln\left(t_{m_{i},DB}^{a}(\lambda)\right) \cdot \frac{\int_{0}^{\infty} \sigma_{m_{i},DB}^{a}(\lambda,z) \cdot N_{m_{i}}(z)dz}{\int_{0}^{\infty} \sigma_{m_{i},DB}^{a}(\lambda,z) \cdot N_{m_{i},DB}(z)dz}, m_{i} = H_{2}O, CO_{2}, O_{3}, CH_{4}, N_{2}O \\
-\ln\left(t_{m_{i},DB}^{a}(\lambda)\right) \cdot \frac{\int_{0}^{\infty} \sigma_{m_{i}}^{a}(\lambda) \cdot N_{m_{i}}(z)dz}{\int_{0}^{\infty} \sigma_{m_{i}}^{a}(\lambda) \cdot N_{m_{i},DB}(z)dz}, m_{i} \neq H_{2}O, CO_{2}, O_{3}, CH_{4}, N_{2}O
\end{cases}$$

$$\tau^{s}(\lambda) = -\ln\left(t_{m,DB}^{s}(\lambda)\right) \cdot \frac{\int_{0}^{\infty} \rho_{m}^{s}(z)dz}{\int_{0}^{\infty} \rho_{m}^{s}(z)dz}$$
(15)

Note that  $m_i$  represents 13 gases (H<sub>2</sub>O, O<sub>3</sub>, N<sub>2</sub>, CO<sub>2</sub>, CO, CH<sub>4</sub>, N<sub>2</sub>O, O<sub>2</sub>, NH<sub>3</sub>, NO, NO<sub>2</sub>, SO<sub>2</sub>, HNO<sub>3</sub>) and the sum of other minor gases (CFC<sub>12</sub>, CFC<sub>13</sub>, CFC<sub>14</sub>, CFC<sub>22</sub>, CFC<sub>113</sub>, CFC<sub>114</sub>, CFC<sub>115</sub>, CLONO<sub>2</sub>, HNO<sub>4</sub>, CHCL<sub>2</sub>F, CCL<sub>4</sub>, N<sub>2</sub>O<sub>5</sub>).

Figure 12 shows the MODTRAN-5 and initial and improved DART TOA nadir radiance spectra over France and Mediterranean Sea. BT MAE is reduced from 3.6 K to 1.0 K for France summer atmosphere, and from 3.7 K to 1.0 K for the Mediterranean Sea summer atmosphere. We can note that the residuals between improved DART and MODTRAN-5 over [3.5  $\mu$ m, 5.0  $\mu$ m] region where solar radiation contributes most to TOA radiance is relatively small (< 0.1 W/m²/sr/ $\mu$ m for both cases). Also, the BT MAE in this region is less than 1.0 K. It confirms the accuracy of DART in this spectral region.



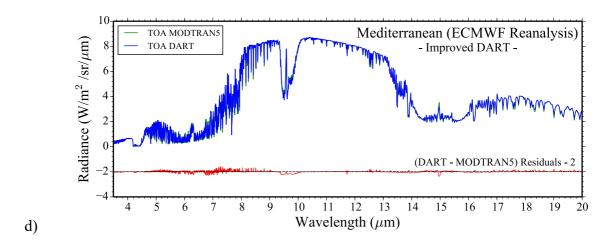


Figure 12. TOA spectral radiance of initial (a, c) and improved (b, d) DART compared to MODTRAN-5 with ECMWF reanalysis profile and surface parameter. a, b) France. c, d) Mediterranean Sea.

## 5.3 Discussion

As indicated in section 4, gas equivalent absorption cross-sections  $\sigma_{m_i}^a(\lambda,z)$  per atmosphere altitude z and gas  $m_i$  are computed with Beer's law. However, Beer's law is less correct in the spectral bands with strong varying spectral absorption. In this case, the absorption extinction coefficient  $\alpha_{j,m_i}^a(\lambda)$  computed by Eq. (9) is slightly smaller than the exact absorption extinction coefficient computed line-by-line, with a difference that depends on the number, strength and width of the absorption lines in the spectral bin. The small BT MAE with MODTRAN-5 validates our strategy. Indeed, if Beer's law is not obeyed, the slightly smaller absorption extinction coefficients lead to slightly lower radiation attenuation and thermal emission that tend to compensate each other, which explains that DART results are accurate. For oblique directions, the longer line-of-sight in each layer increases the issue. Therefore, errors increase with the obliquity of viewing direction at TOA. Conversely, at the BOA, errors decrease with the obliquity of the viewing direction. Indeed, at BOA, the underestimated attenuation

compensates the underestimated thermal emission because the downward vector sources depend more on the thermal emission of the lower atmosphere layers if the line-of-sight is more oblique.

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The equivalent absorption cross-sections were pre-computed for six standard atmospheres that are representative of most pressure and temperature profiles in different seasons over our planet. It explains that DART can simulate accurate TOA radiance spectra for most user-defined atmospheres using the modelling method presented in section 5.2. However, results are less accurate if the actual atmosphere greatly differs from the six standard atmospheres since the pre-computed equivalent absorption cross-sections are for temperature and pressure profiles of standard atmospheres. Although pressure profiles are relatively stable over the Earth, temperature profiles vary with time and space. For this reason, we investigated the variation of DART atmosphere thermal radiance accuracy if the atmosphere vertical profile is offset by  $\Delta T$ at all altitude levels. Figure 13.a illustrates the impact of an offset equal to +15 K for the USSTD76 atmosphere, in thermal emission mode, no aerosol, with Earth skin temperature 0 K and albedo 0.0. As expected, the offset increases the TOA BT MAE to 1.69 K, especially in the [10  $\mu$ m, 13  $\mu$ m] region where the DART adjustment method (Eq. (15)) overestimates vertical optical depth, which leads to overestimated atmospheric TIR radiance. Table 9 shows the MAE of TOA atmospheric TIR radiance of the USSTD76 atmosphere with five temperature offsets  $\Delta T = 3 \text{ K}, 6 \text{ K}, 9 \text{ K}, 12 \text{ K}$  and 15 K. Results are still accurate if the temperature offset relative to the standard atmosphere is not too large. For example, TOA BT MAE is 1.07 K if  $\Delta T = 6$  K and 1.27 K if  $\Delta T = 9$  K.

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We must note the errors in Table 9 decrease if the Earth surface thermal emission and scattering are considered. For example, Figure 13.b shows the DART and MODTRAN-5 TOA total

radiance spectra of the USSTD76 atmosphere with +15 K temperature offset, and a land surface with a skin temperature of 303.1 K (BOA temperature of the USSTD76 atmosphere with +15 K offset) and an albedo of 0.14 (global annual average albedo of the Earth's surface in 2019 derived from ERA-Interim dataset). Results are much better, with TOA BT MAE equal to 1.1 K. Indeed, in the [10  $\mu$ m, 13  $\mu$ m] region, the overestimated vertical optical depth slightly reduces the contribution of Earth surface thermal emission on TOA radiance. Then, the underestimated Earth thermal emission compensates the overestimated atmospheric thermal emission and the total TOA radiance is better.

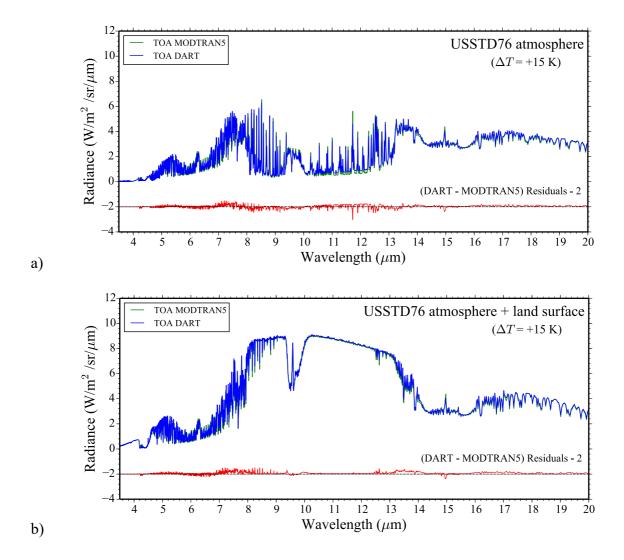


Figure 13. DART and MODTRAN-5 TOA TIR radiance spectra of the USSTD76 atmosphere with temperature vertical profile offset by +15 K. Atmosphere thermal emission only (a), total TOA thermal radiance with Earth surface thermal emission and scattering (b).

Table 9. TOA BT MAE of the USSTD76 atmosphere with six offsets  $\Delta T$  of its temperature vertical profile.

ΔΤ	0 K	+3 K	+6 K	+9 K	+12 K	+15 K
BT MAE (K)	0.68	0.87	1.07	1.27	1.48	1.69

## 6. Concluding remarks

DART TIR atmospheric RT modelling accuracy has been greatly improved by (1) introducing the equivalent absorption cross-section of the five most absorbing gases (H<sub>2</sub>O, CO<sub>2</sub>, O<sub>3</sub>, CH<sub>4</sub>, N<sub>2</sub>O) in six standard atmospheres (USSTD76, TROPICAL, MIDDLATSUM, MIDDLATWIN, SUBARCSUM, SUBARCWIN), and (2) implementing a double-layer thermal emission modelling method. MODTRAN-5, with its atmospheric thermal BT accuracy better than 1 K, is the reference atmospheric RT model to validate this improvement.

With the new RT modelling strategy, the TIR BT average MAE over the whole [3.5  $\mu$ m, 20  $\mu$ m] region, for six standard atmospheres, decreased from 3.1 K to 0.71 K at TOA and from 2.1 K to 0.64 K at BOA, with largest improvements in the TIR absorbing regions (*i.e.*, 3.5-4.5  $\mu$ m, 6-7  $\mu$ m, 9-10  $\mu$ m, 14-16  $\mu$ m). The band BT error in TIR bands of present and future EO satellite missions is also reduced below the NeDT of satellite TIR sensors.

Sensitivity studies showed that DART atmospheric thermal radiance accuracy remains good (<  $1~\rm K$ ) for oblique viewing zenith angle less than  $50^{\circ}$ . This improvement was also verified with atmospheric profiles and surface parameters from the ECMWF reanalysis dataset for two large zones: France and Mediterranean Sea during summer. The average differences of TOA radiance spectra with MODTRAN-5 decreased from  $3.6~\rm K$  to  $1.0~\rm K$  for the France summer atmosphere, and from  $3.7~\rm K$  to  $1.0~\rm K$  for the Mediterranean Sea summer atmosphere. In the spectral region over 3.5- $5.0~\mu m$  where the solar radiation contributes most to TOA radiance, the improved DART still have accuracy better than  $1.0~\rm K$ .

DART atmospheric thermal radiance is less accurate if the user-defined atmosphere temperature profile differs from the six standard atmospheres, because DART uses temperature-dependent equivalent absorption cross-sections that are pre-computed for those standard atmospheres. However, the decrease in accuracy is relatively small. For example, TOA BT MAE only increases from 0.68 K to 1.07 K if the temperature profile of the USSTD76 atmosphere is offset by +6 K. In addition, the MAE decreases if the Earth surface thermal emission and scattering is considered. Future work will investigate a better adjustment method to compute accurate gas optical depth for arbitrary atmosphere profiles.

Due to its accurate TIR RT modelling both in the atmosphere and in 3D urban and natural landscapes, including the Earth-atmosphere radiative coupling, DART meets the requirements of TIR EO satellite missions (*i.e.*, Trishna, Sentinel 3, Landsat 8/9) and LST applications in the remote sensing community, which opens new perspectives for DART model.

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## Appendix. Nomenclature

Symbols	Definitions
ΔS	Surface
$\Delta L$	Horizontal path length
Н	Scale height for major gases of an average atmosphere
Ω	Direction vector
$\Delta\Omega$	Solid angle of direction $\Omega$
heta	Zenith angle
$\mu$	Shorthand of $cos(\theta)$
arphi	Azimuth angle
λ	Wavelength
Δλ	Bandwidth
j	Index of atmosphere layer
J	Number of DART atmosphere layers
k	Index of virtual sub-layer
$k_{j}$	Number of virtual sub-layers in layer j
Z	Altitude
$z_{j-1}$	Lower boundary altitude of layer j

$Z_j$	Upper boundary altitude of layer <i>j</i>
$\Delta z_j$	Thickness of layer j
$\Delta z_k$	Thickness of virtual sub-layer k
$Z_{m_i}^*$	Specific height defined per gas $m_i$ such that under this altitude over 98% of
	gas $m_i$ is concentrated.
h	Relative altitude within a layer $j$ , with $h = 0$ at bottom of layer and
	$h = \Delta z_j$ at top of layer
T(z)	Temperature profile
$\Delta T$	Temperature offset
$T_j(h)$	Temperature at relative altitude $h$ in layer $j$
$T_x, T_y$	Temperature variables in the double-layer method
$T_j^U$	Upper boundary temperature of layer j
$T_j^L$	Lower boundary temperature of layer <i>j</i>
$T_{j}$	Average temperature of layer j
$T_{k-1}$	Lower boundary temperature of virtual sub-layer k
$T_k$	Upper boundary temperature of virtual sub-layer k
$T_{DB}(z)$	Temperature profile in DART atmosphere database
P(z)	Pressure profile
$P_{DB}(z)$	Pressure profile in DART atmosphere database
N(z)	Number density profile
$N_m^s(z)$	Number density profile of scattering gases
$N_{m_i}(z)$	Number density profile of gas $m_i$
$N_{m_i,DB}(z)$	Number density profile of gas $m_i$ in DART atmosphere database
$ \rho_{m,DB}^s(z) $	Relative density profile of scattering gases in DART atmosphere database

$t_{m_i}^a(\lambda)$	Vertical absorption transmittance of gas $m_i$ at wavelength $\lambda$
$t_{m_i}^a(\lambda, z, \Delta L)$	Absorption transmittance of gas $m_i$ at wavelength $\lambda$ along horizontal path $\Delta L$
	at altitude z
$t^a_{m_i,DB}(\lambda)$	Vertical absorption transmittance of gas $m_i$ at wavelength $\lambda$ in DART
	atmosphere database
$t_m^s(\lambda)$	Vertical scattering transmittance of scattering gases at wavelength $\lambda$
$t_{m,DB}^s(\lambda)$	Vertical scattering transmittance of scattering gases at wavelength $\lambda$ in DART
	atmosphere database
$ au_{m_i}^a(\lambda)$	Vertical absorption optical depth of gas $m_i$ at wavelength $\lambda$
$ au^s(\lambda)$	Vertical scattering optical depth of scattering gases at wavelength $\lambda$
$ au_p(\lambda)$	Vertical optical depth of aerosols at wavelength $\lambda$
$ au_{p,DB}(\lambda)$	Vertical optical depth of aerosols at wavelength $\lambda$ in DART atmosphere
	database
$\Delta  au_j(\lambda)$	Total optical depth of gases and aerosols of layer $j$ at wavelength $\lambda$
$ au_{j-1}(\lambda)$	Optical depth of gases and aerosols at bottom of layer $j$ at wavelength $\lambda$
$ au_j(\lambda)$	Optical depth of gases and aerosols at top of layer $j$ at wavelength $\lambda$
$\tau_{k-1}(\lambda)$	Optical depth of gases and aerosols at bottom of virtual sub-layer $k$ at
	wavelength $\lambda$
$ au_k(\lambda)$	Optical depth of gases and aerosols at top of virtual sub-layer $k$ at wavelength
	λ
$\Delta  au_k(\lambda)$	Total optical depth of gases and aerosols of virtual sub-layer $k$ at wavelength
	λ
$\tau_j(\lambda,h)$	Optical depth profile at wavelength $\lambda$ at relative attitude $h$ in layer $j$
$A_j(\lambda), B_j(\lambda),$	Coefficients of optical depth function in layer $j$ at wavelength $\lambda$

$C_j(\lambda), D_j(\lambda)$	
$\alpha^e$	Total extinction coefficient
$lpha^a$	Absorption extinction coefficient
$\alpha^s$	Scattering extinction coefficient
$lpha_0^e$	Total extinction coefficient at bottom of atmosphere
$\alpha^a_{j,m_i}(\lambda)$	Absorption extinction coefficient of gas $m_i$ of layer $j$ at wavelength $\lambda$
$\alpha^a_{j,m}(\lambda)$	Gas absorption extinction coefficient of layer $j$ at wavelength $\lambda$
$\alpha_{j,m}^s(\lambda)$	Gas scattering extinction coefficient of layer $j$ at wavelength $\lambda$
$\alpha^e_{j,m}(\lambda)$	Gas total extinction coefficient of layer $j$ at wavelength $\lambda$
$\alpha^a_{j,p}(\lambda)$	Aerosol absorption extinction coefficient of layer $j$ at wavelength $\lambda$
$\alpha_{j,p}^s(\lambda)$	Aerosol scattering extinction coefficient of layer $j$ at wavelength $\lambda$
$\alpha^e_{j,p}(\lambda)$	Aerosol total extinction coefficient of layer $j$ at wavelength $\lambda$
$\alpha^e_{p,DB}(z)$	Aerosol total extinction coefficient profile at 550 nm in DART atmosphere
	database
$\alpha_j^a(\lambda)$	Total absorption extinction coefficient of gases and aerosols of layer $j$ at
	wavelength $\lambda$
$\alpha_j^s(\lambda)$	Total scattering extinction coefficient of gases and aerosols of layer j at
	wavelength $\lambda$
$\alpha_j^e(\lambda)$	Total extinction coefficient of gases and aerosols of layer $j$ at wavelength $\lambda$
$\alpha_j^e(\lambda,h)$	Extinction coefficient profile of gases and aerosols at wavelength $\lambda$ at relative
	altitude $h$ in layer $j$
$\alpha_{z_{j-1}}^e(\lambda)$	Total extinction coefficient of gases and aerosols at lower boundary of layer j
	at wavelength $\lambda$

Total extinction coefficient of gases and aerosols at upper boundary of layer *j*  $\alpha_{z_i}^e(\lambda)$ at wavelength  $\lambda$  $\sigma_{m_i}^a(\lambda)$ Absorption cross-section of gas  $m_i$  at wavelength  $\lambda$  $\sigma_m^s(\lambda)$ Gas scattering cross-section at wavelength  $\lambda$  $\sigma_{m_i}^a(\lambda, z, \Delta L)$ Equivalent absorption cross-section of gas  $m_i$  at wavelength  $\lambda$  along horizontal path  $\Delta L$  at altitude z  $\sigma_{m_i}^{a(*)}(\lambda, z, \Delta L)$  Rescaled  $\sigma_{m_i}^a(\lambda, z, \Delta L)$  by dividing  $\sigma_{m_i}^a(\lambda, z = 0, \Delta L)$  $\sigma_{m_i}^a(\lambda,z)$ Equivalent absorption cross-section of gas  $m_i$  at wavelength  $\lambda$  along horizontal path  $\Delta L = 7$  km at altitude z  $\omega_{p,DB}(\lambda)$ Aerosol single scattering albedo at wavelength  $\lambda$  in DART atmosphere database  $\omega_i(\lambda)$ Single scattering albedo of mixed gases and aerosols of layer *j* at wavelength λ Vector source of layer j along direction  $\Omega$  at wavelength  $\lambda$  $W_i(\Omega,\lambda)$  $W_i^{\uparrow}(\Omega,\lambda)$ Upward vector source of layer j along direction  $\Omega$  at wavelength  $\lambda$  $W_j^{\downarrow}(\Omega,\lambda)$ Downward vector source of layer j along direction  $\Omega$  at wavelength  $\lambda$  $L_{R}(T,\lambda)$ Planck function at temperature T at wavelength  $\lambda$  $W_{\rm ref}^{\uparrow}(\Omega,\lambda)$ Spectrum of reference upward vector source along direction  $\Omega$  at wavelength λ Threshold corresponds to MODTRAN decimal precision ε Band index q Q Number of spectral bands  $X_{\mathrm{DART}}(q)$ A type of DART product at band q  $X_{\text{MODTRAN}}(q)$  A type of MODTRAN product at band q

	MAE Mean absolute error
	MARE Mean absolute relative error
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644	References
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647	graphs, and mathematical tables. US Government printing office.
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789 List of Figure Captions

Figure 1. DART 3D mock-up and voxel matrix. Atmosphere is separated in three altitude regions: high atmosphere (HA) made of layers, mid-atmosphere (MA) made of voxels of any size, and bottom atmosphere (BA) in the Earth scene. Earth scene elements are made of facets (triangles), and/or fluid and turbid vegetation voxels. The voxel matrix is introduced to optimize ray tracing.

Figure 2. DART horizontally homogeneous atmosphere layer with layer thickness  $\Delta z_j$ . The upper and lower boundary parameters are marked.

Figure 3. Major steps for modelling the RT in the Earth-atmosphere system. Red colour indicates thermal emission (steps 1 and 2), orange colour indicates solar incident radiation, and yellow colour indicates thermal and/or solar radiation that is scattered.

Figure 4. Initial DART and MODTRAN-5 TOA / BOA TIR radiance in [3.5  $\mu$ m, 20  $\mu$ m] region for USSTD76 (a), TROPICAL (b), MIDLATSUM (c) and SUBARCWIN (d) atmospheres. 1 cm<sup>-1</sup> spectral resolution. DART and MODTRAN-5 configurations are detailed in section 3.

Figure 5. CO<sub>2</sub> equivalent absorption cross-section  $\sigma_{m_i}^a(\lambda, z, \Delta L)$  (a, c) and rescaled equivalent absorption cross-section  $\sigma_{m_i}^{a(*)}(\lambda, z, \Delta L)$  (b, d) at 13.4  $\mu$ m (a, b) and 13.1  $\mu$ m (c, d), in a 1 cm<sup>-1</sup> spectral bin, for 4 identical horizontal paths ( $\Delta L = 1$  km, 2 km, 5 km, 10 km) at altitudes up to 25 km for 13.4  $\mu$ m and up to 15 km for 13.1  $\mu$ m, in the USSTD76 atmosphere.

Figure 6. Profiles of DART initial and improved absorption extinction coefficients in the USSTD76 atmosphere. a)  $10.0 \,\mu\text{m}$ . b)  $13.0 \,\mu\text{m}$ . c)  $15.4 \,\mu\text{m}$ . d)  $19.6 \,\mu\text{m}$ . Spectral bin is  $1 \,\text{cm}^{-1}$ .

816 Figure 7. DART atmosphere is made of I layers, with layer optical depth  $\Delta \tau_i$  and layer

817 thickness  $\Delta z_i$ . Each layer j is virtually divided into  $k_i$  sub-layers, with sub-layer thickness

818  $\Delta z_k = \frac{\Delta z_j}{k_j}$  and sub-layer optical depth  $\Delta \tau_k$ , with upper and lower boundary temperature  $T_k$  and

819  $T_{k-1}$ , respectively.

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Figure 8. Difference of DART double-layer upward vector source compared with the reference,

for various numbers of sub-layers.  $T^U$  and  $T^L$  are respectively the upper and lower boundary

temperatures. TRANS represents the layer transmittance. MARE is marked in the legend.

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Figure 9. Improved DART and MODTRAN-5 TOA / BOA TIR radiance in [3.5  $\mu$ m, 20  $\mu$ m]

826 region for USSTD76 (a), TROPICAL (b), MIDLATSUM (c) and SUBARCWIN (d)

atmospheres. 1 cm<sup>-1</sup> spectral resolution. DART and MODTRAN-5 configurations are detailed

828 in section 3.

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Figure 10. Improved DART and MODTRAN-5 TOA / BOA TIR radiance in [3.5  $\mu$ m, 20  $\mu$ m]

region for the USSTD76 atmosphere. Viewing zenith angle  $\theta = 30^{\circ}$  (a) and  $\theta = 60^{\circ}$  (b).

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Figure 11. a) Vertical profiles of pressure (mb), temperature (K), and H<sub>2</sub>O, O<sub>3</sub> and CO<sub>2</sub> number

densities (atm-cm/km) for three summer atmospheres: France, Mediterranean Sea and

MIDLATSUM atmosphere. b) Maximum difference of vertical profiles.

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837 Figure 12. TOA spectral radiance of initial (a, c) and improved (b, d) DART compared to

838 MODTRAN-5 with ECMWF reanalysis profile and surface parameter. a, b) France. c, d)

839 Mediterranean Sea.

Figure 13. DART and MODTRAN-5 TOA TIR radiance spectra of the USSTD76 atmosphere with temperature vertical profile offset by +15 K. Atmosphere thermal emission only (a), total

TOA thermal radiance with Earth surface thermal emission and scattering (b).