Consistently Simulating a Wide Range of Atmospheric Scenarios for K2-18b with a Flexible Radiative Transfer Module

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Abstract

The atmospheres of small, potentially rocky exoplanets are expected to cover a diverse range in composition and mass. Studying such objects therefore requires flexible and wide-ranging modeling capabilities. We present in this work the essential development steps that lead to our flexible radiative transfer module, REDFOX, and validate REDFOX for the solar system planets Earth, Venus, and Mars, as well as for steam atmospheres. REDFOX is a k-distribution model using the correlated-k approach with the random overlap method for the calculation of opacities used in the δ-two-stream approximation for radiative transfer. Opacity contributions from Rayleigh scattering, UV/visible cross sections, and continua can be added selectively. With the improved capabilities of our new model, we calculate various atmospheric scenarios for K2-18b, a super-Earth/sub-Neptune with ~8 $M_{\oplus}$ orbiting in the temperate zone around an M star, with recently observed H$_2$O spectral features in the infrared. We model Earth-like, Venus-like, and H$_2$-He primary atmospheres of different solar metallicity and show resulting climates and spectral characteristics compared to observed data. Our results suggest that K2-18b has an H$_2$–He atmosphere with limited amounts of H$_2$O and CH$_4$. Results do not support the possibility of K2-18b having a water reservoir directly exposed to the atmosphere, which would reduce atmospheric scale heights, and with it the amplitudes of spectral features, making the latter inconsistent with the observations. We also performed tests for H$_2$–He atmospheres up to 50 times solar metallicity, all compatible with the observations.

Unified Astronomy Thesaurus concepts: Radiative transfer simulations (1967); Radiative transfer (1335); Computational methods (1965); Exoplanets (498); Extrasolar rocky planets (511); Exoplanet atmospheres (487); Planetary atmospheres (1244); Mini Neptunes (1063); Super Earths (1655)

1. Introduction

Exciting recent discoveries in exoplanetary science include the TRAPPIST-1 system (Gillon et al. 2017), Proxima Centauri b (Anglada-Escudé et al. 2016), and potential super-Earths/warm sub-Neptunes like LHS 1140b and c (Ment et al. 2019), K2-18b (Montet et al. 2015), and GJ 1214b (Charbonneau et al. 2009). Exoplanet science is transitioning from detection into first atmospheric characteristics from spectral observations, giving us insights into their composition and possible formation and evolution. Numerous spectral observations of Jupiter-sized to warm Neptune-sized planets have been reported and discussed in recent years (see, e.g., Sing et al. 2016; Crossfield & Kreidberg 2017), but the first detection of water features in the atmosphere of the temperate ($T_{\text{eq}} \sim 272$ K) super-Earth/sub-Neptune K2-18b (Benneke et al. 2019b; Tsiaras et al. 2019) orbiting an early-type M star is especially exciting, as it offers an unprecedented possibility of gaining insights into the atmosphere and climate of objects in the regime between rocky and gas planets that do not exist in the solar system. Detailed understanding of atmospheric processes, such as radiative transfer, convection, and disequilibrium chemistry, is key for the interpretation of such spectral detections.

The atmospheres of terrestrial planets lying in the habitable zone of their respective host stars could be from H$_2$–He-dominated, to H$_2$O-, CO$_2$-, and N$_2$-dominated, or even O$_2$- or CO-dominated for warmer and cooler planets, respectively (see, e.g., Forget & Leconte 2014; Madhusudhan et al. 2016).

A main motivation for our model development is as follows. The radiative transfer schemes, based on the k-distribution method, implemented in previous versions of our model, as well as other similar models developed for the study of terrestrial planets (e.g., Segura et al. 2010; Kopparapu et al. 2013), rely on premixed k-tables for atmospheric conditions, such as pressure, temperature, and composition. Especially the latter can be a considerable restriction for simulating atmospheres that are more and more different from that of Earth. Adding radiation-absorbing constituents often requires a recalculation of all k-tables. The same applies for including updates of line lists, for example, for one constituent. There are, however, multiple ways of treating the overlap of spectral absorption lines of gaseous components in k-distribution radiative transfer calculations for more flexibility, assuming perfect correlation, random overlap, or disjoint lines (see, e.g., Pierrehumbert 2010). Lacas & Oinas (1991) described how the overlap of absorption by gaseous components can be treated quickly and accurately using the random overlap assumption in...
the $k$-distribution method, which has been implemented and tested for hot Jupiter studies by Amundsen et al. (2017). Malik et al. (2017) recently developed a GPU-based open-source radiative transfer model using the faster assumption of perfect correlation between spectral lines of different molecules in the correlated-$k$ approximation for studying hot Jupiters and other planets with primary atmospheres. This assumption, however, becomes less accurate the more absorbers are present. While $k$-distribution models operate in cross-section space, Kitzmann (2017) used opacity sampling in his CO$_2$ cloud studies, which can be seen as a degraded line-by-line (LBL) radiative transfer model. Then, the addition of absorbing gases is fully additive, but opacity sampling is generally computationally more expensive than the $k$-distribution method and becomes less accurate for lower pressures, where many thin absorption lines can be missed by wavelength discretization. Lincowski et al. (2018) adopted a different approach by introducing an LBL radiative transfer module into a climate-chemistry model using the linearized flux evolution approach (Robinson & Crisp 2018) in order to reduce the number of time-consuming radiative transfer calculations for the study of terrestrial climates. This approach is fast as long as changes in important parameters influencing radiative fluxes, such as temperature and composition of major absorbers, are small. In that case, fluxes are approximated by linear flux gradients stored in a Jacobian for the last calculated state, rather than invoking full radiative transfer calculations.

Our new radiative transfer model, REDFOX, using the random overlap assumption, aims to combine the flexibility with regard to stellar spectra and atmospheric conditions similar to an LBL model but with calculation times approaching those of other $k$-distribution models using the correlated-$k$ approach. A central aim of this work is to show our new extensive capabilities for studying terrestrial exoplanets with REDFOX as part of our 1D coupled climate-chemistry model, 1D-TERRA.

In Section 2, we provide information on general climate and chemistry model updates that lead to our new 1D climate-chemistry model 1D-TERRA. Section 2.1 focuses in detail on the essentials of REDFOX, including the $k$-distribution method using the random overlap approximation. Section 3 validates REDFOX against known properties of atmospheres in the solar system. Section 4.2 presents our results for the super-Earth/sub-Neptune K2-18b before our final remarks in Section 5.

2. Methodology

Our 1D coupled climate-chemistry model has a long heritage dating back to, e.g., Kasting & Ackerman (1986), Pavlov et al. (2000), and Segura et al. (2003) for the study of Earth-like planets. Since then, it has been extensively updated in our group by, for example, Rauer et al. (2011), Grenfell et al. (2012), and Scheucher et al. (2020). Von Paris et al. (2008, 2010, 2015) implemented MRAC, a modified version of the rapid radiative transfer model (RRTM; Mlawer et al. 1997) for CO$_2$-dominated atmospheres in the climate module to study, e.g., early Mars or planets at the outer edge of the habitable zone. Our new radiative transfer module, REDFOX, is designed to operate over a wide range of stellar energy spectra, as well as diverse neutral composition (without ion chemistry) and pressure-temperature conditions in terrestrial atmospheres.

Grenfell et al. (2007), Tabataba-Vakili et al. (2016), and Scheucher et al. (2018) implemented parameterizations of cosmic rays and stellar energetic particles into our chemical solver. The latter can be part of an extensive model suite, calculating the precipitation of energetic particles through a magnetosphere and atmosphere, induced atmospheric ionization, and the impact on climate and neutral atmospheric composition, as described in Herbst et al. (2019). In conjunction with the companion paper (Wunderlich et al. 2020), we briefly describe in Section 2.3 key aspects of our extensively updated chemical reaction scheme that can simulate diverse terrestrial atmospheres.

The new model with updated climate and chemistry will be referred to as 1D-TERRA. Figure 1 provides a schematic overview of the 1D-TERRA model.

For postprocessing, we use the Generic Atmospheric Radiation Line-by-line Infrared Code (GARLIC; e.g., Schreier et al. 2014, 2018a, 2018b) to calculate planetary transit and emission spectra as described in, e.g., Scheucher et al. (2018) and Wunderlich et al. (2020).

2.1. Radiative Transfer Module REDFOX

REDFOX calculates radiative transfer for discrete intervals, or bands, in the spectral range from $v = 0$ to $10^{4}$ cm$^{-1}$, where any of the spectral intervals can be used for the short-wave (SW) and long-wave (LW) treatment of radiative transfer to allow for, e.g., more complete coverage of the irradiation of late-M dwarfs. Also, in the LW, the choice of the spectral interval is now flexible to include colder, temperate, and warmer planets alike. In addition, we extended the pressure and temperature range for the correlated-$k$ calculations so that absorption by, for example, O$_3$, H$_2$O, CO$_2$, and CH$_4$ can also be treated for planets close to the inner edge of the habitable zone, where evaporation of water can lead to surface pressures higher than 1.5 bars, which was our previous pressure limit for Earth-like atmospheres. Note that von Paris et al. (2010) implemented absorption by CO$_2$ and H$_2$O for pressures up to 1000 bars for a high-CO$_2$ atmospheric study without trace gases in an earlier model version. In contrast, our extended range now includes absorption by all molecules presented in Table 1, which, e.g., also allows for modeling steam atmospheres, habitable zones, and the upper atmospheres of sub-Neptunes or other H$_2$-dominated atmospheres.

2.1.1. Calculation of VIS/IR Cross Sections

In the random overlap method, cross sections calculated for each gas constituent separately are then cross-correlated in the radiative transfer calculations of atmospheric transmission functions. For the calculation of spectroscopic cross sections, we use the HITRAN 2016 line list (Gordon et al. 2017) and the open-source KSPECTRUM code originally developed by Eymet et al. (2016). We downloaded KSPECTRUM1.2.09 in 2017, included the treatment of HITRAN 2016 in KSPECTRUM, and also implemented the Total Internal Partition Sums (TIPS) from Gamache et al. (2017), used to calculate temperature conversion factors applied to line intensities, into what we now refer to as KSPECTRUM_Htr16. In 2018, KSPECTRUM1.3 was released with updates on CO$_2$ treatment. These updates, e.g., removed the possibility of line truncation...
when sub-Lorentzian wings are used. Since we decided to cut line wings and add missing contributions from far wings with collision-induced absorption (CIA), these modifications are not included in our calculations. A short discussion of our approach follows below. Our KSPECTRUM_Htr16 source code is available on our group’s software page. For the spectral discretization of the Voigt profiles, we define line center regions up to 10 half-widths (HWs) from the nominal line center wavenumbers, which are calculated at 8 points per HW and 16 points in the far wings and use a cutoff at 25 cm$^{-1}$ from the line center for every molecule (see below). After extensive testing on numerous computing platforms (not shown), the abovementioned parameter set for spectral discretization represented a reasonable trade-off between accuracy and computing time (<several months for low pressures). KSPECTRUM also has one integrated discretization algorithm that aims to keep the error from discretizing the Voigt profiles below a user-defined value. Unfortunately, this algorithm becomes computationally inefficient for low pressures where lines are very narrow, leading to a sharp increase in points needed for the wavenumber grid discretization. Our choice of discretization showed less than $10^{-5}$ relative deviation in resulting cross sections from results using that error-limited algorithm for tests at 1 Pa (and even less deviation at higher pressures), except for H$_2$O, which showed higher deviations of up to 1%. It is noteworthy that calculation times for cross sections should go down significantly with the use of GPU-based algorithms, such as, e.g., Helios-k (Grimm & Heng 2015). The trade-off between wavenumber discretization and accuracy is a common challenge in molecular absorption modeling, and different LBL codes use different approaches for the grid discretization and interpolation to speed up calculations; see, e.g., Schreier (2006) for a discussion.

Further, one has to be careful with regard to which line cutoff value to choose (Figure 2). Appropriate line-wing cutoff parameterizations, together with the right pressure-broadened wing profiles, are still debated in the literature (see, e.g., Sharp & Burrows 2007; Takagi et al. 2010; Grimm & Heng 2015; Hedges & Madhusudhan 2016). It is beyond the scope of this paper to outline all proposed theories, discussions, and possible assumptions surrounding this topic; instead, we would like to quickly motivate our choices. Assuming we could produce all true line-wing shapes, their deviation from Lorentzian profiles and their changes with temperature, pressure, and composition, adding up the contribution of all absorption lines to infinity may, theoretically, reproduce most known spectral features, including absorption bands, window regions, and possibly some continua. Unfortunately, many line wings differ substantially from the classical Lorentzian approximation. Clough et al. (1992) already argued that the super-Lorentzian nature of H$_2$O absorption is too complex to parameterize with wing shapes and rather developed continuum parameterizations to be used in addition to LBL calculations with a 25 cm$^{-1}$ cutoff. The sub-Lorentzian nature of CO$_2$ line wings has proven to be even more difficult, since numerous major absorption bands need their own parameterization (see, e.g., Perrin & Hartmann 1989; Pollack et al. 1993; Tonkov et al. 1996). Therefore, a multitude of continuum and CIA parameterizations have emerged (see, e.g., Gruszka & Borysow 1997; Baranov et al. 2004). Sharp & Burrows (2007) recommended a general pressure-dependent cutoff, $d = \min(25p, 100)\$cm$^{-1}$, with $p$ being the atmospheric pressure in atm, leading to cutoff values
>25 cm$^{-1}$ for pressures >1 atm and therefore being important for high-pressure atmospheric studies, such as gas planet atmospheres. Wordsworth et al. (2010a) conducted a thorough comparison of a 25 cm$^{-1}$ cutoff versus untruncated line wings for CO$_2$, together with various CIA parameterizations. Following these and similar studies, some authors studying terrestrial atmospheres started adopting larger cutoff values of 500 cm$^{-1}$ (e.g., Kopparapu et al. 2013) or even untruncated line shapes for selected molecules (e.g., Wordsworth et al. 2010b; Wordsworth & Pierrehumbert 2013).

Figure 2 suggests that taking into account the far wings of all absorption lines of a specific molecule over the whole wavenumber range may reproduce certain parts of continuum absorption in specific wavelength ranges but at the same time may overestimate absorption in other spectral regions where the addition of many Lorentzian line wings from the whole absorption spectrum would create additional artificial continua not observed in experiments. For pressures above a few bars, this effect can effectively mask any CO$_2$ or H$_2$O absorption not observed in experiments. For pressures above a few bars, this effect can effectively mask any CO$_2$ or H$_2$O absorption not observed in experiments. For pressures above a few bars, this effect can effectively mask any CO$_2$ or H$_2$O absorption not observed in experiments. For pressures above a few bars, this effect can effectively mask any CO$_2$ or H$_2$O absorption not observed in experiments. For pressures above a few bars, this effect can effectively mask any CO$_2$ or H$_2$O absorption not observed in experiments. For pressures above a few bars, this effect can effectively mask any CO$_2$ or H$_2$O absorption not observed in experiments.

Since we calculate absorption cross sections for pure gases of a given molecule (Table 1) separately, we can only account for self-broadening and not foreign broadening of absorption lines. Since pressure broadening of any given molecule by the total atmospheric gas pressure is therefore approximated by self-broadening for that pressure environment, this could become relevant for trace species in high-pressure environments for which self-broadening coefficients could differ significantly from their foreign-broadening coefficients. That said, one should note that the foreign broadening listed in HITRAN refers to (Earth) air broadening only, which should be used with caution for non-Earth-like atmospheres as discussed, e.g., by Wordsworth & Pierrehumbert (2013). For selected molecules, however, there exist more general pressure-broadening descriptions in the Exomol database (Tennyson et al. 2016). To tackle this problem consistently for any species of interest would require a tabulated parameter for broadening by any possible major constituent in an atmosphere of interest. Then the line wings would have to be calculated in LBL calculations using, e.g., the broadened HW $\gamma = \text{vmr}_{\text{self}} \cdot \gamma_{\text{self}} + \sum_i (\text{vmr}_i \cdot \gamma_i)$, with vmr being the volume mixing ratio and $i$ any atmospheric constituent other than the considered species itself. This then needs to be tabulated in premixed $k$-tables in $n$ dimensions for $n$ major constituents of interest calculated on a discrete volume mixing ratio grid, which would somewhat contradict our main aim here, namely a flexible radiative transfer model that is also straightforward to update with additional molecules of interest.

High-resolution cross-section lists have been calculated in this work for each of the 20 HITRAN 2016 molecules shown in Table 1 on a pressure–temperature grid for a total of 121 points. We thereby considered 11 pressures equally spaced in log($p$) ranging from $10^{-3}$ to $10^3$ bars, or 0.01–1000 Pa, and the following 11 temperatures: $T(K) = [100, 150, 200, 250, 300, 350, 400, 500, 600, 800, 1000]$. Studies calculating the outgoing LW radiation (OLR) of hot atmospheres ($\geq$800 K), e.g., Kopparapu et al. (2013) and Katyal et al. (2019), have shown that these cases may require the calculation of cross sections from databases that focus on high temperatures, such as HITEMP (Rothman et al. 2010) or Exomol (Tennyson et al. 2016).
2016), although our Venus validation (Section 3) suggests that this effect may not be central for the atmospheres studied here.

2.1.2. k-distributions and Spectral Bands

The k-distributions are cross-section ($\sigma$) probability distributions within a frequency band, represented by a small number of k-coefficients and respective weighting quadratures. For a detailed description of the k-distribution method and the implementation of the Random Overlap approximation with the “Ranking and Reblocking” or “Resorting and Rebinning” RORR method, we refer to, for example, Lacis & Oinas (1991) or Amundsen et al. (2017). The assumption behind random overlap is that absorption lines of individual molecules are uncorrelated. Although computationally more expensive than the simple addition of all molecular cross sections with their respective concentrations, this assumption is certainly a good approximation when including multiple molecules of different shapes and sizes as we do here, leading to very different roto-vibrational and translational absorption features. In random overlap, k-distributions—or $\sigma$-distributions, to be more precise—need to be calculated separately for every pressure $p$, temperature $T$, and molecule. To calculate individual k-distributions from cross sections, we make use of the KDISTRIBUTION package, developed by V. Eymet, for easy handling of high-resolution cross-section files previously generated by KSPECTRUM. While we require REDFOX to be as flexible as possible in handling different gas mixtures and atmospheric conditions, note that we will lose any frequency dependence within spectral bands when converting cross sections into k-distributions. The k-coefficients of different gas mixtures within one band will not generally map to the same frequencies as in a different gas mixture. This means that we cannot directly map a given source function such as a stellar spectrum or atmosphere Planck function, or other opacity sources like Rayleigh scattering coefficients, continua, or aerosols, into individual k-coefficients. These have to be added as band-integrated averages. For this reason, individual bands should be as small in frequency range as possible to minimize inaccuracies introduced by using the abovementioned band mean values, while at the same time being fast enough for climate evolution studies. We tested different bandwidths for an Earth-like atmosphere ranging from the original bands (38 for SW, 25 for LW) up to 480 bands over the whole spectral range (not shown). We chose 128 bands in total between $\nu = 0 \text{ cm}^{-1}(\lambda = \infty)$ and $\nu = 10^5 \text{ cm}^{-1}(\lambda = 100 \text{ nm})$, as further increases in band numbers resulted in OLR changes of <1%. Bands are evenly spaced in log($\nu$) above $\nu = 100 \text{ cm}^{-1}$, plus 10 bands with $\Delta \nu = 10 \text{ cm}^{-1}$ in the range $\nu = 0$–100 cm$^{-1}$. The design is such that we can subsequently change the spectral bands for a specific study if accuracy or computational efficiency become an issue. Such a change requires only recalculation of $k$-distributions from the high-resolution (8 points per HW) cross-section files, which takes approximately a total of 24 hr on 100 CPUs on our university server for all 20 molecules and 121 $p-T$ points currently included. Details on band-averaged sources and opacities follow later in this section.

Additionally, one must choose a suitable number of quadrature weights or k-coefficients within a band and the quadrature rule. The quadrature rule used in previous versions of our code dates back to the RRTM (Mlawer et al. 1997) and is a modification of the half Gauss–Legendre weighting, placing more emphasis on the absorption line centers ($g \sim 1$), as described in their paper. We use those quadratures for comparison, since their weighting was specifically designed to well resolve the line center absorption for cooling rates in Earth’s atmosphere. For exoplanet applications, however, we cannot generally assume that the main contribution to cooling rates arises mainly from the line centers alone; there can be additional cooling, e.g., from extensive broadening at higher pressures or temperatures. To test this, we also calculate $k$-distributions by applying the standard Gauss–Legendre quadrature rule using the 16th-order Legendre polynomial $P_{16}(\theta)$ shifted to the [0,1] interval. For transmission $T$ through a homogeneous layer, this is

$$T = \int_0^1 f(g) dg = \frac{1}{2} \sum_{i=1}^{16} w_i \left( \frac{1 + g_i}{2} \right),$$

(1)

with $g_i$ being the $i$th root of $P_{16}$ and $f = \exp(-\Delta \tau/\mu)$, where $\mu = \cos \Theta$ and $\Theta$ is the mean zenith angle used in the two-stream approximation. As given by Abramowitz & Stegun (1972), the associated quadrature weights $w_i$ are a function of the derivatives of $P_{16}$, specifically,

$$w_i = \frac{2}{(1-g_i)^2 P_{16}'(g_i)^2}, \quad \sum_i w_i = 1.$$

(2)
We tested 8th-, 16th-, 20th-, and 24th-order Legendre polynomials and corresponding weights in an Earth atmosphere setting with the 128-band model but did not find any significant differences (<10^{-3} W m^{-2}) in total up/down radiative fluxes above 16th order (not shown). In comparison, Malik et al. (2017) used 20th-order Gauss–Legendre polynomials after comparing to Simpson’s rule integration for their radiative transfer code. Table 2 shows a comparison of the quadrature weights used in the RRTM and the Gauss–Legendre weights (Equation (2)). One can see the emphasis placed in the RRTM upon probability function values close to unity, indicated by very small values for weights \( i > 10 \), together only representing the largest \( \sim 1\% \) of absorption cross sections within a band. On the contrary, Gauss–Legendre weighting is symmetric around medium values of cross sections within the band, and the largest and smallest 1.3\% of values are represented collectively in weights 16 and 1, respectively. The representative cross-section value \( \sigma_i \), or \( k \)-coefficient, corresponding to a quadrature of weight \( w_i \) is then simply the arithmetic mean of the cumulative cross-section function within the respective quadrature.

### 2.1.3. Continuum Absorption

The CIA is taken from the HITRAN CIA database (Karnman et al. 2019). A complete list of the currently implemented CIAs in REDFOX is shown in Table 3. Since the HITRAN CIA formatting is identical, any missing CIA from the list can be flexibly added in REDFOX for a specific study. Additionally, REDFOX utilizes MT_CKD (Mlawer et al. 2012) version 3.2.\(^{11}\) Although originally developed for the H\(_2\)O continuum, this now also includes continua for other molecules. In REDFOX, one can choose which CIA and MT_CKD continua from Table 3 are used. These continua are first calculated on a finer grid with 10 points per band using the same interpolation method as for MT_CKD in LBLRTM (Clough et al. 1992, 2005), which gives the cross sections

\[
\sigma_i = -\sigma_{j-1} \left[ \frac{f_\nu}{2} (1 - f_\nu)^2 \right] + \sigma_j \left[ 1 - (3 - 2f_\nu)f_\nu + \frac{f_\nu^2}{2} (1 - f_\nu) \right] + \sigma_{j+1} \left[ (3 - 2f_\nu)f_\nu + \frac{f_\nu^2}{2} (1 - f_\nu)^2 \right] + \sigma_{j+2} \left[ \frac{f_\nu}{2} (1 - f_\nu) \right],
\]

with

\[
f_\nu = \frac{\nu_i - \nu_j}{\nu_{j+1} - \nu_j},
\]

where \( i \) are the 10 grid points in a band interval and \( j \) are linearly interpolated from tabulated cross sections at neighboring temperatures from either MT_CKD or HITRAN CIA, where applicable. Values at the band boundaries are linearly interpolated from tabulated values at neighboring frequencies. We tested different numbers of points per band for the interpolation, but convergence was found for 10 or more points per band. From these interpolated cross sections, band-integrated averages are calculated via \( 1/(\Delta
\nu_{\text{band}}) \sum_{i=1}^{n}(\sigma_i \Delta
\nu_i) \) and added to other opacity sources with their corresponding volume mixing ratio.

### 2.1.4. UV/ VIS Cross Sections

In the current version of 1D-TERRA, we include 81 absorbers from the MPI Mainz Spectral Atlas (Keller-Rudek et al. 2013) in the visible, UV, and far-UV (FUV) range. These were initially chosen for the photochemistry module as described in Section 2.3 but are also available for radiative transfer in REDFOX. Where available, we follow the recommendation of the JPL Evaluation 18 (Burkholder et al. 2015). Otherwise, we took the latest reference in the JPL report, unless the data coverage was poor. The full list of cross-

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\(^{11}\) http://rtweb.aer.com/continuum_frame.html
Table 4
List of Parameters for the Rayleigh Cross-section Calculations

| Molecule | A   | B   | D       |
|----------|-----|-----|---------|
| CO       | 32.7| 8.1 | $9.49 \times 10^{-3}$ |
| CO₂      | 43.9| 6.4 | $8.05 \times 10^{-2}$ |
| H₂O      | ... | ... | $3.00 \times 10^{-4}$ |
| N₂       | 29.06| 7.7 | $3.05 \times 10^{-2}$ |
| O₂       | 26.63| 5.07| $5.40 \times 10^{-2}$ |

Notes. Here A and B from Allen (1973) and Vardavas & Carver (1984) are used for the refraction approximation; D (Sneep & Ubachs 2005) is for depolarization in the King factor $K_{\lambda}$. * Murphy (1977).

section data used in the climate and chemistry model is given in the companion paper (Wunderlich et al. 2020). These cross sections are arithmetically averaged into the corresponding REDFOX bands and added to the other opacities discussed above. For the remaining HITRAN absorbers in the band, the UV/VIS cross sections are directly added to the $k$-distributions for cross-correlation using the random overlap approach, as described earlier. In this case, UV/VIS cross sections are interpolated and band-averaged from the MPI Mainz Spectral Atlas data with the same method as described in Section 2.1.3 for the continua. They are used in the spectral range from the highest available energies or wavenumbers ($10^7$ cm$^{-1}$ in the current version) up to the band with the first HITRAN data point of the given species. This approach was chosen to avoid accounting for absorption of a given species twice (i.e., in both the HITRAN and MPI Mainz databases). In overlapping data regions, we preferentially chose line list data rather than measured cross sections because the latter could also include experimental noise between absorption features, which would add artificial UV “continua” to our heating rates. For molecules where line list data were not included in a certain band, the cross sections are simply added as mean opacities per band in the same way as the continua are added in Section 2.1.3.

2.1.5. Rayleigh Scattering

Rayleigh scattering is included in our model (see also von Paris et al. 2015) for CH₄, CO, CO₂, H₂, H₂O, He, N₂, and O₂. The Rayleigh scattering cross sections (cm$^2$) for CO, CO₂, H₂O, N₂, and O₂ are calculated using (Allen 1973)

$$\sigma_{\text{Ray, } i}(\lambda) = \frac{32\pi^3}{3n^2} r_i^2 K_{\lambda i},$$

and with number density $n = 2.688 \times 10^{19}$ cm$^{-3}$ for standard temperature and pressure (STP),

$$\sigma_{\text{Ray, } i}(\lambda) = 4.577 \times 10^{-21} r_i^2 K_{\lambda i},$$

where $\lambda$ is in μm, $r_i$ represents the refractive index ($n - 1$) of species $i$, and the “King factor” $K_{\lambda i}$ is a correction for polarization, given by

$$K_{\lambda i} = \frac{6 + 3D_i}{6 - 7D_i},$$

with $D_i$ being the depolarization factor calculated from Sneep & Ubachs (2005) shown in Table 4. Further, for CO, CO₂, N₂, and O₂, the refractive index $r$ is approximated using

$$r = \left(1 + \frac{3 \times 10^{-3} B_i}{\lambda^2}\right),$$

with the two additional parameters $A_i$ and $B_i$, also shown in Table 4, and $\lambda$ again in μm. For H₂O, the refractive index is calculated as $n_{\text{H₂O}} = 0.85 r_{\text{dry air}}$ (Edlén 1966), with the approximation for the refractive index of dry air (Bucholtz 1995):

$$r_{\text{dry air}} = 10^{-8} \left(\frac{5.7918 \times 10^6}{2.38 \times 10^3 - \lambda^2} + \frac{1.679 \times 10^5}{57.362 - \lambda^2}\right).$$

Rayleigh scattering cross sections for H₂, He, and CH₄ are included using reference measurements of $\sigma_{\text{Ray, } i}$ at wavelengths $\lambda_{0,i}$ from Shardanand & Rao (1977) shown in Table 5. These cross sections are then approximated for other wavelengths using the simple $\lambda^{-4}$ relationship:

$$\sigma_{\text{Ray, } i}(\lambda) = \sigma_{\text{Ray, } i}(\lambda_{0,i})^4,$$

where $\sigma_{\text{Ray, } i}$ of species $i$ are given in cm$^2$ molecule$^{-1}$, $\lambda$ is the wavelength of interest in μm, and $\lambda_{0,i}$ is a reference wavelength where $\sigma_{\text{Ray, } i}$ was measured. In REDFOX, we updated the calculation of band-integrated scattering cross sections, which is now performed for all spectral bands, rather than only the SW bands. The band mean values are now calculated from one specific wavelength per band, representative of the band-integrated average. We emphasize that this does not correspond to the band-mid wavelength. Instead, we use the equivalence of the integrals,

$$\int_{\lambda_i}^{\lambda_2} \lambda^{-4} d\lambda = \int_{\lambda_i}^{\lambda_2} \lambda_{\text{Ray}}^{-4} d\lambda = \lambda_{\text{Ray}}^{-4} \int_{\lambda_i}^{\lambda_2} d\lambda$$

$$\Rightarrow \lambda_{\text{Ray}} = \left(\frac{\lambda_i^{-3} - \lambda_2^{-3}}{3(\lambda_2 - \lambda_i)}\right)^{-\frac{1}{3}},$$

to determine the representative wavelength $\lambda_{\text{Ray}}$ for the Rayleigh cross-section calculations in each band ($\lambda$ in Equations (6) and (8)–(10)). Then, the choice of the radiative transfer method (see Section 2.1.7) defines in which bands the Rayleigh scattering opacities are used.

2.1.6. Source Functions

We consider essentially two radiative sources: incident stellar flux and thermal radiation from the planetary surface and the atmosphere. Stellar spectra can be taken either directly from

Table 5
List of Measured Reference Rayleigh Cross Sections $\sigma_{\text{Ray, } i}$ at Wavelength $\lambda_{0,i}$ from Shardanand & Rao (1977)

| Molecule | $\sigma_{\text{Ray, } i}$ (cm$^2$) | $\lambda_{0,i}$ (μm) |
|----------|-------------------------------|-------------------|
| H₂       | $1.17 \times 10^{-27}$        | 0.5145            |
| He       | $8.6 \times 10^{-29}$         | 0.5145            |
| CH₄      | $1.244 \times 10^{-26}$       | 0.5145            |

(Allen 1973)
the MUSCLES database\textsuperscript{12} or from the VPL webpage.\textsuperscript{13} The solar spectrum is taken from Guéymard (2004). Spectra that do not cover the entire wavelength range were extended with the NextGen 4 spectrum of the corresponding effective temperature of the star up to 971 \(\mu\)m (Hauschildt et al. 1999). We first perform a logarithmic interpolation of the spectra to a constant resolution of 1 Å over the entire wavelength range and then bin the data into our 128 bands using an arithmetic mean.

Thermal blackbody emissions from the planetary surface and every atmospheric layer are calculated for 101 points (100 intervals) per band distributed equally in \(\nu\) following Planck’s law in wavenumbers:

\[
B_{\nu}(\nu, T) = \frac{2hc^2\nu^3}{e^{\frac{hc\nu}{kT}} - 1}.
\] (12)

Then, a simple arithmetic mean is taken as the average blackbody source term in the given band and atmospheric layer. We tested this simple method against the computationally slightly more expensive trapezoidal rule in the Earth and Venus atmosphere runs but found no significant (<10\(^{-4}\)) differences in cooling rates or atmospheric temperature structure. This suggests that our band model features sufficiently small bandwidths. For this reason we chose the faster band mean calculations explained above.

2.1.7. Opacities and Transmission Functions

Once all individual \(k\)-coefficients \(\sigma_i\) are calculated, they are mixed for the atmosphere of interest. In random overlap, \(\sigma_{ij,nn,b}\) in units of cm\(^2\) molecule\(^{-1}\) of two molecules \(m\) and \(n\) and their respective quadratures \(i\) and \(j\) in band \(b\) are cross-correlated when performing radiative transfer calculations by

\[
\sigma_{ij,nn,b} = \frac{\sigma_{ij,nn} + \sigma_{ij,nn} - \sigma_{ij,nn} - \sigma_{ij,nn}}{\chi_m + \chi_n},
\] (13)

where \(\chi\) is the respective volume mixing ratio, and individual \(k\)-coefficients \(\sigma\) are linearly interpolated in \(T\) and \(\log(p)\) from the precalculated \(k\)-distributions. The corresponding 16 \(\times\) 16 quadrature weights as a result of mixing the \(k\)-coefficients from two molecules are

\[
w_{ij} = w_iw_j,
\] (14)

with \(i\) and \(j\) each taking integer values from 1 to 16, as shown in Table 2. In REDFOX, we use quicksort (Press et al. 1992) to sort the mixed \(\sigma_{ij}\) and corresponding \(w_{ij}\) again as a monotonically increasing function, or \(k\)-distribution. Before adding new molecules to the mix, we bin the mixed distribution back into the original 16 quadratures (\(g = 1\)–16). For the respective mean \(k\)-coefficients \(\sigma\), individual \(\sigma\)'s are added where the cumulative weights \(w_{c,ij}\) of the mix lie in the range \(w_{c,i-1} < w_{c,ij} < w_{c,i}\) of the original quadrature with weight \(w_i\). The new \(k\)-coefficients are then calculated as

\[
\sigma_{c,nn} = \frac{\sum_{i=1}^{g} w_i w_{ij}}{w_{ij}, w_{ij}, w_{ij}, w_{ij}} \sigma_{ij,nn},
\] (15)

Contributions of mixed quadratures that overlap with the boundaries of the original 16 quadratures are factored into the corresponding \(\sigma\) accordingly. This process is repeated for every molecule added to the gas mixture. Depending on the composition of the atmosphere of interest, one cannot expect that all constituents are accounted for by our absorbers, especially when we choose to exclude specific constituents from radiative transfer calculations e.g., for performance reasons, studies of individual gas contributions, or when noble gases are excluded in calculations because they would not contribute significantly to the radiative energy budget. Since Equation (13) assumes the absorbing contribution of all constituents, we calculate the total mixing ratio of the absorbing species \(\chi_{n_{mix}}\) along with the \(k\)-coefficients and correct the cross sections of the mixture using \(\sigma = \sigma' \cdot \chi_{mix}\). This approach is especially appropriate for Earth’s atmosphere, where \(N_2\) accounts for approximately 78% of molecules while not contributing significantly to absorption. In this case, calculations can be sped up significantly when we exclude nonsignificantly absorbing species from the radiative transfer calculations.

Once opacities \(\tau = \sigma_du\), with \(u\) being the respective column density, are calculated, other previously described band-integrated opacities can be added flexibly. Radiative transfer is solved together with Rayleigh scattering, for which we use the quadrature \(\delta\)-two-stream approximation (Meador & Weaver 1980; Toon et al. 1989) for SW radiative transfer. For the thermal outgoing LW radiative transfer, we have the option to use either the Toon et al. (1989) hemispheric mean two-stream approximation, including Rayleigh scattering and with Planck emissions instead of the stellar component, or the faster diffusivity approximation (Mlawer et al. 1997) without scattering. In this case, the radiative transfer equation is solved for the single angular point \(\mu = \frac{1}{1.66}\), corresponding to a polar angle \(\theta = 52^\circ 95\) (Elsässer 1942), and the linear-in-tau approach for the Planck functions (Clough et al. 1992). While implementations of the abovementioned radiative transfer solvers date back to Pavlov et al. (2000) and Segura et al. (2003), they are still useful in our cloud-free studies. Upcoming model updates including scattering by larger aerosols and cloud particles will include two-stream updates similar to Heng et al. (2018) and an option to use a discrete ordinates method, such as DISORT (e.g., Stamnes et al. 1988; Hamre et al. 2013), which will then allow for treatment of incident stellar beam, scattering, and internal source function, namely the Planck function of each layer, at the same time, ridding us of the SW–LW distinction necessary with the currently used two-stream approximations.

The globally averaged zenith angle \(\theta\) for the effective path lengths of the direct stellar beam through an atmospheric layer can be chosen by the user. Cronin (2014) pointed out that zenith angle and global mean averaged irradiation \(S\) have to be changed together according to the product \(S \cdot \cos \theta = S_0/4\), where \(S_0\) is the total stellar irradiation (TSI), and the factor 1/4 comes from the purely geometric derivation of the planetary cross section over the planetary surface area. Note that a simple

\[
w_{c,i} = \sum_{i=1}^{g} w_i \quad \text{and} \quad w_{c,ij} = \sum_{j=1}^{l} w_{ij}.
\] (16)
daytime-weighted global mean assumption, a zenith angle \( \theta = 60^\circ \) with \( S = S_0/2 \) is commonly used in the literature. Additionally, this approximation assumes a rapidly rotating planet, such that the incident stellar flux is effectively distributed over the entire planetary surface despite only illuminating half of the planet. This would obviously be different for tidally locked planets, where a more general parameter can be introduced that simulates the efficiency of heat redistribution from the permanent day to the nightside (see, e.g., Spiegel & Burrows 2010; Malik et al. 2017).

While aerosols and clouds can be treated to some degree in the two-stream approximation via extinction coefficients that depend on particle sizes, forms, and refractive indices (see, e.g., Kitzmann et al. 2010), we do not explicitly include such particles in the current work. We parameterize cloud behavior in a simple way by increasing the surface albedo and adjusting the effective path length in radiative transfer with a zenith angle deviating from the geometric mean value of 60°. The appropriate choice of albedo and zenith angle, however, is generally a degenerate problem.

With all of the model updates mentioned above, calculation times are nevertheless sufficient for our purposes. While calculating opacities plus radiative fluxes in MRAC for four absorbers in 25 LW bands and 38 SW bands plus Rayleigh scattering took ~180 ms, REDFOX with the same configuration takes ~235 ms. With our long list of LW and SW absorbers in our 128 bands, including MT_CKD and CIAs now takes ~1600 ms, all on a single CPU. This is still fast compared to full LBL calculations, which can take several minutes on a server node of 20 CPUs.

### 2.1.8. Key Features of REDFOX

The following is a summary of the key features of REDFOX in the configuration validated and applied in the current work.

1. Continuous \( k \)-distribution model with 128 spectral bands (16 g Gauss–Legendre).
2. Spectral range \( \nu = 10^5 \) cm\(^{-1} \) (100 nm) – 0 cm\(^{-1} \) (∞).
3. Pressure range 0.01 Pa – 10\(^5 \) bars.
4. Temperature range 100 – 1000 K.
5. 20 absorbers (HITRAN 2016); see Table 1.
6. 81 VIS/UV/FUV absorbers (MPI Mainz Spectral Atlas); see Table 1.
7. CIAs (HITRAN CIA list); see Table 3.
8. MTCKD_3.2; see Table 3.
9. Flexible choice of absorbers (SW/LW, CIA/CKD).
10. Flexible choice of SW/LW ranges for specific study.

### 2.2. Climate Module

The central tasks of the climate module are to calculate atmospheric and surface temperatures in radiative–convective equilibrium and temperature-dependent molecular abundances of condensible species, e.g., H\(_2\)O or CO\(_2\), in convective regions where temperatures change. The governing energy-conserving differential equation determining the temperature \( T \) profiles is (see, e.g., Pavlov et al. 2000

\[
\frac{dT}{dt}(z) = -\frac{g(z)}{c_p(T, z)} \frac{dF(z)}{dp(z)},
\]

where \( d/dt \) is the time derivative, \( g(z) \) is gravitational acceleration, \( c_p \) is the heat capacity of the atmospheric layer, \( F \) is the radiative flux, and \( p \) is the cell-centered pressure of the atmospheric layer at a mid-layer height \( z \). Equation (17) is discretized in the model using finite differences, resulting in \( dt \) being used as the finite time step. After the radiative temperature profile is calculated for a model time step, radiative lapse rates are compared in every layer with adiabatic lapse rates to determine where convective adjustment has to be performed (i.e., Schwarzschild criterion). The decision as to the appropriate adiabatic lapse rate (moist or dry) and whether \( H_2O \) or \( CO_2 \) is the condensing molecule in the moist case is based on the fraction of respective partial pressures over the corresponding saturation vapor pressure. Note that combined moist adiabatic lapse rates are not implemented. If \( CO_2 \) condensation occurs, the resulting lapse rate is a \( CO_2 \) moist adiabat, disregarding any possible \( H_2O \) contribution. The \( H_2O \) moist adiabatic lapse rates are calculated if \( H_2O \) condenses in the absence of \( CO_2 \) condensation. The \( H_2O \) profiles are calculated using prescribed relative humidity (RH) profiles, e.g., by Manabe & Wetherald (1967), for planetary scenarios with a water reservoir, i.e., an ocean, via

\[
\chi_{H_2O}(p) = RH(p) \frac{p_{sat, H_2O}(T(p))}{p},
\]

with \( p_{sat} \) being the saturation vapor pressure. The total surface pressure \( p_0 \) of the atmosphere is calculated via \( p_0 = p_{0, dry} + p_{0, H_2O} \); therefore, atmospheric pressures, and with them the mixing ratios of all atmospheric constituents, are adapted for those convective layers. For a detailed description of convective adjustment and \( CO_2 \) lapse rate calculations in our model, we refer to, e.g., Kasting (1991) and Kasting et al. (1993), as well as von Paris et al. (2008) for the water vapor treatment.

Heat capacities \( c_p \) for temperature and lapse rate calculations have historically been included in our model for different species using different approaches (for details, see, e.g., von Paris et al. 2008, 2010, 2015). The next 1D-TERRA update will come with updated \( c_p \) treatment. Therefore, we only give a brief summary of our currently used \( c_p \) calculations in the Appendix.

### 2.3. Photochemistry Module

The atmospheric composition profile of each species is calculated in the photochemistry module using the continuity-transport equation,

\[
\frac{\partial n}{\partial t} = \frac{\partial}{\partial z} \left(K \cdot \frac{\partial n}{\partial z} \right) + P - nL,
\]

where \( n \) denotes the number density of a certain species (cm\(^{-3} \)), \( P \) is the production term (cm\(^{-3} \) s\(^{-1} \)), \( L \) is the loss rate (s\(^{-1} \)), and \( K \) is the eddy diffusion coefficient (cm\(^2 \) s\(^{-1} \)). The loss and production rates are determined by the kinetic coefficients and boundary conditions. The companion paper (Wunderlich et al. 2020) describes the new photochemistry module BLACKWOLF with a flexible chemical network. The full network consists of 1127 reactions for 115 species, including photolysis for 81 absorbers.

The scheme can consider wet and dry deposition, as well as an upward flux at the surface for each species. Outgassing from volcanoes is treated as an upward flux equally distributed over
the lower 10 km of the atmosphere. At the top of the atmosphere (TOA), the module can calculate escape fluxes and parameterized effusion flux or use predefined values. Usually, we only consider O, H, and H2 to have an upper boundary flux. The profile of K can be either a fixed predefined profile or calculated in the model depending on the planetary atmosphere. See Wunderlich et al. (2020) for the calculation of K and more details on the photochemical module.

3. Model Validation

In this section, we restrict ourselves to the validation of the radiative transfer module, REDFOX, and its integration into the climate part of 1D-TERRA; thus, in some cases, we prescribe the atmospheric composition. The chemistry is validated separately in the companion paper (Wunderlich et al. 2020). We first validate for Earth standard conditions, then go on to Earth climate-change studies with increased amounts of CO2, before validating for other solar system planets, i.e., modern Venus and Mars, and then exoplanetary scenarios (i.e., Earth-like and steam atmospheres). In all cases, we discretize the atmosphere into 100 layers from the surface up to the TOA.

3.1. Modern Earth

Figure 3 shows our 1D-TERRA results in coupled climate-chemistry mode for US standard 1976 Earth atmospheric composition. We tune surface albedo and zenith angle for radiative transfer calculations together to achieve Earth global average surface temperatures of 288.15 K in our cloud-free model and an Earth-like global mean O3 column in the range 300–320 Dobson units (DU; see, e.g., Segura et al. 2010), which is achieved with a surface albedo of 0.255 and an angle \( \theta = 54^\circ 50\); thus, \( S = 0.4305 \ S_0 \), so that \( S \cdot \cos(\theta) = S_0 / 4 \), for all radiative transfer calculations in climate and chemistry. This agrees well with the fact that modern Earth is partially cloudy; this angle lies well in the range for a clear sky and fully cloud-covered planet (see, e.g., Cronin 2014). Note that zenith angles used in climate and chemistry calculations do not necessarily have to be the same; see, e.g., Hu et al. (2012) for a discussion. Unless stated otherwise, we will use this parameter set for all other tests and applications.

Temperature profiles with the original radiative transfer model MRAC (von Paris et al. 2015) were calculated using absorption by H2O, CO2, CH4, and O3, with the addition of O2 in one band (752–784 nm) for stellar absorption. Those with REDFOX are calculated with all 20 HITRAN absorbers from Table 1 with the addition of UV/VIS cross sections for CH2Cl, CH3, CO, CO2, H2O, HNO3, N2O, NO, O2, and O3 for wavenumbers above available HITRAN data, as described in Section 2.1.4. We calculate temperature profiles with two different \( k \)-distribution quadrature settings in REDFOX, as shown in Table 2, to determine which one compares better to observations. For this, we compare to the US standard atmosphere 1976, as well as Earth observation data from MIPAS (von Clarmann et al. 2009) and ACE-FTS (Boone et al. 2005). From both observation data sets, we show (gray shaded regions) the 95\% (2\( \sigma \)) range and the global annual mean temperature profiles (dotted lines). While we see generally good agreement between our calculated low and mid-atmospheric temperature profiles with the US standard atmosphere and the MIPAS and ACE-FTS data (see Figure 3), in all model runs using the double Gaussian quadratures, both updated (blue solid) and original model (black solid), the stratosphere peak lies slightly below US standard atmospheric values in both height and temperature, similar to other cloud-free 1D studies (see, e.g., Segura et al. 2003). Mesospheric temperatures in these cases lie slightly below the MIPAS and ACE-FTS 2\( \sigma \) ranges. Figure 3 suggests that Gauss–Legendre quadratures (orange) result in a temperature profile closer to US standard atmospheric values and global mean averages from observations up to \( \sim 70 \) km. The inclusion of the Gauss–Legendre quadratures therefore represents a major improvement in REDFOX.

Additionally, with the addition of O2 absorption cross sections in the UV Schumann–Runge bands, the model now clearly shows mesopause and thermospheric temperature inversions that were previously lacking (in MRAC). In this range, calculations with REDFOX using the double Gaussian quadratures compare better with the observations. However, we are not taking into account any UV absorption in the atmosphere above our TOA; hence, our O2 absorption might be slightly overestimated, leading to generally warmer mesopause values, especially visible in the calculations with the Gauss–Legendre quadratures. In previous studies with our 1D climate-chemistry model, the TOA was set to \( \sim 6 \) Pa due to the lack of O2 absorption in the UV, similar to, e.g., Segura et al. (2010), Kopparapu et al. (2013), and Ramirez et al. (2014), while other studies (e.g., Meadows et al. 2018) have set isothermal profiles above an arbitrary model pressure where model temperatures would otherwise strongly underestimate temperatures due to the missing physics.

Figure 4 shows the model TOA OLR for the two previously discussed different quadrature weightings (orange and blue) compared to LBL calculations with GARLIC (black). We use GARLIC with HITRAN 2016 and MT_CKD for H2O

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14 www.imk-asf.kit.edu/english/308.php
15 http://ace.scsat.ca/publications/
continuum, as in REDFOX. The spectral grid in GARLIC is discretized with \( \Delta \nu = \gamma / 4 \), and the Voigt profiles are cut at 25 cm\(^{-1} \). The TOA OLR calculated by GARLIC is 260.74 W m\(^{-2} \). Results for REDFOX using Gauss–Legendre quadratures (263.37 W m\(^{-2} \)) show very good agreement within 1.0%, while the double Gaussian quadratures (253.60 W m\(^{-2} \)) differ by 2.7%. Figure 4 suggests that fluxes estimated with the Gauss–Legendre method (orange columns) compare generally better with the LBL fluxes (black columns). Kopparapu et al. (2013) validated their \( k \)-distribution model, using the same double Gaussian quadratures, against a different LBL code, SMART (Meadows & Crisp 1996), for different terrestrial atmospheres, with deviations of the \( k \)-distribution model in the range between 2.7% and 4.0%, similar to our double Gaussian validation. Note that the RRTM (Mlawer et al. 1997), using the double Gaussian quadratures, was validated for Earth conditions to deviate by only \(<1\) W m\(^{-2} \) when compared to the same LBL model, namely LBLRTM, that was used to derive the \( k \)-distributions in the first place. Only in this way can one be certain to not mix in the differences between LBL models; see, e.g., Schreier et al. (2018a, 2018b) for an LBL model comparison. Based on this comparison, we now proceed using the Gauss–Legendre quadratures for the remaining validations and case studies.

### 3.2. Earth’s Climate Response to CO₂ Increase

Here we test our modeled climate response to increased levels of CO₂ and compare to results from studies of climate change on Earth. Rogelj et al. (2012) summarized results from an extensive list of 3D model studies and the International Panel on Climate Change (IPCC) report estimates for a doubling of CO₂ levels from the 1976 values of 326–652 ppm. Their findings suggest a resulting change in global mean surface temperatures in the range from +2.6°C to +3.6°C. Upon doubling CO₂, our resulting change in global mean surface temperatures of +2.8°C agrees very well with these works. Figure 5 presents our results for the 1976 CO₂ value (black) and gradually increased levels of CO₂ by factors of 2, 5, 10, and 100. We further see the typical behavior of CO₂ as a greenhouse gas, confining thermal radiation in the lower atmosphere, thus heating the troposphere while cooling the middle and upper atmosphere.

### 3.3. Steam Atmospheres

To further test H₂O absorption in REDFOX, we compute radiative fluxes output from REDFOX for the scenarios of the model intercomparison study by Yang et al. (2016) with fixed temperatures and atmospheric compositions. We took their values for Earth-like planets having a 1 bar N₂ atmosphere with 376 ppm CO₂ and H₂O steam that varies as a response to global mean surface temperatures between 250 and 360 K at saturation. With these added amounts of steam, the surface pressure changes accordingly (up to +0.5 bar), representing evaporation from oceans. Temperature profiles are set to 200 K isotherms above the tropopause. The study uses Earth-like global mean stellar irradiation of 340 W m\(^{-2} \) for all tests on specifying the abovementioned surface temperatures; thus, OLR does not balance incoming radiation. We specify the boundary parameters with REDFOX and plot output from both studies for different LBL and \( k \)-distribution models as shown in Figure 6. REDFOX compares well with the models shown and suggests the symptomatic OLR flattening for higher
temperatures toward the Kobayashi–Ingersoll limit (see, e.g., Nakajima et al. 1992; lower right), as well as the transition from optically thin to optically thick for thermal radiation in the first atmospheric layer above the surface due to the increased steam (lower left). Note that the compared models show quite large differences in those LW net fluxes for the surface layer (lower left) for the 300 K runs. This analysis for the transition from optically thin to optically thick is generally very sensitive to modeling parameters such as individual layer heights, used line lists and continua, or exact H2O, temperature, and pressure profiles. We read these profiles off the plots in Yang et al. (2016), which may have introduced extra differences in addition to the already large differences of the models originally compared in their study of up to ∼100%. To further clarify this, we plan on doing a thorough k-distribution model intercomparison in the future. For absorption of stellar radiation in the SW, both the radiation reaching the surface (upper left) and the backscattered radiation escaping again at the TOA (upper right) compare well with the other models.

Figure 6. Comparison of radiative fluxes under steam atmosphere conditions against the tested models in Yang et al. (2016).
3.4. Cloud-free Venus

While the above tests were performed for Earth-like planets, Figure 7 shows our temperature profiles for a cloud-free Venus calculated with 1D-TERRA in climate-only mode with prescribed atmospheric composition compared to the Venus International Reference Atmosphere (VIRA-1; Seiff et al. 1985) and a cloud-free Venus model result from Mendonça et al. (2015). For this test, we set the planetary parameters to represent Venus, e.g., with surface gravity \( g = 8.87 \, \text{m s}^{-2} \), surface pressure \( p_0 = 93 \, \text{bars} \), and solar constant \( 1.913 \, S_{\text{Earth}} \). and, due to the lack of cloud treatment in our model, we set the surface albedo to 0.755. Note, however, that due to the thick atmosphere, the influence of the surface albedo on the planetary atmosphere, the in

...
the double Gaussian quadratures (blue) for comparison to confirm that our choice of using the Gauss–Legendre quadratures is also justified for Venus and Venus-like planets.

In conclusion, for our Venus tests, results with REDFOX show slightly lower cooling rates (hence LW absorption) than the LBL model used by Haus et al. (2015) yet slightly higher overall LW absorption than the LBL model GARLIC, and temperatures compare well to measurements and other cloud-free model studies. In summary, we have shown that Venus temperatures, calculated with our new general-purpose climate model, compare very well with observations and other model studies designed to reproduce Venus.

3.5. Aerosol-free Mars

Our final validation, shown in Figure 10, is for an aerosol-free modern Mars scenario (orange). We compare temperatures modeled with 1D-TERRA in coupled climate-chemistry mode against the reference atmosphere of Haberle et al. (2017; black) for a low-dust scenario based on diurnal averages of observations from the MCS instrument (Kleinböhl et al. 2009). Also overplotted (green) are zonally averaged temperature ranges based on Mariner 9 IRIS data (Justus et al. 1996). As initial condition we set a 250 K isoprofile, Martian atmospheric composition of major species is taken from Owen et al. (1977), the water vapor profile and the profiles of minor species are taken from Nair et al. (1994). Mars’s planetary albedo of 0.29 (Clawson & J.P.L., 1991) is for most of the time throughout a Martian year (i.e., without global dust storms) dominated by the surface. Our cloud-free assumption in radiative transfer using a surface albedo of 0.290 is therefore reasonable. As Mars does not have a surface water ocean reservoir, we do not calculate tropospheric H2O profiles from RH profiles.

Our model results shown in Figure 10 compare reasonably well with Martian lower and upper atmospheric temperatures, while middle atmospheric temperatures are 10–30 K lower compared to Mars reference data. We are not parameterizing Mie scattering from aerosols in this work, which would lead to extra heating in the Martian lower to middle atmosphere, as discussed by, e.g., Gierasch & Goody (1972).

Figure 9. Same as Figure 4, but for cloud-free modern Venus conditions.

Figure 10. Validation for a hypothetically aerosol-free Mars. We compare temperatures calculated with 1D-TERRA (orange) to the Haberle et al. (2017) Mars reference atmosphere (black) and Mariner 9 IRIS data (green).

4. Application to K2-18B

We apply 1D-TERRA to the super-Earth/sub-Neptune planet K2-18b with recently analyzed atmospheric infrared features from combined Kepler K2, Hubble WFC3, and Spitzer observations (Benneke et al. 2019b; Tsiaras et al. 2019). This marks the first detection of H2O in the atmosphere of an exoplanet smaller than Neptune and Uranus. Planet K2-18b has a mass of $8.63 \pm 1.35 M_{\oplus}$ and orbits an M2.5 host star $(0.0234 L_\odot)$ at 0.1429 au with a resulting TSI = $1.1459 TSI_\odot$. For the host star, K2-18, we use the stellar spectrum from GJ 176, an M2.5 star similar to K2-18 in stellar properties, available in the MUSCLES database, and prepare it as described in Section 2.1.6. The planetary radius of K2-18b was recently updated from 2.27 to 2.711 $R_{\oplus}$ due to reanalysis of K2-18’s stellar radius by Cloutier et al. (2019). Planetary radius calculations are based on the 4.5 $\mu m$ Spitzer band transit depths. We apply a simple mass–radius
parameterization from Noack et al. (2016) to estimate gravity at the surface–atmosphere boundary layer and find that the original radius estimate of 2.27\(R_\oplus\) could still be interpreted as a rocky planet with an ice-mass fraction of 35%–62% and a core-mass fraction <35%. These estimates lead to a surface gravity of \(g \sim 15 \text{ m s}^{-2}\). The updated radius of 2.71\(R_\oplus\), however, cannot be achieved using this parameterization without a significant atmospheric contribution.

We compare a variety of planetary scenarios and atmospheres calculated with the extensive capabilities of 1D-TERRA against the published observations. Our main goals here are to show the large application range of our new model and provide possible explanations and constraints when interpreting the observed spectral features of K2-18b.

### 4.1. Scenarios

(1) For our first scenario shown in Table 6, we start with an Earth-like atmosphere based on the US standard atmosphere 1976. As a starting condition, we assume Earth’s atmospheric mass, which, with the elevated gravity, leads to a surface pressure of 1.55 bars. Recent modeling studies have shown that surface temperatures of Earth-like planets around M stars would increase relative to Earth for Earth’s TSI because of the redshifted spectrum of cooler stars, different UV environments, and atmospheric and ocean responses (see, e.g., Scheucher et al. 2018). Consequently, we expect a theoretically Earth-like K2-18b, receiving somewhat higher TSI than Earth, to significantly warm up, evaporating parts of the ocean H\(_2\)O reservoir, resulting in a thick steam atmosphere. For this reason, we use the constant RH profile of 0.95 used in Equation (18) for the H\(_2\)O calculation over all convective layers. For this scenario, we use 1D-TERRA in fully coupled climate-chemistry mode to capture details of the impact of increased H\(_2\)O in the atmosphere.

(2) Due to the higher TSI and the size of the planet, the accumulation of a significant atmosphere and a past runaway greenhouse state are plausible; therefore, our second atmosphere of interest is an exo-Venus. As with Venus, we do not assume an H\(_2\)O reservoir, and, to retain Venus’s atmospheric mass, we increase the surface pressure accordingly to 143.6 bars. All Venussian scenarios (2)–(4) are run in climate-only mode, as we focus here on the resulting H\(_2\)O features in the modeled transmission spectra influenced by temperatures, pressures, and H\(_2\)O amounts, rather than the full photochemistry of other trace gases. Our initial temperatures for the Venus-like runs are 500 K isoprofiles.

(3)–(4) To increase the amplitude of absorption features, we increase the atmospheric scale heights by adding H\(_2\) to our exo-Venus atmospheres. First, we triple (=279 bars \(p_0\)) our original (=93 bars \(p_0\)) Venus atmosphere by adding 186 bars of H\(_2\) (3), and in another scenario, we add 800 bars of H\(_2\) on top of the 93 bars of Venus for comparison (4). This was chosen to stay within our limit of calculated \(k\)-distributions of 1000 bars.

(5) Next, we move on to hydrogen-dominated primary atmospheres, which we model with 1D-TERRA in climate-only mode with a prescribed atmospheric composition. We have calculated the equilibrium chemical composition for an isothermal atmosphere with an equilibrium temperature of \(T_{\text{eq}} = 320 \text{ K}\) using the NASA CEA model (McBride & Gordon 1992) with initial solar elemental abundances by Asplund et al. (2009). The chemical composition is subsequently kept fixed. Radiative-convective equilibrium is calculated down to 10 bars, although the atmosphere might extend further down to higher pressures. We choose this limit because we expect H\(_2\)O absorption features in the Hubble WFC3 spectral range to result from pressures up to a few hundred mbar, and we cannot make any assumption on the actual extent down to a possible surface. For all H\(_2\)-dominated atmospheres, we start with a linear temperature gradient from the surface up to the TOA, in order to speed up climate calculations.

(6) We repeat the same with a potential H\(_2\)O reservoir (ocean) at the lower atmospheric boundary at 10 bars, which can evaporate and mix into the atmosphere dependent on temperature, H\(_2\)O saturation pressure, and assumed constant RH of 95% for convective layers as in scenario (1), due to the expected warm temperatures in the lower atmosphere. To stay well within our valid model temperature range (\(T < 1000 \text{ K}\)), we limit the H\(_2\)O saturation vapor pressure, i.e., the amount of water the atmosphere can hold in gas phase, to its value at the critical point at 647 K for temperatures above, leading to a maximum of 220 bars of H\(_2\)O in the atmosphere. As in scenario (5), the chemical composition is kept fixed, except for the changes in H\(_2\)O, which changes all mixing ratios accordingly.

(7) Lastly, we calculate a 50 times solar metallicity atmosphere with the NASA CEA model and perform climate calculations similar to scenario (5) without any H\(_2\)O reservoir to study the effect of metallicity on atmospheric scale heights, impacting the amplitude of the resulting absorption features.

### 4.2. Results

Table 6 shows the different planetary scenarios modeled in this work, plus the resulting bottom-of-atmosphere (BOA) pressures after the climate, or climate-chemistry calculations, respectively, as well as the respective BOA temperatures. The BOA pressures can only change in our model when mass conservation is broken by additional in- or outfluxes. This is invoked, e.g., for scenarios with an H\(_2\)O reservoir, evaporating extra molecules into the atmosphere when the atmosphere is heating up or condensing them out.
Figure 11. Temperature profiles for our K2-18b model atmospheres (see Table 6).

Figure 11 shows the resulting atmospheric temperature profiles for all scenarios described above. Almost all scenarios lead to global mean temperatures in the thick lower atmosphere that are too hot to be habitable. That said, at the 1 bar level, all runs, except the hydrogen-dominated cases, yield moderate temperatures with the possibility of liquid water, as also discussed by Benneke et al. (2019b). At higher pressures, temperature profiles become adiabatic. At low atmospheric pressures, UV heating leads to the temperature inversions in the upper layers.

Our main results are shown in Figure 12. We supply the modeled atmospheric compositions and temperatures from Figure 11 to calculate forward-modeled transmission spectra in GARLIC and compare them with the Kepler, Hubble, and Spitzer data of K2-18b from Benneke et al. (2019b). We plot the planetary transit depth, \( \delta(\lambda) = \left[\frac{(r_p + h(\lambda))}{r_p}\right]^2 \), with \( r_p \) being the planetary radius, \( r_s \) the stellar radius, and \( h(\lambda) = \sum_i (1 - T_i(\lambda)) \Delta h_i \) the effective height of the atmosphere for a given wavelength. Note that all spectra shown can, in principle, be shifted vertically within the error in the 4.5 \( \mu \)m Spitzer observation, from which radius estimates for K2-18b were derived, but it was rather our aim to focus on the amplitudes of spectral features, rather than the closest observational fit. Such a shift could arise due to the lack of knowledge regarding, e.g., the interior structure and location of the planet–atmosphere boundary. Spectral absorption features in the modeled solar composition atmosphere (purple) and the 50 times solar metallicity results (pink) match the observations well within \( \pm 1 \sigma \), with the exception of the 3.6 \( \mu \)m Spitzer band. A distinction between 1 and 50 times solar metallicities from the observations is difficult. Other considered scenarios cannot produce features strong enough to explain the apparent 1–2 \( \mu \)m \( \text{H}_2\text{O} \) absorption observations with a strength of \( \approx 100 \text{ ppm} \) and a \( 1 \sigma \) of \( \approx 23 \text{ ppm} \). For example, our \( \text{H}_2 \)-dominated Venus-like case (4), shown in red, produces feature strengths of only \( \approx 35 \text{ ppm} \).

Furthermore, the addition of extra \( \text{H}_2\text{O} \) due to a hypothetical water-world ocean reservoir (brown) would increase atmospheric mean molecular weights, thus drastically decreasing scale heights. For the solar metallicity case with ocean reservoir (6), the features would reduce to \( < 15 \text{ ppm} \). Even if one were to shift these spectra vertically in Figure 12, it is clear that the amplitudes of features seen in any model scenarios (other than the \( \text{H}_2-\text{He} \) atmospheres without an ocean reservoir) would still not be compatible with the observations. A further test run with an Earth-like RH profile with 80% humidity at the surface and a very dry upper atmosphere to calculate the \( \text{H}_2\text{O} \) profile after Manabe & Wetherald (1967) suggested no significant changes in planetary climate and atmospheric spectral appearance. Madhusudhan et al. (2020) recently argued that the amount of \( \text{H}_2\text{O} \) mixed into an \( \text{H}_2-\text{He} \) atmosphere consistent with the Hubble Space Telescope measurements would not significantly change the planetary radius, and further, that a habitable ocean world with liquid water underneath an \( \text{H}_2-\text{He} \) atmosphere is possible for K2-18b. While it may be true that the observed radius can be achieved in such a scenario, our study considers the effect such a large \( \text{H}_2\text{O} \) reservoir would have upon the atmosphere due to strong evaporation and thereby on the observed spectral features. Our results suggest that an ocean world scenario would not fit the observed spectral features. This includes all of our terrestrial atmospheres, as well as the hypothetical Venus runs with added \( \text{H}_2 \), although the Venus run with 800 bars of added \( \text{H}_2 \) (red) already shows distinguishable features. While it is clear that larger scale heights are needed to explain the observations, it is interesting that our results suggest that large amounts of the heavy molecule \( \text{CO}_2 \) can also be excluded by observations, as well as the existence of a hypothetical surface ocean at our BOA temperatures. The contrast gradient between the two Spitzer observations at 3.6 and 4.5 \( \mu \)m could come from extensive amounts of \( \text{CO}_2 \) or other absorbers in the 4.5 \( \mu \)m band, e.g., \( \text{O}_3 \), \( \text{N}_2\text{O} \), or \( \text{CO} \) (all not shown), but all of which would further bring down scale heights. Another possibility is reduced \( \text{CH}_4 \) in the middle and upper atmosphere, e.g., by freezing it out (at \( \approx 91 \text{ K} \)), and in doing so reducing the 3.6 \( \mu \)m \( \text{CH}_4 \) absorption feature. The CEA solar composition atmosphere contains \( \approx 460 \text{ ppm} \) \( \text{CH}_4 \) (50 times solar \( \approx 2.48\% \) \( \text{CH}_4 \)). In Figure 13, we show how a transmission spectrum without \( \text{CH}_4 \) contribution would look by comparison. Our results suggest that the depletion of \( \text{CH}_4 \) could indeed explain the discrepancy between model results and observations. Benneke et al. (2019b) could only limit \( \text{CH}_4 \) to \( < 0.25\% \), while our results with 1D-TERRA limit \( \text{CH}_4 \) to \( < 460 \text{ ppm} \).

5. Summary

We describe in this work our new radiative transfer module, REDFOX, implemented in our 1D climate-chemistry model, 1D-TERRA. The model also uses the updated photochemistry reaction scheme, BLACKWOLF, which is described in depth in the companion paper (Wunderlich et al. 2020). The radiative transfer update included the user’s choice of absorbing species, extended wavelength ranges of stellar and thermal calculations, flexible inclusion of ClAs, additional continua and UV absorbers, and broader pressure–temperature ranges, among others. We show an extensive verification and validation of REDFOX and 1D-TERRA against terrestrial-type solar system atmospheres and previously published modeling results for other theoretical atmospheres.

With our new model, we study the exoplanet K2-18b, with its first-ever observed atmospheric absorption features of \( \text{H}_2\text{O} \)
in an exoplanet with mass \(< 10 \, M_\oplus\), and calculate climate and transmission spectra for different atmospheric and planetary scenarios.

We confirm the findings of Benneke et al. (2019b) that K2-18b likely has an H$_2$–He atmosphere and additionally exclude the existence of a large H$_2$O ocean reservoir exposed to the atmosphere. This rules out a water layer at the top of the mantle for possible interior structures, as it would decrease the atmospheric scale height, despite the newly described effect of increased radii for H$_2$O steam atmospheres by Turbet et al. (2020). We further confirm that the Hubble WFC3 observations between 1 and 2 \(\mu\)m can be explained by H$_2$O absorption in a hydrogen-dominated primary atmosphere. Both solar and 50 times solar metallicity results alike can explain the observations. With the recent radius update for K2-18b and the need for a significant atmospheric contribution to the planetary radius, a hypothetical H$_2$O reservoir would likely be a supercritical fluid at such high temperatures, implying an envelope rather than a solid or liquid surface. This suggests that K2-18b is unlikely to be a water world or even an icy world. We also argue that significant amounts of CH$_4$ are excluded by the Spitzer observations.

Figure 12. Comparison of planetary transmission spectra for K2-18b calculated with GARLIC for our 1D-TERRA model atmospheres (Table 6 and Figure 11) with Kepler, Hubble, and Spitzer data taken from Benneke et al. (2019b). Here \(\delta(\lambda)\) is the wavelength-dependent transit depth of the planet.

Figure 13. Transmission spectra for the solar metallicity atmosphere (purple) as in Figure 12 compared to the same atmosphere but without CH$_4$ contribution (orange).

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Software: GARLIC (Schreier et al. 2014, 2018a, 2018b), HITRAN 2016 (Gordon et al. 2017), MPI Mainz Spectral Atlas (Keller-Rudek et al. 2013), KSPECTRUM1.2.0 (Eymet et al. 2016), 1D climate-chemistry model legacy (Kasting et al. 1993), and the simulations were performed on the supercomputer JUQUEEN (Jülich Supercomputing centre) and the Leibniz Supercomputing Centre (LRZ) with the support of the German Research Foundation (Deutsche Forschungsgemeinschaft, DFG) under grant no. JSC4142/1.
Table A1. Parameters $s_i$ and $T_s$ for Heat Capacity Calculations with the Shomate Equation (Equation (A2)), Together with the Respective Validity Range

| Coef. | CH$_4$ | CO$_2$ | H$_2$O | N$_2$ | O$_3$ |
|-------|-------|-------|-------|-------|-------|
| $s_1$ | $-0.703$ | 7.7 | 30.992 | 6.76 | 8.27 |
| $s_2$ | 108.477 | $5.3 \times 10^{-3}$ | 6.832 | $6.06 \times 10^{-4}$ | $2.58 \times 10^{-4}$ |
| $s_3$ | $-42.522$ | $-8.3 \times 10^{-7}$ | 6.793 | $1.3 \times 10^{-7}$ | ... |
| $s_4$ | 5.863 | ... | $-2.534$ | ... | ... |
| $s_5$ | 0.679 | ... | 0.082 | ... | $1.877 \times 10^{7}$ |
| $T_s$ (K) | 1000 | 1 | 1000 | 1 | 1 |
| Valid (K) | 298–1300 | | 500–1700 | | |

Notes.

1. Chase (1998); https://webbook.nist.gov/chemistry/.

2. Kasting (1991).

Ackerman 1986; Pavlov et al. 2000; Segura et al. 2003; von Paris et al. 2015, and others), NASA CEA (McBride & Gordon 1992).

Appendix

Heat Capacities

There are in total nine heat capacities, $c_p$ (J mol$^{-1}$ K$^{-1}$), considered in our model: Ar, CH$_4$, CO, CO$_2$, H$_2$, H$_2$O, He, N$_2$, and O$_2$. These had been implemented by various researchers over several decades, most recently by Dr. Philipp von Paris in 2011 and used in, e.g., Godolt et al. (2016, 2019), Gebauer et al. (2017, 2018), Keles et al. (2018), Scheuerer et al. (2018, 2020), and Wunderlich et al. (2019). Two of the $c_p$ values are implemented as temperature-independent: $c_{p,Ar} = 20.78600$ and $c_{p,He} = 20.78603$ (Chase 1998). Heat capacities for CO and H$_2$ are calculated based on the empirical formula (Deming & Shupe 1931),

$$c_p(T) = \frac{7R}{2} + \frac{T_{ref}}{T} \left( \frac{T}{T_{ref}} \right)^2 \frac{e^{T_{ref}}}{e^T - 1},$$

(A1)

with the gas constant $R$ and the reference temperatures $T_{ref,CO} = 3090$ K and $T_{ref,H_2} = 6100$ K, respectively. Other heat capacities are calculated using the Shomate equation (Parks & Shomate 1940),

$$c_p \left( \frac{T}{T_s} \right) = s_1 + s_2 \cdot \left( \frac{T}{T_s} \right) + s_3 \cdot \left( \frac{T}{T_s} \right)^2 + s_4 \cdot \left( \frac{T}{T_s} \right)^3 + s_5 \cdot \left( \frac{T}{T_s} \right)^{-2},$$

(A2)

with parameters $s_i$ and temperatures $T_s$ for different molecules shown in Table A1. For CH$_4$, Equation (A2) is only used above 300 K within the respective validity range of parameters in Table A1. Below, we use the linear interpolation

$$c_{p,CH_4}(T) = \frac{c_{p,2} - c_{p,1}}{T_2 - T_1} (T - T_1) + c_{p,1}$$

(A3)

of calculations from Gurvich et al. (1989) of heat capacities $c_{p,1}$ and $c_{p,2}$ at temperatures $T_1$ and $T_2$, respectively, shown in Table A2.

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Table A2. CH$_4$ Heat Capacities $c_{p,1}$ (J mol$^{-1}$ K$^{-1}$) from Gurvich et al. (1989), Used in Equation (A3)

| Regime | $T_1$ (K) | $T_2$ (K) | $c_{p,1}$ | $c_{p,2}$ |
|--------|----------|----------|----------|----------|
| 100–200 K | 100 | 200 | 33.28 | 33.51 |
| 200–300 K | 200 | 300 | 33.51 | 35.76 |

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