

*На правах рукописи*

Разумовский Михаил Владимирович

Разработка параметризаций молекулярного  
поглощения с минимальным количеством  $k$ -членов  
для моделирования переноса излучения в атмосфере  
Венеры

Специальность 1.3.1 Физика космоса, астрономия

## АВТОРЕФЕРАТ

диссертации на соискание ученой степени  
кандидата физико-математических наук

Москва — 2026

Работа выполнена в \_\_\_\_\_.

Научный руководитель: Фомин Борис Алексеевич, доктор физико-математических наук, доцент

Ведущая организация: \_\_\_\_\_  
\_\_\_\_\_  
\_\_\_\_\_

Защита состоится \_\_\_\_\_ 2026 года в \_\_\_\_\_ часов \_\_\_\_\_ минут на заседании диссертационного совета \_\_\_\_\_.

С диссертацией можно ознакомиться в библиотеке \_\_\_\_\_  
и на сайте организации \_\_\_\_\_.

Автореферат разослан «\_\_\_\_\_» \_\_\_\_\_ 2026 года.

Ученый секретарь диссертационного совета \_\_\_\_\_

As a manuscript

Mikhail Vladimirovich Razumovskiy

Development of molecular absorption parameterizations  
using a minimal-set  $k$ -distribution scheme for radiative  
transfer modeling in the atmosphere of Venus.

Specialty: 1.3.1 Space Physics, Astronomy

## ABSTRACT

of the dissertation for the Degree of  
Candidate of Physical-Mathematical Sciences  
(equivalent to PhD in Physical and Mathematical Sciences)

Moscow — 2026

The work was carried out at \_\_\_\_\_.

Scientific supervisor: Boris Alekseevich Fomin, Doctor of Physical  
and Mathematical Sciences, Docent

Leading organization: \_\_\_\_\_  
\_\_\_\_\_  
\_\_\_\_\_

The defense will take place on \_\_\_\_\_ 2026 at \_\_\_\_\_ h \_\_\_\_\_ min at a  
meeting of dissertation council \_\_\_\_\_.

The dissertation is available at the library of \_\_\_\_\_  
and on the organization's website \_\_\_\_\_.

The abstract was distributed on "\_\_\_\_" \_\_\_\_\_ 2026.

Academic secretary of the dissertation council \_\_\_\_\_

**Relevance of the work.** Accurate radiative transfer modeling with sufficient computational efficiency remains a challenging problem for Venus climate studies and other applications, involving broad spectral analysis of radiative transport in Venus atmosphere. Molecular absorption — a central component in radiative transfer schemes — must be represented under conditions of strong vertical inhomogeneity, high pressures and temperatures, uncertain continuum behavior and incomplete spectroscopic constraints. At the same time, full line-by-line calculations are too computationally expensive for direct use in general circulation models or time-marching radiative-convective models. Consequently, the development of compact but physically justified parameterizations of molecular absorption is a significant and independent research problem. This problem is especially important for Venus, where the accuracy of heating and cooling rates directly affects the interpretation of atmospheric energetics and circulation, while the available radiative schemes often rely either on correlated- $k$  approaches with a large number of terms or on simplified parameterizations (e.g. Mendonça et al. [2015]). The present work addresses this gap by developing parameterizations that require the minimum number of radiative transfer solver calls for a given level of accuracy. These parameterizations, constructed with the flux-fitting  $k$ -distribution approach outperform existing correlated- $k$ -based solutions by 1-2 orders of magnitude. Parameterizations are provided in a form suitable for implementation in radiative transfer schemes for the ultraviolet and thermal infrared spectral ranges.

The work also introduces MARFA, a newly developed flexible high-resolution line-by-line tool for efficient calculation of atmospheric absorption cross-sections. The method is based on an efficient interpolation technique [Fomin, 1995], which makes it possible to perform high-resolution calculations over wide spectral ranges, including the far wings of spectral lines, which is particularly important under conditions of uncertain continuum absorption, as in the case of Venus. In addition, a web-based implementation of the MARFA tool has been developed, providing online access to high-resolution calculations (up to  $5 \times 10^{-4} \text{ cm}^{-1}$ ), with fast computation times, interactive plotting capabilities, and the ability to download computed cross-sections. While several online tools for spectroscopic calculations already exist, the proposed solution provides competitive performance at very high spectral resolution together with convenient access to computed data. More broadly, Venus serves as a natural benchmark for dense  $\text{CO}_2$ -dominated atmospheres and therefore it is an interesting reference case for modeling Venus-like terrestrial exoplanets [Kane et al., 2019]. In this sense, the methods developed in this work may be adapted for applications in comparative planetology and

exoplanet climate studies.

**Dissertation goals and objectives.** The aim of the dissertation is to develop parameterizations of molecular absorption for radiative transfer modeling in the atmosphere of Venus that require the minimum possible number of radiative transfer solver calls for a given level of accuracy with respect to reference line-by-line calculations.

To achieve this aim, the following objectives were addressed:

1. To adapt and formulate the flux-fitting  $k$ -distribution technique for the conditions of the Venus atmosphere and to identify its differences from the conventional correlated- $k$  method.
2. To develop a flexible and efficient line-by-line tool for recalculation of molecular absorption cross-sections under uncertain spectroscopic and atmospheric conditions and at high resolution. The tool is intended to support both the construction of parameterizations, reference calculations of fluxes and sensitivity studies.
3. To develop the reference radiative transfer model, based on the Monte-Carlo method, to calculate fluxes and cooling/heating rates across various atmospheric, spectroscopic and geometry parameters.
4. To construct compact parameterizations of shortwave absorption for the main absorbers of Venus, including the unknown UV absorber, and to determine representative spectral points for Rayleigh scattering and cloud optical properties.
5. To construct a longwave parameterization for the 10–6000  $\text{cm}^{-1}$  spectral range for the main gaseous absorbers of Venus, with effective absorption coefficients suitable for direct use in radiative transfer solvers and climate models.
6. To validate the obtained parameterizations against reference radiative transfer calculations for representative Venus atmospheric profiles.
7. To develop software implementations of the proposed parameterizations to make them accessible to the scientific community and suitable for integration into existing radiative transfer models.

**Scientific novelty.** The scientific novelty of the dissertation lies in the development and application of the flux-fitting  $k$ -distribution technique for Venus

atmospheric radiative transfer, aimed explicitly at minimizing the number of radiative transfer evaluations in parameterized model, while retaining control over accuracy through comparison with reference line-by-line calculations. Unlike the conventional correlated- $k$  method [Lacis and Oinas, 1991], the proposed approach does not rely on the assumption of inter-level correlation of monochromatic absorption and is formulated in terms of vertically resolved effective absorption coefficients constrained by fluxes and cooling rates, computed with reference line-by-line model.

For the ultraviolet region of Venus, an effective parameterization of absorption by gaseous species and the unknown UV absorber was obtained for 125–400 nm. It was shown that the entire UV range can be represented using only eight effective absorption coefficients, while maintaining flux discrepancies below 3% and heating-rate discrepancies below 1% in the tested cases. For the thermal infrared region, a new parameterization was developed for 10–6000  $\text{cm}^{-1}$ , based on 16 spectral bands and requiring only 32 radiative transfer evaluations for the whole longwave range. It was shown that this compact representation reproduces upward fluxes within about 2% below 95 km and cooling rates with acceptable accuracy below 90 km for representative Venus atmospheric profiles. The efficiency of the parameterization in the longwave region has a substantial performance advantage over existing solutions (e.g. Takahashi et al. [2023], Eymet et al. [2009]).

An additional element of novelty is release of the MARFA line-by-line tool as a flexible computational backend for planetary molecular absorption studies under uncertain spectroscopic conditions. The tool combines high spectral resolution with efficient multi-grid interpolation, support for large line cut-offs and wing corrections, and open-source implementation suitable for reproducible sensitivity analysis. Over the course of this work, the development evolved from a local tool into a complete computational platform for molecular absorption, which has already been used in planetary research [Marleau et al., 2025].

**Theoretical and practical significance.** The theoretical significance of the work is connected with the further development of alternative  $k$ -distribution methods for strongly non-Earth-like atmospheres. The dissertation demonstrates that, for Venus conditions, molecular absorption can be parameterized not only within the standard correlated- $k$  framework, but also through a flux-fitting approach that directly targets the accuracy of radiative fluxes and cooling rates and yields compact minimal sets of effective coefficients. Essentially, the suggested numerical scheme for the flux-fitting  $k$ -distribution technique can be considered as a viable alternative to

correlated- $k$  method, overcoming some of its limitations in non-homogeneous atmospheres (e.g. [Pincus et al., 2019]). This is important for the theory of radiative transfer parameterization in vertically inhomogeneous, high-pressure CO<sub>2</sub>-dominated atmospheres.

The practical significance of the work lies in the fact that the developed parameterizations are suitable for direct insertion into radiative transfer modules of Venus climate models and related numerical tools. Parameterizations are presented as collection of effective absorption coefficients  $k_{i,j}^*(z)$ . However, the temperature dependence of the parameterizations must be taken into account. In the longwave spectral region, this dependence is handled using an interpolation procedure, since climate models compute temperature profiles at each time step. For this purpose, a publicly available Fortran module has been developed, which accepts temperature profiles as input and computes the corresponding effective absorption coefficients  $k_{i,j}^*(z)$  together with band-averaged Planck function values. These quantities are required as inputs for radiative transfer modules within climate models. The parameterization for the UV region was found to be temperature-independent. This makes the developed parameterizations directly transferable to general circulation models and radiative-convective models with minimal modification of the host code.

The practical significance is further enforced by the creation of the MARFA open-source software and web platform, which make it possible to recalculate molecular absorption spectra efficiently for varying atmospheric profiles, line-shape assumptions, and spectroscopic datasets. This is especially valuable for Venus, where uncertainties in continuum absorption, line-wing behavior, and available line databases remain substantial [Haus et al., 2013]. The tool is available both as a source code and as a web platform. Its deployment provides convenient access for both offline calculations and online use.

**Research methods** of this study belong to the domain of theoretical atmospheric physics, molecular spectroscopy and numerical radiative transfer modeling. The central methodological element is the flux-fitting  $k$ -distribution technique, in which effective absorption coefficients are constructed by matching line-by-line reference radiative fluxes and cooling rates within selected spectral intervals.

Reference radiative fields were computed using high-resolution line-by-line Monte Carlo radiative transfer modeling [Liou, 2002] for representative Venus atmospheric profiles. The calculations account for the main gaseous absorbers relevant to the corresponding spectral ranges and use realistic assumptions for cloud optical properties and atmospheric structure. The val-

idation criterion was the agreement of parameterized and line-by-line fluxes and heating/cooling rates.

To compute molecular absorption spectra used in the construction and testing of the parameterizations, the MARFA line-by-line code was employed. MARFA uses a multi-grid interpolation approach, supports user-defined atmospheric profiles, line-shape functions, and wing corrections, and is designed for rapid recalculation under uncertain spectroscopic inputs. The code is written in Modern Fortran [Metcalf et al., 2024], which provides high computational performance together with modular program structure and portability across computing platforms. In benchmark comparisons, its computational speed was shown to be about two orders of magnitude higher than that of HAPI [Kochanov et al., 2016] for the tested setup, while preserving accuracy sufficient for radiative applications.

### Statements submitted for defense.

1. A flux-fitting  $k$ -distribution approach is introduced for the atmosphere of Venus to construct compact parameterizations of molecular absorption with a minimal number of effective absorption coefficients  $k_{i,j}^*(z)$ , while avoiding the inter-level correlation assumption inherent in the standard correlated- $k$  method.
2. A reference Monte Carlo radiative transfer model for vertically inhomogeneous atmospheres has been developed and used for the construction and validation of the proposed parameterizations.
3. In the ultraviolet spectral range 125–400 nm, absorption by the main relevant species of Venus atmosphere, including the unknown UV absorber, can be represented with only eight effective radiative transfer evaluations, while preserving agreement with reference line-by-line calculations at the level required for climate-model applications.
4. In the thermal infrared spectral range 10–6000  $\text{cm}^{-1}$ , molecular absorption in the lower and middle atmosphere of Venus can be represented by a 16-band parameterization requiring only 32 radiative transfer evaluations, with flux errors below about 2% and acceptable cooling-rate accuracy below 90 km.
5. Efficient construction and validation of such parameterizations for Venus require a flexible line-by-line computational tool capable of handling uncertain spectroscopic inputs, large line cut-offs, and line-wing corrections; this requirement is satisfied by the developed MARFA code.

6. The developed parameterizations and computational tools are publicly available in the form of open-source repositories, including implementation modules and documentation, and are suitable for integration into radiative transfer blocks of Venus climate models. The developed methods can also serve as a methodological basis for studies of Venus-like terrestrial planets and dense CO<sub>2</sub>-dominated exoplanet atmospheres.

**Personal contribution.** The main results presented in the dissertation were obtained by the author either personally or with his direct participation. The author personally introduced and formulated the flux-fitting  $k$ -distribution technique in its present form for application to the atmosphere of Venus, including its mathematical formulation, its distinction from the conventional correlated- $k$  method, and the quantitative framework for efficiency comparison based on the parameter  $\eta$ . The author participated in the development of ultraviolet and thermal-infrared parameterizations of molecular absorption for the atmosphere of Venus, in their construction and validation against reference line-by-line radiative transfer calculations, and in the preparation of the corresponding publications.

A major part of the dissertation is associated with the development of the MARFA line-by-line tool, which was designed and implemented by the author from the ground up. The author's contribution included the conceptual design of the code, development of the numerical methodology, software architecture and implementation, validation, data curation, web-platform development, project administration, and manuscript preparation. The earlier exoplanet study performed by the author is considered as a preliminary stage that helped shape the broader planetary-atmosphere context of the present dissertation.

### **Compliance with Passport of Speciality 1.3.1 Space physics, astronomy**

The dissertation complies with the passport of speciality 1.3.1 *Space Physics, Astronomy* and corresponds primarily to passport items 1, 5, and 14, and additionally to item 6. Item 1 covers research on the generation, propagation, and absorption of radiation in cosmic media and particularly — in planetary atmospheres; item 5 covers theoretical and experimental studies of Solar System bodies, including the structure and composition of planetary atmospheres; item 6 includes exoplanet research; and item 14 covers experimental methods, scientific instruments, methods of computational astrophysics, and data-processing algorithms for space and astronomical studies.

Below is the correspondence between the statements submitted for defense

and the items listed in the speciality passport.

**Statements 1, 3 and 4** correspond to passport items 1 and 5, since they are devoted to the development of methods for parameterizing molecular absorption and radiative transfer in the atmosphere of Venus in the ultraviolet and thermal infrared spectral ranges. These results concern the study of radiation absorption and radiative transfer in a cosmic medium, as well as the investigation of the structure, composition, and radiative properties of a planetary atmosphere of the Solar System.

**Statement 2** corresponds to passport items 1 and 14, since it involves the development and application of a Monte Carlo radiative transfer model for vertically inhomogeneous planetary atmospheres. This relates to the study of radiation propagation and absorption in cosmic media (item 1), as well as to computational astrophysics methods and numerical algorithms for radiative transfer modeling (item 14).

**Statement 4** corresponds to passport items 1 and 5, because This also falls within the study of absorption of radiation in planetary atmospheres and theoretical research on Solar System planets.

**Statement 5** corresponds primarily to passport item 14, and also supports item 1, since the MARFA code is a computational tool for high-resolution line-by-line calculation of molecular absorption in planetary atmospheres under uncertain spectroscopic conditions. Therefore, this result belongs to the development of methods of computational astrophysics and algorithmic tools for space and astronomical research and at the same time serving radiative transfer studies of planetary media.

**Statement 6** corresponds to passport item 5 and 14, in a broader comparative planetology sense, to item 6, because the developed parameterizations are aimed primarily at the atmosphere of Venus but are methodologically applicable to Venus-like terrestrial exoplanets as well.

**Approbation of the results.** The main results of the dissertation were presented and discussed at international and national conferences and seminars, including:

- 22nd All-Russian Open Conference “Modern Problems of Remote Sensing of the Earth from Space (Physical Foundations, Methods and Technologies for Environmental Monitoring, Potentially Hazardous Phenomena and Objects)”, Moscow, Russia, 2024.

- 11th Moscow Solar System Symposium (11M-S3), Moscow, Russia, October 5–9, 2020.
- Seminar of Department 53 “Planetary Physics”, Space Research Institute of the Russian Academy of Sciences (IKI RAS), Moscow, Russia.
- 62nd All-Russian Scientific Conference of MIPT, Dolgoprudny, Russia, 2019.
- 1st International Aerospace Symposium *Silk Road 2018* (IASS “Silk Road” 2018), Dolgoprudny, Russia, December 6–8, 2018.

**Structure of the dissertation.** The dissertation is organized into an introduction, three chapters, a conclusion, a bibliography, a glossary of symbols and abbreviations, a list of figures, and supplementary materials.

## The contents of the work

In **Chapter 1**, the physical and computational foundations of the MARFA line-by-line tool are presented. The calculation of molecular absorption is based on the classical line-by-line approach, in which the absorption coefficient is obtained by summing contributions from individual spectral lines:

$$k(\nu; p, T) = n(p, T) \sum_j S_j(T) f_j(\nu - \nu_0; \gamma(p, T)), \quad (1)$$

where  $S_j(T)$  is the temperature-dependent line intensity,  $f_j$  is the line shape function (Lorentz, Doppler, or Voigt profile),  $\nu_0$  is the line center, and  $\gamma(p, T)$  is the pressure- and temperature-dependent half-width. The number density  $n(p, T)$  is determined from the atmospheric pressure and temperature profiles. In MARFA, Lorentz, Gaussian, and Voigt line profiles are implemented. These correspond to pressure broadening, Doppler broadening, and the combination of both effects, respectively. Particular attention is given to numerical schemes for the evaluation of the Voigt function, because these are usually the most computationally expensive. MARFA implements its own numerical scheme for Voigt function evaluation. Special emphasis is placed on the treatment of far line wings, which are especially important in dense CO<sub>2</sub> atmospheres such as the atmosphere of Venus. Experimental data suggest that the far wings of spectral lines deviate from Lorentz or Voigt behavior,

and to account for this, so-called  $\chi$ -correction functions [Burch et al., 1969] are introduced:

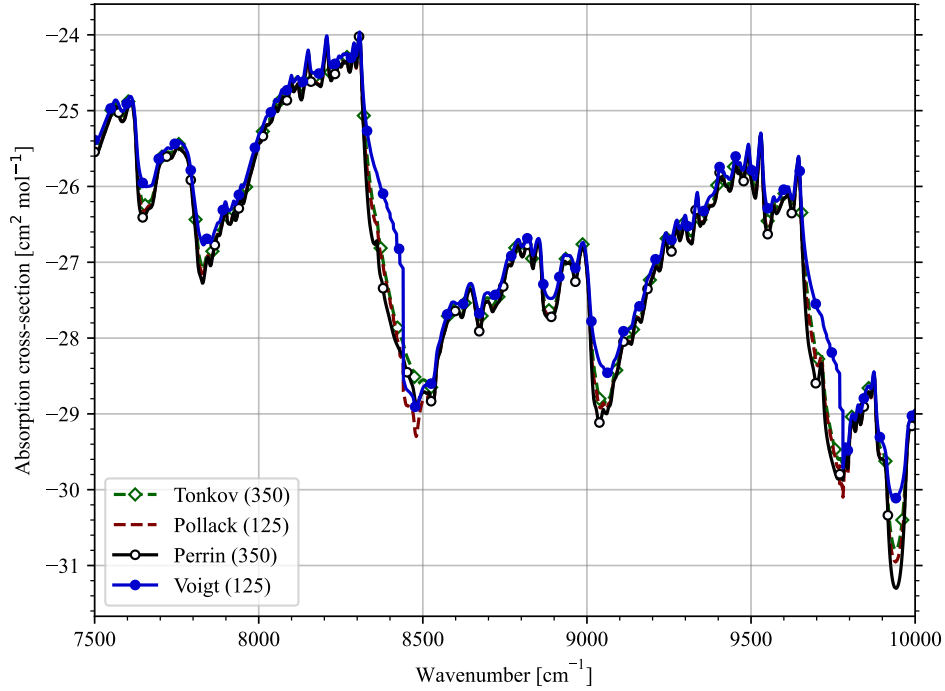
$$f_{\text{corrected}}(\nu - \nu_0) = f_{\text{L}}(\nu - \nu_0)\chi(\nu - \nu_0), \quad (2)$$

MARFA supports user-defined line-shape functions and  $\chi$ -correction factors.

A review of existing computational tools for line-by-line modeling is provided, and the main computational challenges are discussed, including the high computational cost of line-by-line calculations when large line cut-offs are required and when continuum absorption is poorly constrained. These conditions are typical for planetary atmospheres with incomplete spectroscopic data. Chapter 1 further discusses the interpolation technique algorithm by Fomin [1995] which is considered fast and suitable for calculations with various line contour models. MARFA employs the scheme with 11 grids with increasing resolution, as it was independently confirmed that in presence of large line cut-offs, 2 or 3 grids are not enough to achieve the desired balance between speed and accuracy. Interpolation technique is performed on  $10 \text{ cm}^{-1}$ -length intervals. Number of points in the finest grid is set to  $N = 20481$  leading to a resolution of  $10/(N - 1) \approx 4.88 \cdot 10^{-4} \text{ cm}^{-1}$ . This is usually sufficient to resolve typical Doppler lines in upper atmosphere in IR-region.

The chapter also describes the spectral data used in the calculations, including spectroscopic databases. MARFA relies on HITRAN2020 database [Gordon et al., 2022], while other spectral data sources, such as HITEMP database [Rothman et al., 2010a] can also be incorporated due to the flexible code architecture. Total internal partition sums (TIPS) are needed to determine temperature-dependent spectral line intensities. In MARFA, TIPS data are set in an external file and are implemented based on the study by Gamache et al. [2016]. A notable feature of MARFA, which makes it suitable for use within larger radiative transfer frameworks, is that a full atmospheric pressure–temperature profile can be provided as input, and the corresponding absorption cross-sections can be computed on the same vertical grid simultaneously for all atmospheric levels.

A separate section of the chapter is devoted to the validation and benchmarking of the MARFA code. The accuracy of the calculations is evaluated through comparison with reference line-by-line calculations performed using the HAPI Python package [Kochanov et al., 2016]. The comparison shows that MARFA provides comparable accuracy while achieving a significant increase in computational speed, especially for large line cut-off values. The Venus atmosphere is used as a benchmark test case due to the high tempera-

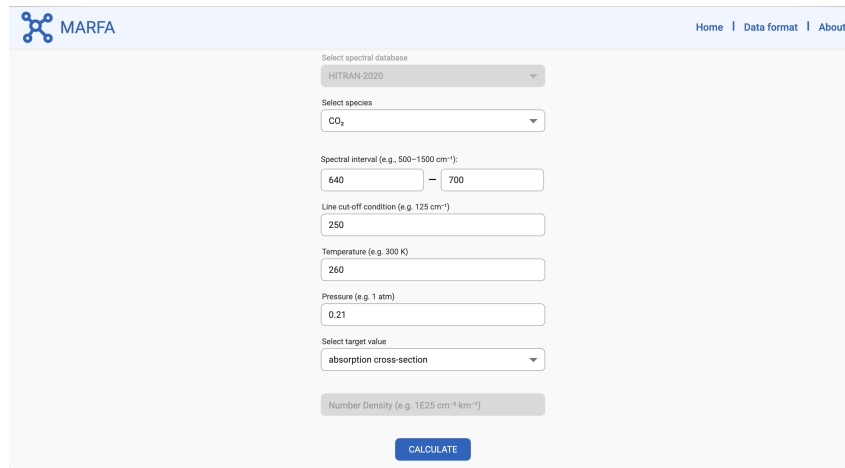


**Figure 1:** Monochromatic absorption cross-sections of  $\text{CO}_2$  at 92.1 bar and 735.3 K as a function of wavenumber in dependence on sub-Lorentzian profile and line-cut condition. Continuum absorption is neglected.

ture, high pressure, and uncertainty in spectroscopic parameters, which make it a challenging environment for radiative transfer modeling. An example calculation of monochromatic absorption cross-sections for several  $\chi$ -factors and line cut-off values is shown in Fig. 1.

The final part of the chapter describes the software architecture of the MARFA project, with emphasis on the modular organization of the source code, the compilation and execution workflow, and the principles adopted to ensure extensibility, transparency, and open-source development. The MARFA code is organized as a collection of Fortran modules responsible for specific physical and numerical tasks, which improves readability, maintainability, and further development. Particular attention is given to the refactoring of the initial legacy implementation into a more structured Modern Fortran codebase. In this context, the dissertation also discusses a number of practical principles referring to the use and avoidance of specific Fortran language features in the development of scientific software. The source code, documentation, installation instructions and usage examples are publicly available in the project repository.<sup>1</sup>

<sup>1</sup><https://github.com/Razumovskyy/MARFA>



**Figure 2:** User interface of the MARFA web platform for molecular absorption calculations

A separate part of the chapter is devoted to the MARFA web platform<sup>2</sup>, which provides browser-based access to a lightweight version of the MARFA kernel. The web interface allows users not only to perform molecular absorption calculations online, but also to visualize the results and download the generated datasets. Example of the web interface is presented on Fig.2.

MARFA is distributed through several public scientific platforms. The code is registered in the Astrophysics Source Code Library (ASCL), which provides a persistent software record and facilitates citation and discoverability. MARFA has also been invited for inclusion in the Exoplanet Modeling and Analysis Center (EMAC) at NASA Goddard Space Flight Center, where migration of the code and associated data is currently in progress. Additional visibility is provided through the NASA Astrophysics Data System (ADS), which links the software to the corresponding publication and related materials.

Chapter 1 concludes with a discussion of the current scope of application of MARFA, its present limitations, and directions for future development.

**Chapter 2** of the dissertation is devoted to the reference radiative transfer model based on the Monte-Carlo method, which is used as a benchmark tool for validating the developed absorption parameterizations. However, it has a significant standalone importance, due to limited number of such tools developed by Venus scientific community. The reference model provides a physically complete solution of the radiative transfer problem in a vertically inhomogeneous atmosphere with absorption, multiple scattering, and cloud extinction, and therefore serves as a standard against which radia-

<sup>2</sup><https://marfa.app>

tive schemes based on parameterized absorption are tested. A key advantage of the Monte-Carlo method is that multiple scattering is treated explicitly, while the statistical error of the solution decreases proportionally to  $K^{-1/2}$ , where  $K$  is the number of photon histories, and does not depend on the number of spectral grid points [Fomin, 2006]. This makes the method particularly suitable for optically thick and strongly scattering media such as the Venus cloud layer.

Particular attention in the dissertation is given to the specification of physically realistic input data for the reference modeling, using atmospheric and spectroscopic parameters consistent with modern studies of the Venus atmosphere. In the shortwave spectral region, the atmospheric setup follows the general approach of Haus et al. [2015] and includes gaseous absorption, Rayleigh scattering, and the optical properties of sulfuric-acid cloud particles. Absorption cross-sections for the main UV-active species are assembled from datasets summarized in the MPI-Mainz spectral atlas [Keller-Rudek et al., 2013], while the unknown UV absorber is introduced using baseline retrieved parameterization of Haus et al. [2015]. The model also incorporates representative abundance profiles of the main minor absorbers [Tsang et al., 2008], VIRACONSISTENT pressure–temperature structure [Zasova et al., 2006], and a four-mode sulfuric-acid cloud model based on the modern Venus cloud description of Haus et al. [2013]. The incident solar spectrum is taken from the COSI model. Overall, this setup provides a physically realistic benchmark model for validating shortwave absorption parameterizations against line-by-line calculations.

In the thermal infrared region, the reference model is formulated as a line-by-line Monte-Carlo solver for thermal radiation in a plane-parallel layered atmosphere with a thick cloud layer. Its general configuration follows mentioned above line-by-line Venus studies of Haus et al. [2015, 2016], while the Monte-Carlo implementation is based on the methods developed earlier for accurate radiative transfer calculations. The reference atmosphere is constructed from representative VIRACONSISTENT-like temperature profiles, and the main absorbers are restricted to  $\text{CO}_2$ ,  $\text{H}_2\text{O}$ , and  $\text{SO}_2$ , which dominate the broadband thermal energetics of the lower and middle atmosphere of Venus. The corresponding monochromatic absorption coefficients are precomputed using the MARFA code from modern molecular databases, primarily HITEMP for  $\text{CO}_2$  and  $\text{H}_2\text{O}$  [Rothman et al., 2010b] and HITRAN2020 for  $\text{SO}_2$  [Gordon et al., 2022]. In the treatment of far-wing absorption and continuum-related effects, the model follows the Haus-type approximation, including sub-Lorentzian  $\chi$ -factors and finite line cut-off, which was shown to be suitable for broadband flux and heating/cooling-rate calculations in Venus con-

ditions. Cloud optical properties in the thermal infrared are taken from the physically realistic Venus cloud framework [Haus et al., 2013].

The reference Monte-Carlo model plays a central role in the dissertation, since the developed minimal-set  $k$ -distribution is directly constrained by the radiative fluxes and heating (or cooling) rates obtained from these benchmark calculations. The reference solutions are used to determine optimal spectral intervals and to identify dominant absorbers in each spectral band, and to evaluate the accuracy of the reduced radiative transfer model. Chapter 2, overall, shows that in both shortwave and longwave regimes, the reference calculations are based on atmospheric, cloud, and spectroscopic inputs consistent with the current state of Venus atmospheric research.

**Chapter 3** of the dissertation is devoted to the development and application of the *flux-fitting  $k$ -distribution* technique for parameterizing gaseous absorption in the atmosphere of Venus. This technique is introduced as an alternative to the conventional correlated- $k$  method. In contrast to the latter, it does not rely on spectral reordering or on the assumption of inter-level correlation of monochromatic absorption coefficients. Instead, it uses radiative fluxes and heating/cooling rates obtained from reference line-by-line calculations as an organizing principle for constructing compact sets of effective absorption coefficients. As a result, the parameterization is controlled directly by the target radiative characteristics of the atmosphere.

The technique consists of two main stages. At the preparatory stage, high-resolution spectral absorption cross-sections are precomputed and the spectral range is divided into bands according to the smoothness of cloud optical properties and the Planck function within each band. At the second stage, a *vertical iterative procedure* is applied in each band to construct effective absorption profiles  $k_{i,j}^*(z)$  that reproduce the radiative fluxes of the reference line-by-line model. For each spectral band  $I_i$ , the method constructs a set of vertically resolved effective absorption coefficient profiles

$$K = \{K_i\}_{i=1}^n, \quad K_i = \{k_{i,j}^*(z)\}_{j=1}^{N_i}, \quad N = \sum_{i=1}^n N_i, \quad (3)$$

where  $N$  is the total number of radiative transfer solver evaluations required to cover the full spectral range. The main idea of the method is to replace computationally expensive line-by-line integration by a finite number of representative calculations with preconstructed effective coefficients  $k_{i,j}^*(z)$ .

In the iterative procedure, the effective cross-section profile is retrieved by

**Table 1:** Parameterization details for the absorption of thermal infrared radiation

Band	Spectral region (cm <sup>-1</sup> )	Dominant absorber	$\tilde{\nu}_i^{\text{eld}}$ (cm <sup>-1</sup> )	$N_i$
1	10–200	H <sub>2</sub> O	100	2
2	200–400	H <sub>2</sub> O	300	2
3	400–500	CO <sub>2</sub>	450	1
4	500–600	CO <sub>2</sub>	550	1
5	600–760	CO <sub>2</sub>	680	10
6	760–900	CO <sub>2</sub>	830	2
7	900–1100	CO <sub>2</sub>	1000	5
8	1100–1210	CO <sub>2</sub>	1150	1
9	1210–1300	CO <sub>2</sub>	1250	1
10	1300–1400	CO <sub>2</sub>	1350	1
11	1400–1800	H <sub>2</sub> O	1600	1
12	1800–2650	CO <sub>2</sub>	2000	1
13	2650–3000	CO <sub>2</sub>	2800	1
14	3000–4100	CO <sub>2</sub>	3500	1
15	4100–4400	H <sub>2</sub> O	4300	1
16	4400–6000	CO <sub>2</sub>	5000	1
Total $n = 16$				32

vertical inversion from the downward line-by-line reference flux:

$$\sigma_{\text{eff}}(z_l) = \frac{1}{\rho \Delta z} \ln \frac{F_{\text{lbl}}^\downarrow(z_l)}{F_{\text{lbl}}^\downarrow(z_{l-1})}, \quad (4)$$

where  $\rho$  is the absorber mass concentration,  $\Delta z$  is the layer thickness, and  $F_{\text{lbl}}^\downarrow$  is the downward flux obtained from the reference line-by-line Monte-Carlo model. For a spectral subset dominated by one absorber, the resulting effective absorption coefficient is written as

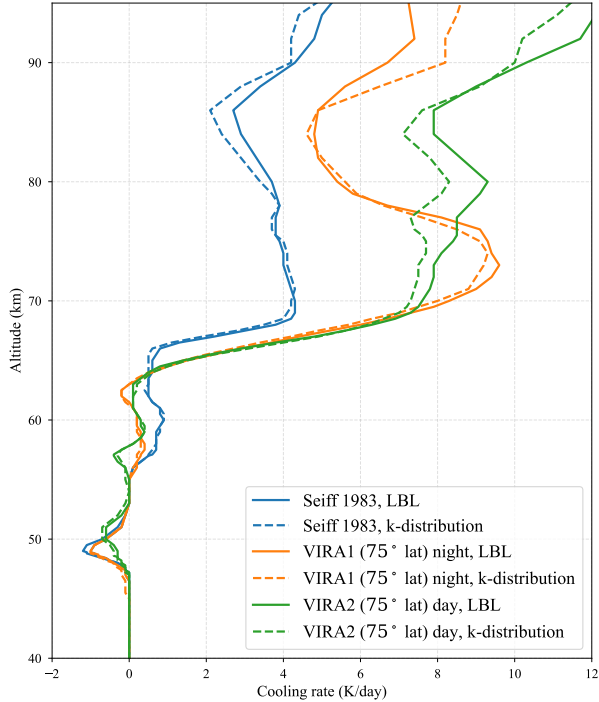
$$k_j^*(z) = \rho_{\text{dom}} \sigma_{j,\text{eff}}^{(\text{dom})}(z) + \sum_{s \in S_{\text{other}}} \rho_s \sigma_{j,\text{eff}}^{(s)}(z), \quad (5)$$

which makes it possible to account for overlapping absorption by the dominant and secondary species within the same spectral subset.

A separate part of the chapter compares the proposed flux-fitting  $k$ -distribution technique with the conventional correlated- $k$  framework. In the correlated- $k$  method, radiative transfer in a spectral band is represented using quadrature over the reordered absorption coefficient distribution,

$$T_{\Delta\nu} = \sum_{j=1}^{N_i^{(\text{ck})}} w_j \exp \left[ - \int k(g_j, z) dz \right], \quad (6)$$

where  $k(g_j, z)$  are tabulated absorption coefficients and  $w_j$  are quadrature weights. In the flux-fitting approach, the same quantity is represented as a



**Figure 3:** Comparison of radiative cooling-rate profiles obtained with the flux-fitting  $k$ -distribution scheme (dashed lines) and the line-by-line Monte-Carlo reference calculations (solid lines) for representative Venus atmospheric profiles.

sum over a set of effective absorption coefficients,

$$T_{\Delta\nu} = \sum_{j=1}^{N_i^{(\text{fkD})}} \exp \left[ - \int k_j^*(z) dz \right], \quad (7)$$

where each function  $k_j^*(z)$  represents absorption over a corresponding subset of the spectral interval. In this formulation, the total number of terms,

$$N = \sum_i N_i, \quad (8)$$

is exactly the number of radiative transfer solver calls required to cover the full spectral range. Unlike the correlated- $k$  method, where the number of quadrature points is fixed by the numerical integration scheme, in the flux-fitting technique this number is controlled directly during the construction of the effective absorption coefficients. To quantify the efficiency gain relative to correlated- $k$ , the parameter

$$\eta = \frac{N^{(\text{ck})}}{N^{(\text{fkD})}} \quad (9)$$

is introduced. The obtained values of  $\eta$  indicate that the proposed technique is more efficient by one to two orders of magnitude than modern Venus radiative schemes based on correlated- $k$ .

**Table 2:** Parameterization details for the absorption of ultraviolet radiation

Band	Spectral region ( $10^4 \text{ cm}^{-1}$ )	Dominant absorber	$\tilde{\nu}_i^R$ ( $\text{cm}^{-1}$ )	Incident solar flux ( $\text{W m}^{-2}$ )
1	5.00–8.00	CO <sub>2</sub>	66000	0.20
2	3.(3)–5.00	SO <sub>2</sub> , CO <sub>2</sub>	36000	27.74
3	3.10–3.(3)	SO <sub>2</sub> , UVA	32000	28.19
4	3.00–3.10	SO <sub>2</sub> , UVA	30000	19.91
5	2.90–3.00	UVA, SO <sub>2</sub>	30000	20.20
6	2.70–2.90	UVA, SO <sub>2</sub>	28000	52.40
7	2.55–2.70	UVA, SO <sub>2</sub>	26250	17.64
8	2.50–2.55	UVA, SO <sub>2</sub>	25250	47.27
Total $n = 8$				213.55

The chapter also discusses the role of temperature dependence in the developed parameterizations. In the thermal infrared region, the effective absorption coefficients must be adjusted to the temperature profile used in a climate model. For this purpose, a dedicated interpolation procedure and a corresponding Fortran implementation module are introduced, allowing the coefficients to be recalculated for arbitrary temperature profiles on the same vertical grid. In the shortwave region, by contrast, the temperature dependence of molecular absorption cross-sections can be neglected for the adopted level of accuracy. Therefore, the ultraviolet parameterization is formulated in a simpler form.

The method was applied to the thermal infrared spectral range 10–6000  $\text{cm}^{-1}$  for the lower and middle atmosphere of Venus. The resulting longwave parameterization consists of 16 spectral bands and requires only 32 radiative transfer solver evaluations to cover the entire thermal infrared range. Comparison with the reference line-by-line Monte-Carlo calculations shows that the developed longwave parameterization reproduces upward radiative fluxes with errors below 2% below 95 km, while discrepancies in cooling rates do not exceed about 1.2  $\text{K day}^{-1}$  below 90 km and decrease to about 0.3  $\text{K day}^{-1}$  below 75 km. A representative comparison of the cooling-rate profiles is shown in Fig. 3. The corresponding band structure of the longwave parameterization is given in Table 1.

In the ultraviolet region, the same general approach is applied. The 125–400 nm interval is divided into eight spectral bands, for which effective absorption coefficients are constructed for the dominant absorbers and representative spectral points are selected for the calculation of Rayleigh scattering and cloud optical properties. Validation against the reference line-by-line Monte-Carlo model showed discrepancies of less than 3% in radiative fluxes and less than 1% in heating rates. Thus, the developed shortwave parameterization correctly reproduces the solar-radiation budget of the Venus atmo-

sphere. The corresponding band structure of the ultraviolet parameterization is summarized in Table 2.

Thus, Chapter 3 of the dissertation presents a unified methodological framework for parameterizing molecular absorption in both the shortwave and thermal infrared spectral regions of the Venus atmosphere, together with the resulting parameterizations. The developed flux-fitting  $k$ -distribution technique combines the physical consistency of line-by-line reference calculations with the computational efficiency required for climate modeling. It provides a practical alternative to correlated- $k$  schemes for dense vertically inhomogeneous atmospheres.

## Conclusion

In this dissertation, the problem of constructing and validating efficient parameterizations of molecular absorption for radiative transfer modeling of the Venus atmosphere in the shortwave and thermal infrared spectral regions is addressed. The study combines three intersected components: high-resolution line-by-line modeling of molecular absorption, reference line-by-line simulations based on the Monte-Carlo method, and the development of compact parameterizations suitable for use in radiative-convective and climate modeling.

The flux-fitting  $k$ -distribution technique is developed and applied to the Venus atmosphere. In contrast to the conventional correlated  $k$ -distribution approach, the proposed technique does not require the assumption of inter-level correlation of monochromatic absorption coefficients, naturally accounts for vertical inhomogeneity of the atmosphere, and directly controls the accuracy-efficiency trade-off through fitting to benchmark fluxes and cooling rates.

A major result of the dissertation is the development of the MARFA line-by-line code for calculating molecular absorption coefficients and cross-sections in planetary atmospheres. The implemented eleven-grid interpolation technique provides efficient calculation of high-resolution spectra for large line cut-offs and under conditions of uncertain spectroscopic data, which are typical for the Venus atmosphere. Apart from source code in a public repository, MARFA can be accessed as a web-based platform and can be considered as an online laboratory for investigating absorption in planetary atmospheres.

A benchmark line-by-line radiative transfer model based on the Monte-Carlo method is used throughout the dissertation for validation of the developed

parameterizations. In the ultraviolet spectral region, this model is applied to calculate solar radiative fluxes and heating rates in the Venus atmosphere. In the thermal infrared region, it is used to calculate upward thermal fluxes and cooling rates. The use of a benchmark Monte-Carlo model makes it possible to validate the parameterizations directly against physically complete line-by-line radiative transfer solutions.

For the ultraviolet spectral region, an effective parameterization of solar-radiation absorption in the 125–400 nm interval is developed. It is shown that the entire ultraviolet spectral range can be represented using only eight effective absorption coefficients. There are different dominant absorbers in different spectral bands: CO<sub>2</sub> in the far ultraviolet, CO<sub>2</sub> and SO<sub>2</sub> in the middle ultraviolet, and SO<sub>2</sub> together with the unknown ultraviolet absorber in the near-ultraviolet region. For Rayleigh scattering and cloud optical properties, eight representative spectral points are introduced. As a result, the full ultraviolet range is reduced to eight radiative transfer evaluations while preserving high accuracy suitable for climate modeling: the discrepancies are below 3% for radiative fluxes and below 1% for heating rates.

For the thermal infrared spectral region, in the 10–6000 cm<sup>-1</sup> interval, a parameterization based on 16 spectral bands and requiring only 32 radiative transfer evaluations is constructed for the main absorbers CO<sub>2</sub>, H<sub>2</sub>O, and SO<sub>2</sub>. Validation of the developed longwave parameterization demonstrates that the upward thermal fluxes are reproduced with errors below 2% below 95 km, while the discrepancies in cooling rates remain within acceptable limits throughout the lower and middle atmosphere of Venus, not exceeding approximately 1.2 K day<sup>-1</sup> below 90 km and decreasing to about 0.3 K day<sup>-1</sup> below 75 km. These results confirm that the proposed parameterization is suitable for use in Venus general circulation models and radiative–convective models.

## Author’s publications on dissertation topic

1. Fomin, B. A., Razumovskiy, M. V. The flux-fitting  $k$ -distribution technique: An application to thermal infrared absorption in the atmosphere of Venus // *Journal of Quantitative Spectroscopy and Radiative Transfer*. 2026. Article 109912.
2. Razumovskiy, M. V., Fomin, B. A., Astanin, D. A. MARFA: An effective line-by-line tool for calculating molecular absorption in planetary atmospheres // *Journal of Quantitative Spectroscopy and Radiative*

*Transfer*. 2025. Vol. 346. Article 109599.

3. Фомин Б.А., Разумовский М.В. Моделирование переноса тепловой радиации в атмосфере Венеры // Материалы 21-й Международной конференции «Современные проблемы дистанционного зондирования Земли из космоса». Москва: ИКИ РАН, 2023. С. 441.
4. Fomin, B. A., Razumovskiy, M. V. Effective parameterization of absorption by gaseous species and unknown UV absorber in 125–400 nm region of Venus atmosphere // *Journal of Quantitative Spectroscopy and Radiative Transfer*. 2022. Vol. 286. Article 108201.
5. Разумовский, М. В., Родин, А. В. Моделирование атмосфер гравитационно-захваченных супер-Земель, вращающихся вокруг маломассивных родительских звезд, с использованием негидростатической модели общей циркуляции // *Письма в Астрономический журнал*. 2020. Т. 46, № 6. С. 427–434.
6. Razumovskiy, M. V., Fomin, B. A., Rodin, A. V. Development of radiation block for non-hydrostatic GCM of Venus' atmosphere // *The Eleventh Moscow Solar System Symposium*. 2020. P. 371.

## References

- Darrell E. Burch, David A. Gryvnak, Richard R. Patty, and Charlotte E Bartky. Absorption of infrared radiant energy by CO<sub>2</sub> and H<sub>2</sub>O. iv. shapes of collision-broadened CO<sub>2</sub> lines. *JOSA*, 59(3):267–280, 1969.
- Vincent Eymet, R Fournier, J-L Dufresne, Sébastien Lebonnois, Frédéric Hourdin, and Mark A Bullock. Net exchange parameterization of thermal infrared radiative transfer in Venus' atmosphere. *Journal of Geophysical Research: Planets*, 114(E11), 2009. doi: 10.1029/2008JE003276.
- B.A. Fomin. Effective interpolation technique for line-by-line calculations of radiation absorption in gases. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 53(6):663–669, 1995. doi: 10.1016/0022-4073(95)00029-K.
- BA Fomin. Monte-Carlo algorithm for line-by-line calculations of thermal radiation in multiple scattering layered atmospheres. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 98(1):107–115, 2006. doi: 10.1016/j.jqsrt.2005.05.078.

- Robert R. Gamache, Michaella Farese, and Candice L. Renaud. A spectral line list for water isotopologues in the 1100-4100 cm<sup>-1</sup> region for application to CO<sub>2</sub>-rich planetary atmospheres. *Journal of Molecular Spectroscopy*, 326:144–150, 8 2016. ISSN 1096083X. doi: 10.1016/j.jms.2015.09.001.
- I. E. Gordon, L. S. Rothman, R. J. Hargreaves, et al. The HITRAN2020 molecular spectroscopic database. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 277:107949, 1 2022. ISSN 00224073. doi: 10.1016/j.jqsrt.2021.107949.
- R. Haus, D. Kappel, and G. Arnold. Radiative heating and cooling in the middle and lower atmosphere of Venus and responses to atmospheric and spectroscopic parameter variations. *Planetary and Space Science*, 117: 262–294, 2015. ISSN 00320633. doi: 10.1016/j.pss.2015.06.024.
- R. Haus, D. Kappel, S. Tellmann, G. Arnold, G. Piccioni, P. Drossart, and B. Häusler. Radiative energy balance of Venus based on improved models of the middle and lower atmosphere. *Icarus*, 272:178–205, 2016. doi: 10.1016/j.icarus.2016.02.048.
- Rainer Haus, David Kappel, and Gabriele Arnold. Self-consistent retrieval of temperature profiles and cloud structure in the northern hemisphere of Venus using VIRTIS/VEX and PMV/VENERA-15 radiation measurements. *Planetary and Space Science*, 89:77–101, 2013. doi: 10.1016/j.pss.2013.09.020.
- Stephen R Kane, Giada Arney, David Crisp, Shawn Domagal-Goldman, Lori S Glaze, Colin Goldblatt, David Grinspoon, James W Head, Adrian Lenardic, Cayman Unterborn, et al. Venus as a laboratory for exoplanetary science. *Journal of Geophysical Research: Planets*, 124(8):2015–2028, 2019.
- H. Keller-Rudek, G. K. Moortgat, R. Sander, and R. Sörensen. The MPI-Mainz UV/VIS spectral atlas of gaseous molecules of atmospheric interest. *Earth System Science Data*, 5(2):365–373, 2013. doi: 10.5194/essd-5-365-2013.
- Roman V Kochanov, IE Gordon, LS Rothman, P Weisło, C Hill, and JS Wilzewski. HITRAN application programming interface (hapi): A comprehensive approach to working with spectroscopic data. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 177:15–30, 2016.
- Andrew A Lacis and Valdar Oinas. A description of the correlated  $k$  distribution method for modeling nongray gaseous absorption, thermal emission,

- and multiple scattering in vertically inhomogeneous atmospheres. *Journal of Geophysical Research: Atmospheres*, 96(D5):9027–9063, 1991. doi: 10.1029/90JD01945.
- Kuo-Nan Liou. *An introduction to atmospheric radiation*, volume 84. Elsevier, 2nd edition, 2002.
- Gabriel-Dominique Marleau, Thomas Henning, Roy van Boekel, Myriam Benisty, Yuhiko Aoyama, and Inga Kamp. Hydrogen-line profiles from accreting gas giants and their cpds. *arXiv preprint arXiv:2511.10751*, 2025.
- JM Mendonça, PL Read, CF Wilson, and C Lee. A new, fast and flexible radiative transfer method for Venus general circulation models. *Planetary and Space Science*, 105:80–93, 2015. doi: 10.1016/j.pss.2014.11.008.
- Michael Metcalf, John Reid, Malcolm Cohen, and Reinhold Bader. *Modern Fortran Explained: Incorporating Fortran 2023*. Oxford University Press, 2024.
- Robert Pincus, Eli J Mlawer, and Jennifer S Delamere. Balancing accuracy, efficiency, and flexibility in radiation calculations for dynamical models. *Journal of Advances in Modeling Earth Systems*, 11(10):3074–3089, 2019.
- L. S. Rothman, I. E. Gordon, R. J. Barber, H. Dothe, R. R. Gamache, A. Goldman, V. I. Perevalov, S. A. Tashkun, and J. Tennyson. Hitemp, the high-temperature molecular spectroscopic database. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 111:2139–2150, 10 2010a. ISSN 00224073. doi: 10.1016/j.jqsrt.2010.05.001.
- Laurence S Rothman, IE Gordon, RJ Barber, H Dothe, Robert R Gamache, A Goldman, VI Perevalov, SA Tashkun, and J Tennyson. HITEMP, the high-temperature molecular spectroscopic database. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 111(15):2139–2150, 2010b. doi: 10.1016/j.jqsrt.2010.05.001.
- Yoshiyuki O Takahashi, Yoshi-Yuki Hayashi, George L Hashimoto, Kiyoshi Kuramoto, and Masaki Ishiwatari. Development of a line-by-line and a correlated k-distribution radiation models for planetary atmospheres. *Journal of the Meteorological Society of Japan. Ser. II*, 101(1):39–66, 2023. doi: 10.2151/jmsj.2023-003.
- C. C.C. Tsang, P. G.J. Irwin, F. W. Taylor, and C. F. Wilson. A correlated-k model of radiative transfer in the near-infrared windows of Venus. *Journal*

*of Quantitative Spectroscopy and Radiative Transfer*, 109(6):1118–1135, 2008. doi: 10.1016/j.jqsrt.2007.12.008.

L. V. Zasova, V. I. Moroz, V. M. Linkin, I. V. Khatuntsev, and B. S. Maiorov. Structure of the Venusian atmosphere from surface up to 100 km. *Cosmic Research*, 44(4):364–383, 2006. doi: 10.1134/S0010952506040095.