BENCHMARK CALCULATIONS OF RADIATIVE FLUXES AND INFLUXES IN THE ATMOSPHERE: HISTORY, METHODS, STATE OF THE ART, AND PROSPECTS

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Of concern in the paper is the problem of benchmark calculations of infrared and solar radiation fluxes in the atmosphere: history of the problem and the reliability and applications of benchmark calculations for testing radiation codes of climate models. In addition, exact numerical techniques for benchmark calculation are reviewed and validated against experiment.

INTRODUCTION

Radiative processes play a central role in climate formation by furnishing energy exchange between the sun, space, and atmosphere, so even slight changes in these processes may affect appreciably the climatic system of the Earth. As an example, ice ages had resulted from a mere 1% (14 W·m^{-2}) decrease in solar constant.[1] Same order of magnitude has the relative value of radiative forcing (i.e., the change of effective radiative flux at the tropopause level) due to doubling of atmospheric carbon dioxide content.[2] Obviously, radiative flux calculations for climate studies should be accurate to within 1%.

And what is the characteristic accuracy in current radiation codes of climate models? This question has been settled by the working group on Intercomparison of Radiation Codes in Climate Models (ICRCCM) organized under the auspices of Joint Scientific Committee on the World Climate Research Programme (WCRP) and International Commission on Radiation (IRC) of the International Association of Meteorology and Atmospheric Physics (IAMAP) on the basis of projects that have been implemented in the USA and Europe since 1982. The ICRCCM was headed by F. Luther (USA) (thermal radiation calculations) and J. Fouquart (France) (solar radiation calculations). After Luther's death in 1986, R. Ellingson (USA) become ICRCCM Co-Chief.

TABLE I. Intercomparison of the results obtained by different groups with the use of different methods for ICRCCM conditions ($F^{-}(0)$ is the integrated flux incident on the underlying surface (W·m^{-2}), *and Q is the effective difference between fluxes at the atmospheric boundaries* (W·m^{-2})).

Calculation case	27 from Ref. 4		31 from Ref. 1		50 from Ref. 1		54 from Ref. 1		49 from Ref. 1	
Number of calculations	39		21		10		10		15	
Physical quantities	$F^{-}(0)$	Q	$F^{-}(0)$	Q	$F^{-}(0)$	Q	$F^{-}(0)$	Q	$F^{-}(0)$	Q
Rms error, %	2.4	–	2	6	1	5	18	13	9	9
Spread, %	12	–	5	21	4	16	61	46	43	35
Average over calculations	343.2	204.0	943.7	206.2	936.2	214.7	444.4	601.2	537.5	255.5
Benchmark calculation[7,9]	348.9	212.5	946.1	197.3	937.8	202.8	444.6	595.5	531.5	255.5

About half hundred scientific research groups participated in the ICRCCM project. They did a series of test flux calculations for a set of atmospheric conditions (cases). In all, 61 cases were considered to test long-wave radiation calculations, and 57 cases – to test solar radiation calculation, each with distinct temperature and pressure stratifications as well as distribution (horizontally uniform) of optically active atmospheric constituents: gases (water vapor, carbon dioxide, ozone, and oxygen), aerosols, and clouds (when present). For example, case 27 for long-wave calculations assumes standard mid-latitude summer atmosphere model with CO_2 content of 300 ppmv (including ozone and water vapor). Case 28 is for

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doubled CO_2 content relative to case 27, and so on. In its turn, case 31 for solar radiation calculations is the same as case 27 for thermal radiation at a solar zenith angle of 30° and surface albedo of 0.2 (Lambertian reflection). Case 50 and 54 differ from case 31 in the presence of thinner and thicker layers of standard aerosols (oceanic and so on). Case 49 is the same as 31 but with a homogeneous cloud layer (for more details, see Refs. 4 and 1 describing infrared and solar radiation calculations, respectively). Results from various groups were intercompared, analyzed, and summarized in Refs. 1, 3, and 4 (special issues of the Journal of Geophysical Research published in 1991 that reported the main results of the ICRCCM project). Some results for the above-considered cases are reproduced in Table I herein; listed are downward integrated fluxes at the lower atmospheric boundary, $F^{-}(0)$, and the differences Q between effective fluxes of infrared (see Ref. 4) and solar radiation (see Ref. 1) at atmospheric top and bottom in the wave number ranges $0 - 2600$ cm^{-1} and $2000 - 33333$ cm^{-1}. Value of Q in the case of solar radiation flux is equal to flux absorbed by the atmosphere itself. Such quantities are chosen because they furnish insights into the absorbing–emitting properties of the atmosphere and illustrate the accuracy of atmospheric radiation calculations by different methods. For each case the table indicates the number of independent calculations being intercompared, average over the calculations, rms deviation, and spread (maximum to minimum difference); the last two are given in per cent of the average.

The spread of the results of flux calculations in Table I is much greater than 1% (particularly for cases 54 and 49 with strong scattering in the atmosphere). Clearly this is indicative of insufficient accuracy of current parametric methods for radiation calculations used in climate models. Unfortunately, based on such a simple comparison, it is impossible to assess the accuracy of individual calculations and hence of the methods themselves, so their refinement or development of more sophisticated methods is presently difficult or even impossible. These methods must be compared against high-precision field experiments, which is the primary objective of the familiar DOE-ARM program,[5] as well as against benchmark calculations. By benchmark calculations are meant calculations based on rigid calculation techniques for solving the equation of radiative transfer in the atmosphere whose optical properties are defined on the rigorous basis of modern understanding of its optically active components and interaction of radiation with gases, aerosols, cloud particles, and the like, that is, *ab initio* calculations. From aforesaid it is clear that benchmark calculations must have controllable accuracy of the order of several fractions of per cent to avoid interference between calculation errors and errors due to lack of understanding of radiation processes in the atmosphere. Such high accuracy calls for highly laborious computational techniques, such as line-by-line (LBL), Monte Carlo methods, etc. to do benchmark calculations. This explains why the problem of benchmark calculation has yet to be solved, in spite of the ten-year effort of many scientific groups equipped with supercomputers. As to the cases, ICRCCM knows only a few independent LBL calculation results for infrared fluxes that agree to within 1–2% (see Refs. 4 and 7). For solar radiation, no one benchmark calculation in scattering (by aerosols and clouds) atmosphere had been done until 1992. Only one LBL computation of solar radiation in the cloudy atmosphere[6] was done for the case similar to the above ICRCCM case 49. The time taken for calculations on CYBER–205 supercomputer was about one hundred hours. To cope with the problem of benchmark calculations to test parametric methods for radiation calculations, E.M. Feigel'son inspired organization of two working groups of experts from ten institutions of the former USSR. The first group, having worked since 1986 till 1989 under leadership of Yu. M. Timofeev, dealt with infrared radiation calculation,[7] while the second, having worked since 1989 till 1993 and headed by me, dealt with solar radiation calculation.[8,9] Both had same aims as ICRCCM, but from the very beginning the emphasis was on the methods for validation against benchmark calculations rather than on the intercomparison. Work of these groups has aided the Kurchatov Institute Russian Scientific Center under my leadership to develop fast benchmark calculation methods. For instance, the calculation mentioned above took only 30–40 hours on IBM–486 computer rather than 100 hours on CYBER–205 computer. Application of these methods has resulted to date in several tens of benchmark infrared and solar radiation calculations. These methods have already been used for validation of radiation codes and other purposes. Examples of such calculations are shown in the lower row of Table I. In the following sections we consider the physical grounds for the developed efficient techniques of benchmark calculations, accuracy limits of benchmark calculations themselves stemming from our insufficient modern knowledge of optical properties of the atmosphere, prospects for using benchmark results and developed numerical techniques, as well as other questions.

PHYSICAL GROUNDS FOR THE EFFICIENT METHODS OF BENCHMARK CALCULATIONS

This section discusses (for integrity of presentation) only basic distinctive features of the developed efficient numerical methods for benchmark calculations, since their detailed description can be found elsewhere.[10a] In developing these methods three types of hindrances were removed: (1) those connected with the necessity of considering many absorption lines of atmospheric gases (several hundred thousand); (2) those connected with atmospheric heterogeneity; and,

(3) those arising from accounting simultaneously for the selective gaseous absorption and scattering.

Hindrance of the first type is important for calculation of selective gaseous absorption coefficients involving the summation of shapes of individual spectral lines. The computation time here is proportional to the product of the number of lines considered (of the order of 10^5) and the number of points taken for each line shape. Spectral line width is normally about 10 cm^{-1} (contributions from line wings at large distances from their centers can readily be accounted for in terms of continuum absorption[12]). For uniform frequency grids used to resolve fine structure of the molecular gas spectrum (with a step of the order of a line halfwidth, 10^{-3} cm^{-1}), for a single standard computation of absorption coefficient it takes several weeks on IBM–486 type computer. (The computer time may be easy evaluated given that a line shape computation at a point involves about ten algebraic and logic operations each at a speed of about 10^{-6} s, and the computation itself is repeated at roughly a hundred levels in the atmosphere.) That is why of so much importance is minimization of the number of points of line shape computation and application of interpolation in between. It can be shown[10b] that for efficient interpolation of line shape, grid points must form a geometric progression. This is difficult to implement in practice, however, particularly in case of line overlapping. Even the FASCOD algorithm,[11] one of the fastest algorithms, employs an interpolation grid far from efficient. So we succeeded in algorithm efficiency improvement[10] by 2–3 times in comparison with the algorithm of Ref. 11, and by one – two orders of magnitude in comparison with algorithms employing uniform grids. (This requires ten grids with steps of the order of 0.001, 0.002, 0.004, ..., 0.001×2^{10} = = 1.024 cm^{-1} and doubled or tripled computer memory.) Using our algorithm, it took about 10 h on an IBM–486 computer to do these calculations.

Difficulty of the second type stems from the atmospheric heterogeneity. In many algorithms the atmosphere is divided into a series of homogeneous layers. However, long-wave radiation calculation in Ref. 7 implemented algorithms with much more efficient line altitude interpolation of atmospheric optical properties. Importantly, with the piecewise-constant altitude profile of the (volume) absorption coefficient, the computation of optical thicknesses between arbitrary levels was accomplished by analytical integration and in practice reduces to a small number of quick algebraic operations. This proved to be very important for determining photon optical paths between scattering events in Monte Carlo computation of solar radiation. In the long-wave radiation calculation, the Plank function was taken to be constant within about 1 cm^{-1} wave number intervals (a standard trick that introduces controllable and negligible error). The integration of relevant fast oscillating functions of wave number over these intervals at the altitude points of a nonuniform interpolation grid was followed by numerical altitude integration of the result multiplied by the Plank function over a uniform grid with 10 m step. (This small step was necessary for reliable benchmark calculations). The integration convergence was improved with the aid of special procedures[7]. Overall, the infrared benchmark calculation (without accounting for scattering processes in the atmosphere) took day or so on an IBM–486 computer.

Difficulty of the third type is the necessity of joint consideration of the processes of selective gaseous absorption and scattering in the atmosphere, due to which the monochromatic transfer equation had to be solved about 10^6 times in infrared run and 10^7 times in solar run. (The figures follow from comparison of 10^{-3} cm^{-1}, the characteristic line halfwidth in the atmosphere, with 100–3000 and 2000–20000 cm^{-1}, the widths of spectral intervals in the infrared and solar runs, respectively.) Most difficult is to solve the radiative transfer equation in such a complex scattering medium as a turbid or cloudy atmosphere. In some cases, as pointed out in the Introduction, it took several hundred hours on a supercomputer (when using combination of LBL and doubling-adding techniques[6]). This problem, however, is surprisingly easy solved by means of the said efficient LBL method in combination with the Monte Carlo technique, taking into consideration atmospheric heterogeneity as described above.[13] Highly useful in this regard has proven to be photon simulation in both space and frequency (which was alluded to the author by A.N. Rublev). Due to this, benchmark calculation of solar radiation has been found to take only one day or so even on moderately fast computer (like IBM–486). What is the reason for high efficiency of Monte Carlo method for atmospheric selective absorption calculation? The point is that Monte Carlo method effectively compensates for errors, predominantly random ones. A useful practical consequence is that about 10^6 photons will be sufficient to run, irrespective of the width of spectral range and spectral resolution. (This claim has been carefully tested by independent calculations based on single scattering approach,[13] and the like.) Thus, by Monte Carlo method, one integral quantity (say, downward flux at a given level) is calculated with 0.1% accuracy from a combination of one million solutions of the transfer equation obtained at different frequencies with about 100% accuracy, whereas the use of a method like doubling-adding technique for the same purpose requires, as much as 10^7 figures obtained with the same 0.1% accuracy (for subsequent numerical integration over frequency). The number of figures can be reduced by several orders of magnitude with the use of *K*-distribution approach or the like.[14] However, even doing so, the volumes of computation are obviously incomparable, thereby confirming the advantage of the Monte Carlo approach. (Evidently, Monte Carlo method becomes less efficient when spectral rather than integral quantity is sought.)

VALIDATION OF BENCHMARK CALCULATIONS

Central question is the accuracy of the benchmark calculations themselves, in view of our insufficient current knowledge of the interaction of radiation with the atmosphere. In particular, how sensitive are benchmark results to the presently used incomplete data bases, namely the HITRAN–86 (see Ref. 15) and HITRAN–92 (see Ref. 16) spectral line databases. Reference 17 provides data answering this question. In particular, the results from solar radiation calculation may vary by several fractions of per cent, while the results from influx calculations – by 2–3% for alternating databases. For infrared calculations, the upward flux at tropopause altitude changes from 295.1 (HITRAN–16) to 294.0 W·m^{-2} (HITRAN–92), while downward flux – from 20.79 to 21.23 W·m^{-2} (for case 27). These results, together with others, indicate that these databases are nearly completed as the revealed disagreement is within the 1% error of flux calculation.

Even more complex is the question: what accuracy can be obtained in benchmark calculations based on the modern knowledge of the shape of line far wings and continuum absorption? It can be answered only with availability of accurate field data. Fortunately, such data came from field experiment SPECTRE made as part of DUE ARM program.[18] They have clarified the situation with infrared radiation calculations. This experiment was recently used in continuation of the ICRCCM study for validation of infrared radiation measurements. The validation was headed by Dr. Ellingson, ICRCCM Co-Chief, of the University of Maryland, USA. Measured in the experiment was the spectrum of infrared radiation, incident normally on the Earth's surface [W/(m^2·sr·cm^{-1})], with about 1 cm^{-1} resolution. Simultaneously, the profiles of pressure, temperature, humidity, carbon dioxide, etc. required for LBL calculations were measured at 45 levels between 0 and 30 km. It is important to note that the accuracy of experimental data was within 1%. As comparison showed, the discrepancy between the LBL results (including my results) and the experimental data for the entire examined spectral range (520–2500 cm^{-2}) was within 1– 2%. This indicates satisfactory agreement (although for individual spectral regions, the discrepancy was in excess of 5%). The comparison is exemplified in Fig. 1 (region of 15 μm CO_2 band and edge of the transparency window) and Table II. The table considers separately spectral intervals encompassing 15 μm CO_2 band (520–800 cm^{-1}), transparency window and 9.6 μm ozone band (800 – 1200 cm^{-1}), 6.3 μm water vapor absorption band (1200 – 2000 cm^{-1}), and 4.3 μm CO_2 band (2000 – 2500 cm^{-1}). Computations employed an advanced continuum model[20] and that used previously in benchmark calculations.[7] As noted above, overall, the results of Table II satisfactorily agree with the experiment (mainly as a result of reasonable agreement in the region of strong bands). This allows us to conclude that at the present stage of physics the benchmark calculations ensure satisfactory accuracy of about 1 per cent for the infrared range. Unfortunately, experimental validation of benchmark calculations of short-wave radiations remains a challenge for future research. Meanwhile, the intercomparison of LBL results mentioned above was encouraging: 500 and 499.4 W·m^{-2} for downward fluxes at the atmospheric bottom, and 431 and 424.1 W·m^{-2} for upward fluxes at the atmospheric top, as given by Ref. 9 and 6, respectively.

TABLE II. An example of comparison of nadir intensity of thermal atmospheric emission (W·m^{-2}·sr^{-1}) *calculated theoretically with that measured in experiment for continuum absorption models of Roberts, et al.*[19] (*water vapor only*) *and Clough et al.*[20] ($H_2O + CO_2 + O_2$). *Experiment* (*upper curve*), *calculation with the Clough continuum* (*middle curve*), *and calculation with the Roberts continuum* (*lower curve*) (*SPECTRE field experiment*[18]).

Spectral interval, cm^{-1}	Intensity, W·m^{-2}·sr^{-1}	Absolute difference, W·m^{-2}·sr^{-1}	Relational difference, %
520–800	22.93		
	22.65	–0.29	1.26
	22.78	–0.16	0.70
800–1200	2.30		
	2.20	–0.10	4.62
	2.41	0.10	4.39
1200–2000	8.52		
	8.63	0.12	1.40
	8.35	–0.17	1.96
2000–2500	0.256		
	0.246	0.010	3.85
	0.233	0.022	8.77
520–2500	34.02		
	33.73	0.29	0.85
	33.78	0.25	0.73

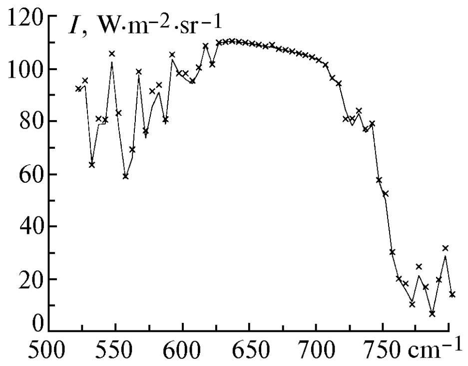

FIG. 1. Calculated (crosses) and experimental (solid curve) nadir intensities of thermal atmospheric emission (W·m^{-2} sr^{-1}) *(SPECTRE field experiment*[18]).

Summarizing, the modern physical modeling of atmospheric radiation for benchmark calculations can be acknowledged as satisfactory.

CONCLUSION

A set of results of benchmark calculations done to date was published in Ref. 7 (infrared radiation calculations for five standard models of a clean cloudless atmosphere), Ref. 8 (fluxes and influxes of solar radiation with an account of the molecular scattering for standard models of a clean atmosphere), and Ref. 9 (fluxes and influxes of solar radiation for five aerosol atmospheric models and three models of clouds). The result of these benchmark calculations has already been used for testing and refining model radiation codes, which substantially altered the modeled climates, thereby warranting the importance of such tests. For instance, Ref. 21 makes use of benchmark results to account for the temperature dependence in radiation code intended to describe infrared radiation in two-dimensional energy-budget radiation-convection climate model. Such an approach was equivalent to introduction of the extra feedback and resulted in 0.5° decrease of greenhouse warming due to CO_2 doubling in the troposphere (i.e., 20% of standard response for this model). (For the lower stratosphere in tropics this resulted in 2–3° change.) Unfortunately, work on updating radiation codes is presently far from completion, in view of only recent appearance of documented benchmark calculations themselves, as well as due to difficulties with developing fast and accurate parameterization (particularly so for solar radiation calculations). Furthermore, the parameterization development most likely will require much more benchmark calculations to form a database (I hope for its appearance during the year to come).

Benchmark calculations of concern in the paper encompass only plane-layered vertically stratified atmospheric models. Their underlying numerical techniques, however, are easy generalized to account for horizontally heterogeneous atmosphere (especially so when using supercomputers). The central task I would like to emphasize here is the development of atmospheric models for radiation calculation in horizontally inhomogeneous atmospheres; these models must describe real atmospheric properties (such as broken cloudiness), but also be straightforward to incorporate them in climate models. (They are supposed to be developed by appropriate working group.)

In conclusion, I would like to note that the developed numerical techniques are highly promising for different applications such as radiative forcing study.[2] They may be especially useful for solving atmospheric sensing problems such as space research of the Earth. (Here high-precision calculations are required for their subsequent use in solving the inverse problems of experimental data processing.) Overall, the set of techniques developed provides a powerful tool for studying atmospheric radiation processes *ab initio* using available computers.

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