Development of an Internet accessible software: Optics and spectroscopy of gas-aerosol media

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ABSTRACT

A description of an Internet accessible software «Optics and spectroscopy of gas-aerosol media» is represented. The new software is focused on research in the field of direct and inverse problems of optics and spectroscopy of gas-aerosol media.

Internet resource, gas-aerosol medium, database, spectral line parameters, spectral characteristic

1. INTRODUCTION

Over the past two decades, a large number of Internet resources devoted to solving various problems in the field of optics and spectroscopy of gas-aerosol medium was created. A small part of such resources is shown on the website of HITRAN database (DB) [1]. They provide the data deal with experimental or calculated spectral characteristics of atoms, molecules and aerosols, meteorological and optical models.

At present there are different spectroscopic databases. A list of the well-known DB includes the following: NIST [1], GEISA [1], JPL [1], CDMS [1], HITRAN [2], HITEMP [3], VALD [4]. They are constantly updated and supplemented with new data that leads to an increase of their volumes and, as a consequence, to the complexity of their processing, analysis and verification. A large number of software for the calculation of the various spectral characteristics and modeling the radiation transfer in the gas-aerosol media was created [5]. Some programs are now available in the form of Internet resources. These include SpectralCalc [1], SPECTRA [1], HITRAN on the Web [6] and others.

The authors of this paper developed a number of physical and mathematical models and algorithms deal with the solution of direct and inverse problems of optics and spectroscopy of gas-aerosol media. Particular attention is paid to calculate the spectral lines parameters (SLP) of the high-temperature gases, unrepresented in the literature. The information of high-temperature SLP is needed to develop the methods for remote sensing the jet engine operation by means of the analysis of the plume spectra. On the other hand, the methods for simulation the spectral characteristics of gas-aerosol media, consisting of several layers, are also created.

Calculations of SLP are performed, using the sets of the empirical parameters of the effective rotational Hamiltonian and the interaction operators, taken from the recent experimental studies. For computing the line positions and intensities the transitions between the vibrational-rotational (VR) levels with a total change of the vibrational quantum numbers, not greater than two are considered For this purpose, the sets of the parameters of the dipole moment function up to the second order inclusive are determined on the basis of the experimental vibrational transition moments. The perturbation effects in line intensities are taken into account. To calculate the air-broadening, as well as self-broadening coefficients of the spectral lines, the approximation expressions from literature and obtained by authors of this work are applied.

In this work, the creating of the Internet available software of the information-calculation system «Optics and spectroscopy of gas-aerosol media» (ICS «INTRAVA») is presented.

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21st International Symposium on Atmospheric and Ocean Optics: Atmospheric Physics,
edited by G. G. Matvienko, O. A. Romanovskii, Proc. of SPIE Vol. 9680, 96800N

2. ARCHITECTURE OF ICS «INTRAVA»

Operation of ICS is provided by the two servers (Fig. 1). The first of them is responsible for the web interface ICS, and the second - for the management of the Grid, performing computing tasks.

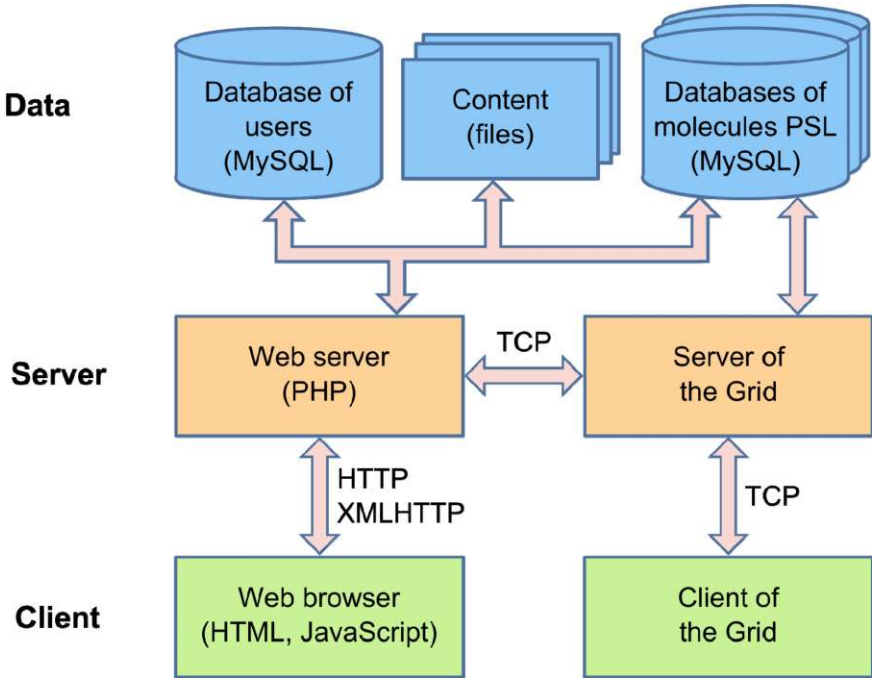

Figure 1. Architecture of the information-calculation system «Optics and spectroscopy of gas-aerosol media».

The implementation of running the software on the web server is carried out on the PHP language, and executed by the client browser - in JavaScript using the library jQuery, simplifying the development of the application. Interacting the client with the web server takes place via AJAX-requests. The user's database contains the data for the functioning of the Internet resource (user accounts, requests for modeling, simulation results, and more). Spectral line parameters of the molecules are placed into separate databases. The content of the Internet resource is stored in files.

To fulfil grid computing written in C language the client-server application (Grid management system (GMS) and client of the Grid (CG)) is used. The interaction of the web server with GMS is provided by written in PHP scripts. GMS produces decomposition coming from a web server computing tasks into subtasks, which are sent to the CG, and the subsequent compilation of the results of calculations. CG caries out the necessary calculations using implemented in C++ software including modified algorithms of software «TRAVA» [7]. For the parallelization of computational algorithms OpenMP is used. CG provides the setting time limits and priority of using the compute node ? resources on which it is installed.

3. FUNCTIONALITY OF ICS «INTRA VA»

Information part of the Internet resource primarily provides access to developed by our research group the databases of SLP of molecules such as H_2O, SO_2, H_2S, NO_2, CO_2 [8, 9, 10]. Data can be presented in tabular and graphical form, sorted and filtered according to the values of the parameters of the spectral lines of molecules.

The web interface of the computation part of the Internet resource provides input of values of the input parameters required for the calculation of the spectral characteristics (absorption coefficients of gases; scattering, absorption and extinction coefficients of aerosols; optical thicknesses; absorption and transmission functions; radiances) (Fig. 2), and present of them in a format used by computer software.

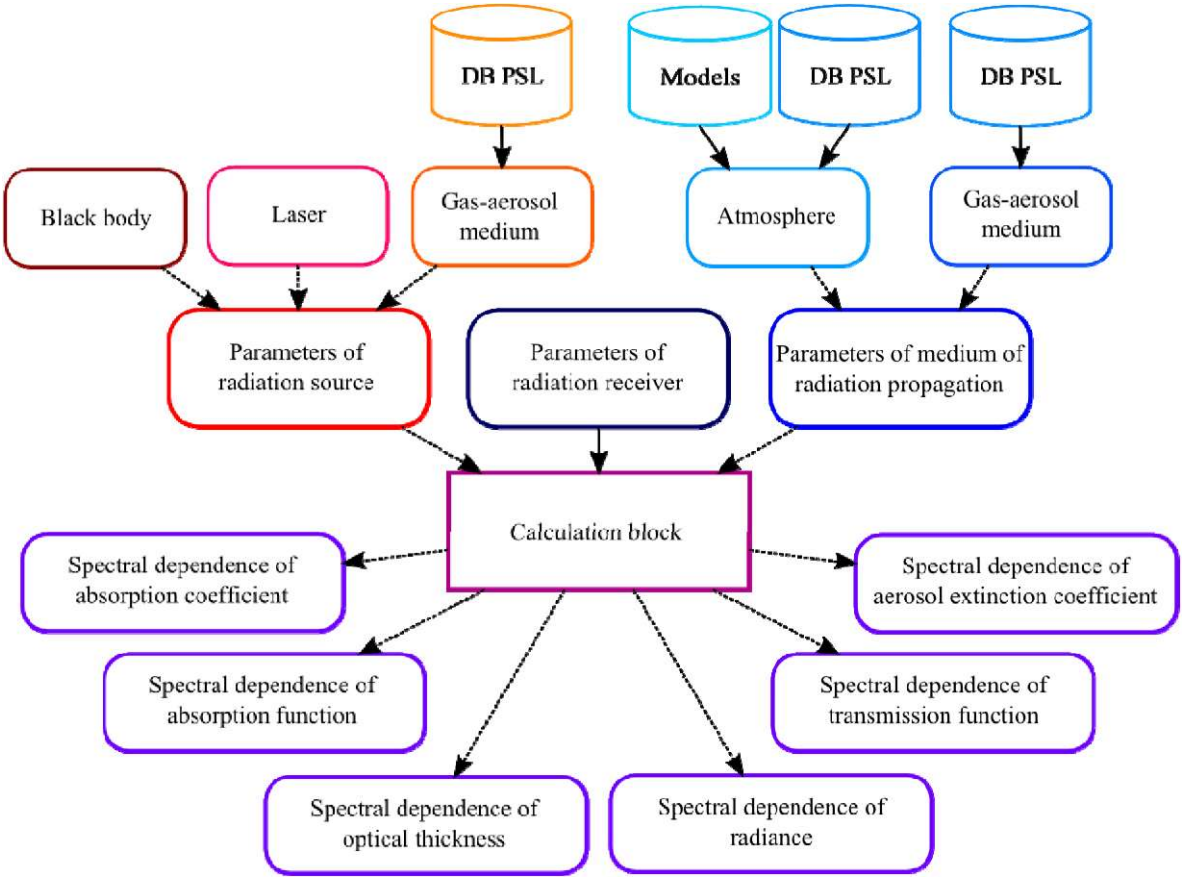

Figure 2. Functionality of the information-calculation system «Optics and spectroscopy of gas-aerosol media».

The calculation of the spectral characteristics of molecules is carried out by line-by-line method, which involves a summation of the contributions of each individual spectral lines to determine the amount of absorption. Spectral characteristics of aerosols are calculated according to the Mie theory. The simulation may last a considerable period of time, so all of the computing tasks are queued. User has the ability to track the progress of his tasks in the queue and the status of their implementation on the page of Internet resource and through notices are sent to his e-mail address.

4. CONCLUSION

A description of the creating Internet available information-calculation system «INTRAVA» is given. The system is built by means of the Internet and network technologies. Internet resource may be interesting for specialists in the field of optics and spectroscopy of gas-aerosol media.

ACKNOWLEDGMENTS

This study was conducted with the support from Russian Foundation for Basic Research, grant numbers 13-07-98027 and 15-01-03176.

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