PROPER ORTHOGONAL DECOMPOSITION USED TO EVALUATE ABSORPTION LINE BLACK BODY DISTRIBUTION FUNCTION.

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Proper Orthogonal Decomposition (POD) technique has been used in many application for more than a century and appears under many names: Karhunen-Loeve Decomposition, Principal Component Analysis, or Singular Value Decomposition. The overview of the POD related literature, theory and history has been recently described[1]. POD offers elegant way to build low dimensional description of large and correlated data sets consisting of a sequence of vectors of the same dimensions. The most striking feature of the POD is its optimality: it provides the most efficient way of capturing the dominant components of a data set using only few degrees of freedom. The technique is similar to discrete Fourier expansion of function. In both cases the approximated function is expressed as a linear combination of orthogonal vectors (modes). The scalar coefficients of this combination are referred to as amplitudes. While the Fourier modes are user defined, the POD modes are calculated by a procedure which extracts the correlation between the members of the vectors sequence.

Absorption Line Black Body Distribution Function (ALBDF) term has been first time introduced by Denison and Webb in their work on Spectral Line-based Weighted sum of gray gases model (SLW)[2]. ALBDF defines absorption cross section (C_{abs}, proportional to the absorption coefficient) which is cumulated over entire spectrum and weighted by Planck function. This function allows to redefine way of integration of the radiative transfer equation (RTE). Instead of integrating with respect to the wavenumber, the RTE is integrated with respect to the absorption cross section. Such approach reduces substantially computational time, however it provides exact solution only for homogenous and isothermal media.

Soufiani[3], and later Modest[4] used similar approach defining cumulation of the absorption coefficient in slightly different way. It can be proved that all methods gives the same result when introduced to the solution of RTE.

Since generation of the cumulated function requires long spectral calculation, ALBDFs have been preprocessed and suitable correlations have been generated[2]. Since implementation of these correlations in the RTE solvers introduces error, their accuracy is of great importance.

In current work POD method is employed to reproduce cumulated functions. The technique proved to produce results in excellent agreement with the original data (i.e. line by line calculations). The first step of the POD application for radiative properties evaluation requires generation of sequence of the ALBDF referred as snapshots. The accurate generation of ALBDF requires good representation of absorption cross section spectral histogram. Here, most up to date spectroscopic data bases CDSD-1000 and HITEMP are employed. ALBDF are generated for 500 discrete values of absorption cross section (logarithmically distributed), separately for CO2 and H2O. Procedure is repeated for different gas and black body temperature and for different concentration in case of H2O. Set of ALDBF defines snapshot matrix **U**. Rows in matrix **U** correspond to discrete value of ALBDF and columns correspond to given combination of gas and black body temperature and concentration in case of H2O. POD technique defines **U** as linear

combination of basis matrix $\mathbf{\Phi}$ and amplitude matrix **A**

$$\mathbf{U} = \mathbf{\Phi} \cdot \mathbf{A} \tag{1}$$

The basis matrix $\mathbf{\Phi}$ can be evaluated by solving eigenvalue problem

$$\mathbf{C}\boldsymbol{\varphi}_i = \lambda_i \boldsymbol{\varphi}_i \tag{2}$$

where $\mathbf{C}=\mathbf{U}\cdot\mathbf{U}^T$. Since the vectors of basis matrix are orthogonal, one can immediately evaluate the amplitudes matrix **A** from

$$\mathbf{A} = \mathbf{\Phi}^T \cdot \mathbf{U} \tag{3}$$

The eigenvalues λ_i of covariance matrix **C** decrease rapidly, thus matrix **U** can be reproduced with good accuracy using only first few modes of $\mathbf{\Phi}$ matrix

$$\mathbf{U} \approx \overline{\mathbf{\Phi}} \cdot \overline{\mathbf{A}} \tag{4}$$

where truncated basis matrix $\overline{\mathbf{\Phi}}$ contains only first K columns of matrix $\mathbf{\Phi}$ and truncated amplitude matrix $\overline{\mathbf{A}}$ contain only first K rows of matrix $\mathbf{A}$. Using formula (4) only original ALBDF (snapshots from **U** matrix) can be reproduced. In order to generate ALBDF for arbitral set of temperature, amplitudes needs to be parameterized. Parameters of the model (denoted as excitation vector **f)** are gas and black body temperature and concentration in case of H2O. Amplitude matrix is defined as linear combination of predefined interpolation matrix **G**, and unknown coefficients **B**

$$\overline{\mathbf{A}}\mathbf{(f)} = \mathbf{B} \cdot \mathbf{G(f)} \tag{5}$$

G is the interpolation matrix gathering the values of the interpolation functions (here Radial Basis Functions) evaluated for different sets of excitation vectors. For original set of data coefficient matrix **B** can be evaluated after simple mathematical manipulation of the formula (5). Finally, ALBDF can be evaluated for arbitral excitation vector from formula

$$\mathbf{u(f)} \approx \overline{\mathbf{\Phi}} \cdot \mathbf{B} \cdot \mathbf{g(f)} \tag{6}$$

Procedure has been tested for numerous values of the excitation vector. In all cases ALBDF reproduced by POD procedure is in perfect agreement with line by line calculations for values of C_{abs}>1e-4 m^2/mol. For C_{abs}<1e-4 m^2/mol error reaches up to 20%. This behavior is a combined effect of the truncation of the POD basis matrix and finite representation error caused by very low values of the reproduced ALBDF. The relatively big error in evaluated ALBDF for the C_{abs}<1e-4 m^2/mol do not affect much global radiative analysis since low values of the C_{abs} represent close to transparent part of the spectrum. Evaluation time of ALBDF with POD method compared to the standard correlations[2] is around 10 times slower. The evaluation time of ALBDF can be reduced by further truncation of the basis matrix. Figure 1 shows comparison of the error between ALBDF evaluated for CO2 from POD model and using line by line calculations for different level of the basis matrix truncation. The lowest number of eigenvectors used (ev=7) to reproduce function effects in error not higher then 2% for the value of C_{abs} >1e-4 m^2/mol.
Reproduced ALBDF have been used to calculate total emisivities and directional intensity in propagating ray of radiation through non-isothermal and non-homogenous media. In both cases comparison to the line by line calculation shows error in predicted values below 2%.

Final remarks

The accuracy reached with present POD model in evaluating ALBDF is very high. This has been proved by comparing the POD results with the benchmark LBL solutions. The precision can readily be controlled by appropriate truncation of the POD basis matrix $\mathbf{\Phi}$. The developed method of evaluating cumulated function can be applied to any similar model of evaluating radiative properties of the gases. The extensive description of the method presented here can be found in recent authors' publication[5].

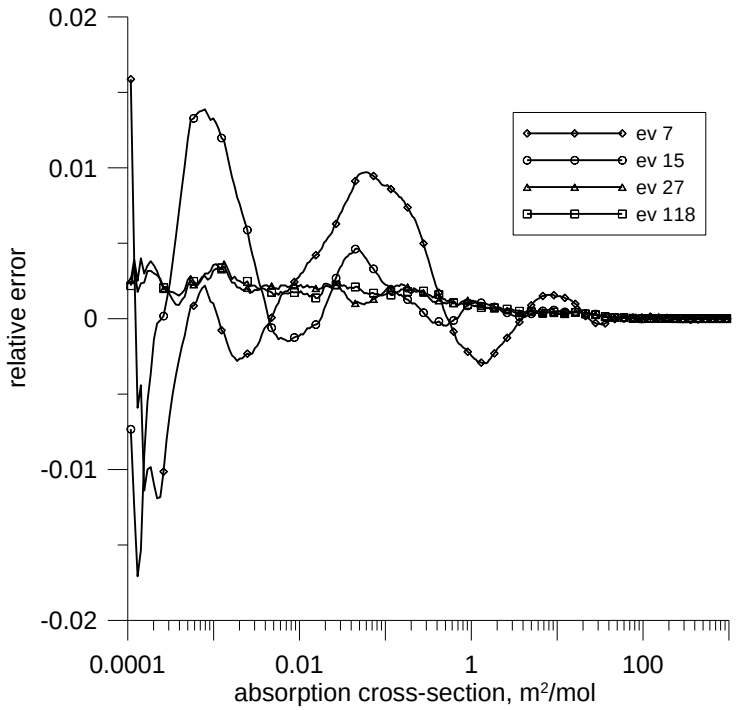

Figure 1. Error between ALBDF generated with LBL and POD for CO2 (gas temperature Tg = 1058 K, black body temperature Tb = 1566 K)

REFERENCES

1. Ostrowski, Z., *Application of Proper Orthogonal Decomposition to the Inverse Problems*, PhD thesis, Silesian Univ. of Technology, Gliwice, (2005).
2. Denison, M.K., Webb, B.W. , An absorption-line blackbody distribution function for efficient calculation of total gas radiative transfer, *Journal of Quantitative Spectroscopy and Radiative Transfer* Volume 50, Issue 5, Pages 499-510, 1993.
3. Riviere, Ph., Soufiani, A., Perrin, M.Y., Riad, H., Gleizes, A., Air mixture radiative property modelling in the temperature range 10,000-40,000 K, *Journal of Quantitative Spectroscopy and Radiative Transfer* Volume 56, Issue 1, Pages 29-45, 1996.
4. Modest, M. F. and Zhang, H., The Full-Spectrum Correlated-k Distribution For Thermal Radiation from Molecular Gas–Particulate Mixtures, *ASME Journal of Heat Transfer*, Vol. 124, pp. 30–38, 2002.
5. Węcel, G., Ostrowski, Z., Białecki, R., A novel approach of evaluating absorption line black body distribution function employing proper orthogonal decomposition, *Journal for Quantitative Spectroscopy and Radiative Transfer*, 111:2 (2010) pp 309-317