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Transformation of the data base to calculate the relation characteristics of steam

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Abstract—Initial spectral data in the form of files for two parameters of the spectrum narrow band model are transformed into integral intermediate values. An example of the transformation is given for emissivity in the entire spectrum. Calculations are simplified without a considerable loss in accuracy.

THE BASE data for calculating the radiation and absorption of energy for steam are represented by the files of two parameters based on the spectrum narrow band model [1]. It is expedient to transform them into intermediate values, which would be integral over parts of the spectrum or over the entire spectrum, and to approximate at least a part of the quantities by formulae in elementary functions. This shortens the calculations without a significant loss of accuracy. Of independent importance are also intermediate quantities. In what follows, an example is given for steam emissivity in the entire spectrum. As a matter of fact, this paper repeats a previous paper [2] of one of the present authors, but on a new basis which was in the stage of development at that time. The initial data are borrowed from ref. [3].

The emissivity is expanded in a series with respect to the absorption coefficients

$$\varepsilon = \alpha_1 x - \alpha_1\alpha_2 x^2/m_2 + \cdots (-1)^{i+1}(x^i/m_i)\prod_{k=1}^{i}\alpha_k,$$

$$i \to \infty. \tag{1}$$

This series is well known in the approximations of small optical thickness. However, the thickness limit can be substantially increased by extrapolating the sum of the series rejected remainder on the basis of an appropriate function [2]. It was proved earlier [4] that at $m_i = i!$ the sequence $\alpha_1, \alpha_2, \ldots$ grows up to a certain limit. Therefore, the converging higher coefficients can be averaged. With the use of $\bar{\alpha}$ for $i > 1$ at $m_i = i$ equation (1) yields

$$\varepsilon = \frac{\alpha_1}{\bar{\alpha}}(\bar{\alpha}x - \bar{\alpha}^2x^2/2 + \bar{\alpha}^3x^3/3 - \cdots).$$

The series is curtailed exactly

$$\varepsilon = \frac{\alpha_1}{\bar{\alpha}}\ln(1+\bar{\alpha}x). \tag{2}$$

The coefficient $\bar{\alpha}$ is the matching parameter with the limit $\bar{\alpha}|_{x=0} = \alpha_2$. In ref. [2] other extrapolation formulae were tried. In particular, at $m_i = i!i$

$$\varepsilon = \frac{\alpha_1}{\bar{\alpha}_*}[\ln(\gamma v) + E_1(v)], \quad v \equiv \bar{\alpha}_* x.$$

According to equation (1), $\bar{\alpha}_*|_{x=0} = 2\alpha_2$. Taking into account the approximation [5]

$$E_1(v) = \ln\left(1 + \frac{\gamma v + 3.5}{v+3.5}\mathrm{e}^{-v}/\gamma v\right)$$

results in

$$\varepsilon = \frac{\alpha_1}{\bar{\alpha}_*}\ln\left(\gamma v + \frac{\gamma v + 3.5}{v+3.5}\mathrm{e}^{-v}\right) \tag{3}$$

i.e. the same function (2) but with a complicated argument which has turned to be less successful than in the previous work [2]. It can be assumed that other versions of the argument will give better results, for the present the consideration will be confined to function (2).

The integral coefficients are expressed in terms of spectral quantities by

$$\prod_{k=1}^{i}\alpha_k = \frac{m_i}{i!}\frac{\pi}{\sigma T^4}\int_0^\infty I_{0\omega}\alpha_\omega^i\,\mathrm{d}\omega$$

where α_ω's are unknown. Below, the second definition—in terms of the emissivity—is realized.

According to equation (1)

$$\prod_{k=1}^{i}\alpha_k = (-1)^{i+1}(m_i/i!)(\partial^i\varepsilon/\partial x^i)_{x=0}.$$

Substitution of the function $\varepsilon\,(x, T, P_*)$ according to ref. [3] yields

$$\prod_{k=1}^{i}\alpha_k = (-1)^{i+1}\frac{m_i}{i!}\frac{\pi\Delta\omega}{\sigma T^4}\sum_{j=1}^{439}I_{0j}(T)(\partial^i\varepsilon_j/\partial x^i)_{x=0} \tag{4}$$

where

$$\varepsilon_j = 1 - \exp(-k_jx/\sqrt{(1+k_jx/a_j)})$$

$$k_j = k_{0j}273/T$$

$$a_j = 4b_0P_*\sqrt{(273/T)}/d_j$$

NOMENCLATURE

a	$4b/d$
b	halfwidth of lines, $b_0 P_* \sqrt{(273/T)}$ [cm^{-1}]
d	mean distance between lines [cm^{-1}]
E_1	$\int_1^\infty t^{-1} \exp(-vt)\, dt$
I	Planck function [cm W m^{-2} sr^{-1}]
k	first parameter of narrow band model [(cm atm)$^{-1}$]
P_*	effective pressure [atm]
t	temperature [°C]
T	temperature [K]
x	optical thickness based on steam partial pressure, $\int p\, dl$ [cm atm].

Greek symbols

α_1	mean Planckian coefficient of absorption [(cm atm)$^{-1}$]
α_2	spectrum-averaged directed coefficient of gas absorption on interaction of two optically thin neighbouring gas volumes [(cm atm)$^{-1}$]
α_i	as above but with energy re-radiation taken into account, $i > 2$ [(cm atm)$^{-1}$]
γ	Euler constant, 1.781
ε	emissivity over the entire spectrum
ε_j	emissivity in the jth range of the spectrum
ω	wave number [cm^{-1}].

Subscripts

i	number of series term
j	number of spectrum range
k	number of the term in the product of i, j, ω
0	normal conditions
ω	spectral quantity.

Superscript

$\bar{}$	averaging.

$$\pi I_{0j} = \frac{37.412(\omega_j/1000)^3}{\exp(1.4388\omega_j/T)-1}$$

and k_{0j} and $1/d_j$ are the tabulated parameters. Let the first five derivatives be written as

$$(\partial\varepsilon_j/\partial x)_{x=0} = k_j$$

$$-(\partial^2\varepsilon_j/\partial x^2) = k_j^2(1+1/a_j)$$

$$(\partial^3\varepsilon_j/\partial x^3)_{x=0} = k_j^3[1+3/a_j+9/(4a_j^2)]$$

$$-(\partial^4\varepsilon_j/\partial x^4)_{x=0} = k_j^4[1+6/a_j+12/a_j^2+15/(2a_j^3)]$$

$$(\partial^5\varepsilon_j/\partial x^5)_{x=0} = k_j^5[1+10/a_j+24/a_j^2 + 60/a_j^3+525/(16a_j^4)].$$

Calculations by equation (4) showed a monotonous increase of the sequence $\alpha_1, \alpha_2, \ldots$ at $m_i = i!$ in accordance with the theorem of ref. [4].

Separation of the effective pressure $a_j \sim P_*$ leads from equation (4) to the polynomial

$$\prod_{k=1}^{i} \alpha_k = C_0 + C_1/P_* + \cdots C_{i-1}/P_*^{i-1} \tag{5}$$

where coefficients C_i depend only on temperature.

In constrast to α_i, the averaged coefficients $\bar{\alpha}$ in equation (2) or (3) depend on all three arguments, including the pressure raised to a fractional power.

The parameters k_{0j} and $1/d_j$ are tabulated at seven temperatures: 300, 600, 1000, 1500, 2000, 2500 and 3000 K which are called nodal. The same name will be given to all the quantities at these points. This separates the problem of the interpolation of quantities for concrete values of temperature for any portion of the spectrum or for the entire spectrum. In Table 1 are entered the examples of the nodal values

Table 1. Integral coefficients of absorption α_i (cm atm)$^{-1}$ at $m_i = i!$ (upper) and $m_i = i$ (lower values)

	i				
θ	1	2	3	4	5
0.6	0.1407	10.721	37.94 18.97	65.66 21.89	90.83 22.71
1	0.05631	2.245	8.526 4.263	16.22 5.41	22.99 5.75
1.5	0.02383	0.5670	2.240 1.120	4.376 1.459	6.031 1.508
2	0.01196	0.1938	0.7705 0.3852	1.449 0.383	1.804 0.451
2.5	0.006863	0.08719	0.2970 0.1485	0.4984 0.1661	0.5628 0.1407
3	0.004154	0.05323	0.1562 0.0781	0.2261 0.0754	0.2570 0.0643

of the coefficients α_1 at $P_* = 1$ atm. They differ greatly from those published in ref. [2] because of the change of the base data. At $m_i = i$ the sequence of α_i rapidly aligns, thus explaining the success of the series curtailment according to equation (2). The coefficient $\bar{\alpha}'$ is obtained by iteration and approximated by a set of equations with constants dependent only on temperature

$$\bar{\alpha}' = \alpha_2'(1+gx)^{-a_0}$$

$$g = 378\exp(-2.76\theta), \quad a_0 = a_1 - a_2 x/1000$$

$$\theta = T/1000,$$

$$x \text{ cm atm}; \bar{\alpha}' = \bar{\alpha}|_{P_*=1},$$

$$\alpha_2' = \alpha_2|_{P_*=1}. \qquad (6)$$

Table 2 lists the constants which are needed to calculate the emissivity at $P_* = 1$ atm with the argument step of 50 K. Along with equations (2) and (6), this table represents a transformed file of data. The coefficients α_1 and α_2 are obtained by interpolating the initial data with the aid of cubic splines within each interval of wave numbers with subsequent summing over the spectrum ranges. The coefficients a_1 and a_2 at the nodal points are obtained by matching, while for the rest of the points a parabola was calculated from the three nearest nodal values of the coefficients.

Table 3 shows the error of the new data base at the most internodal remote points. The emissivity, calculated from the initial file of data with their interpolation within each interval of $\Delta\omega_j$, is compared with that calculated from the new data base. The error is typical of the vast field obtained at all the temperatures with a step of 50 K and at 26 values of the optical thickness from 0.1 to 1000 cm atm. The error of the new base incorporates interpolation deviations; as a rule, it is smaller at nodal points. The fields of the error smaller than 1, 4 and 10% are shown in Fig. 1. It is seen that the method, developed as an approximation of small optical thicknesses, can be used up to 1000 cm atm.

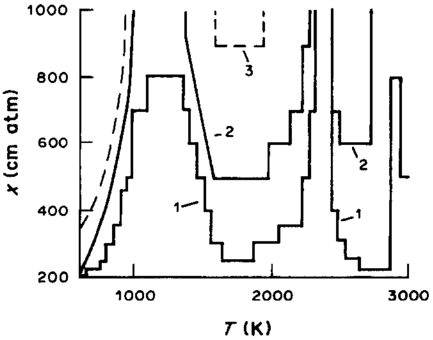

FIG. 1. The error of the transformed file of data at $P_* = 1$ atm when calculated by equations (2) and (5). The lines bound the error field: 1, <1%; 2, <4%; 3, <10%.

Table 2. Coefficients of the transformed data base, $P_* = 1$ atm

T (K)	α_1 (m atm)$^{-1}$	α_2 (m atm)$^{-1}$	a_1	a_2
600	14.07	1072.1	0.1880	0.0990
650	12.42	861.9	0.1825	0.0860
700	11.02	700.0	0.1773	0.0740
750	9.801	573.0	0.1724	0.0631
800	8.730	471.4	0.1678	0.0533
850	7.787	382.3	0.1646	0.0446
900	6.960	322.6	0.1598	0.0370
950	6.243	268.4	0.1562	0.0304
1000	5.631	224.5	0.1530	0.0250
1050	5.112	182.4	0.1506	0.0251
1100	4.664	161.2	0.1484	0.0254
1150	4.270	138.4	0.1465	0.0257
1200	3.917	119.8	0.1448	0.0260
1250	3.597	104.5	0.1432	0.0265
1300	3.306	91.71	0.1420	0.0270
1350	3.041	80.92	0.1409	0.0277
1400	2.800	71.69	0.1400	0.0284
1450	2.581	63.69	0.1394	0.0291
1500	2.383	56.70	0.1390	0.0300
1550	2.204	50.54	0.1397	0.0330
1600	2.043	45.11	0.1404	0.0357
1650	1.897	40.31	0.1412	0.0380
1700	1.764	36.08	0.1420	0.0399
1750	1.645	32.35	0.1427	0.0414
1800	1.537	29.02	0.1436	0.0425
1850	1.439	26.15	0.1444	0.0432
1900	1.350	23.60	0.1452	0.0435
1950	1.270	21.35	0.1461	0.0434
2000	1.196	19.38	0.1470	0.0430
2050	1.128	17.65	0.1479	0.0421
2100	1.066	16.12	0.1488	0.0409
2150	1.007	14.78	0.1498	0.0393
2200	0.9529	13.58	0.1508	0.0373
2250	0.9015	12.53	0.1517	0.0349
2300	0.8531	11.59	0.1528	0.0321
2350	0.8074	10.75	0.1538	0.0289
2400	0.7645	9.997	0.1548	0.0253
2450	0.7242	9.323	0.1559	0.0213
2500	0.6863	8.719	0.1570	0.0170
2550	0.6508	8.176	0.1606	0.0194
2600	0.6174	7.689	0.1646	0.0227
2650	0.5860	7.253	0.1692	0.0269
2700	0.5565	6.863	0.1742	0.0321
2750	0.5288	6.515	0.1796	0.0381
2800	0.5028	6.207	0.1856	0.0451
2850	0.4784	5.935	0.1920	0.0529
2900	0.4557	5.698	0.1988	0.0617
2950	0.4346	5.494	0.2062	0.0714
3000	0.4154	5.327	0.2140	0.0820

Table 3. Emissivity errors at the internodal points at $P_* = 1$ atm, $(\varepsilon - \varepsilon_{\text{apr}})100/\varepsilon$ (%)

x (cm atm)	T (K) 800	1250	1750	2250	2750
10	−0.9	−1.0	−0.1	−0.3	−0.3
100	−1.2	−0.9	0.5	−0.1	−0.7
200	−1.1	−1.9	0.6	0.1	−1.3
500	4.9	−2.1	3.4	1.1	−3.5
700	10.9	−0.7	6.5	2.1	−4.7
1000	26.3	2.6	11.8	4.4	−5.5

The pressure effect manifests itself only via the broadening of lines. Calculations from the initial data of ref. [3] readily reproduce the family of curves $c(P_*, x, t)$ from ref. [1] where $c = \varepsilon(P_*)/\varepsilon(P_* = 1)$. An attempt to transform the base has not been satisfactory yet.

Equation (5) easily takes into account pressure but only for coefficients α_1. Moreover, coefficients C_i are strongly dependent on temperature. According to Table 1, $C_0 = \alpha_1$, $C_0 + C_1 = \alpha_1 \cdot \alpha'_2, \ldots$, etc. An attempt to generally describe emissivity by the same equation (2) yields the following relations:

$$\bar{\alpha} = \alpha'_2 \frac{1+fP_*}{(1+f)P_*}(1+g_* x)^{-a_*}$$

$$f = 0.36\sqrt{(0.273/\theta)}\exp(1.984\theta - 2.012)$$

$$g_* = \exp[n + m(P_*^{k_*} - 1)]$$

$$k_* = 0.645(1.3 + 2.6\theta - \theta^2)$$

$$a_* = a_{*1}P_*^r + a_{*2}(1 - P_*^r),$$

$$x \,\text{cm atm}, \quad \exp n \,(\text{cm atm})^{-1}. \tag{7}$$

The files of the values for α_1 and α'_2 are given in Table 2. The nodal values of n, m, a_{*1}, a_{*2} and r are listed in Table 4. It is seen that analytical properties of the coefficients especially of a_{*2} and r, are disturbed. Starting from 2500 K, the function $f(T)$ grows very rapidly, the pressure effect decreases quickly in all the terms of equation (7). When $P_* \to 1$, equation (7) should go into equation (6). Actually, this takes place with an additional error, since $a_1 \neq a_{*1}$ and $\exp n \neq g$. An example of the errors at $P_* = 5$ atm is given in Table 5. This is typical of other pressures.

In conclusion, interpolation of the files of numbers depending on temperature will be considered. The preliminary logarithmic operation with numbers is obligatory, because the differences between them are leveled out and the effect of small numbers grows. Interpolation by the Lagrange equation to all the nodes turned out to be unreliable. It is seen on the example of the mean Planck coefficient of absorption.

Table 4. Error of interpolation of the mean Planck coefficient of absorption $100(\alpha_{12} - \alpha_{1i})/\alpha_{12}$, where i is the order of the derivative $\partial^i \ln k_{0j}/\partial T^i$ prescribed at the ends of the interpolation segment. The value at $i = 2$ is taken to be standard. The last column lists the errors of the values according to Lagrange as compared with the standard values

	Splines		
T (K)	$i = 1$	$i = 3$	Lagrange
373	0.08	−0.1	−2.1
473	0.10	−0.1	−2.7
873	−0.06	0.09	2.1
1273	0.02	−0.03	−0.06
1873	−0.003	0.004	−0.06
2273	0.01	−0.02	−3.4
2773	−0.04	0.06	0.9
2873	−0.05	0.06	1.3

Table 5. Emissivities of steam at $P_* = 1$ atm with infinite dilution by nitrogen. The lines from above: 1, according to Leckner; 2, from the data base of ref. [4] with interpolation according to Lagrange; 3, from the data base of ref. [4] with interpolation by cubic splines at $i = 2$; 4, by the nomogram of ref. [1]. The digits after the point are given

x (cm atm)	T (K) 873	1273	1873	2273
1	0399	0255	0126	0083
	0394	0257	0126	0086
	0399	0256	0127	0083
	0390	0260	0125	0082
2	0623	0432	0235	0158
	0611	0438	0235	0165
	0616	0438	0235	0159
	0620	0440	0230	0155
10	147	119	0836	0621
	142	122	0832	0650
	142	122	0836	0628
	143	120	0850	0630
20	200	170	131	103
	192	174	131	108
	192	175	132	105
	200	175	130	103
100	357	330	302	268
	343	338	303	286
	342	339	304	274
	355	345	310	275
200	435	413	397	368
	418	421	400	400
	416	422	402	380
	420	430	410	380

In Fig. 2 the right-hand scale denotes the index δ of the remainder term of the approximate formula

$$\ln \alpha_1 = 2 - 1.075(t/1000) + \exp \delta.$$

The scale increases the deviation of numbers.

The interpolation according to Lagrange led to oscillations of values that increased with temperature. For interpolation of the initial data use was made of

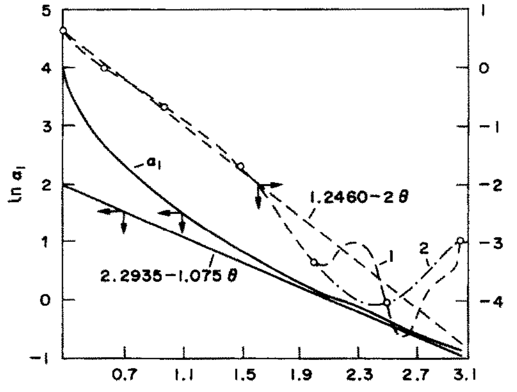

FIG. 2. The plot of the mean Planck coefficient of absorption, α_1 (m atm)$^{-1}$, $\theta_* = t/1000$; 1, interpolation of initial data by the Lagrange equation; 2, by cubic splines.

the cubic splines with boundary conditions of the second kind, i.e. with prescribed values of the second derivative at the ends of the interpolation segment [6]. For the tabulated function, the second derivative was approximated by separated differences of the second order. The oscillations of the values of α_1 were eliminated. The growth of α_1 near 3000 K is probably connected with the excitation of 'hot' bands.

According to Fig. 2, $\delta = 0.7-2\theta_*$, $\theta_* = t/1000$. This yields

$$\ln \alpha_1 = 2-1.075\theta_*+\exp(0.7-2\theta_*). \qquad (8)$$

The discrepancy between the calculations made by equation (8) within the range from 300 to 3000 K changes the sign four times. Therefore, refinement of this equation will lead to its substantial complication after which this equation will be unable to substitute the column in Table 2. At 3000 K a maximum relative deviation (underestimation) is equal to 4.35%. Nevertheless, equation (8) can be used in simple calculations. Its merit lies in the fact that, though extrapolation to high temperatures is not reliable, the limit $\theta_* \to \infty$ does not disagree with the physical sense of α_1.

The method offers promise when applied to the spectrum intervals which are narrow enough to take into account the superposition of the bands of other gases, the entire spectrum of bodies, to take the Planck function outside the sum which determines integral absorption. It is desirable to include in the intervals strong bands entirely or their halves.

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TRANSFORMATION DE LA BASE DE DONNEES POUR CALCULER LES CARACTERISTIQUES RADIATIVES DE LA VAPEUR D'EAU

Résumé—Les données expérimentales spectrales initiales sous forme de fichiers pour deux paramètres du modèle spectral à bande étroite sont transformées en valeurs intermédiaires intégrales. Un exemple de la transformation est donné par l'émissivité dans le spectre complet. Des calculs sont simplifiés sans une perte considérable de précision.

TRANSFORMATION DES DATENBESTANDES ZUR BERECHNUNG VON EIGENSCHAFTEN DES WASSERDAMPFS

Zusammenfassung—Anfängliche Spektraldaten in Form von Files für zwei Parameter des spektralen Schmalband-Modells werden in integral dazwischenliegende Werte überführt. Es wird ein Beispiel für die Umformung der Emissionsfähigkeit im Gesamtspektrum angegeben. Die Berechnungen werden ohne merklichen Genauigkeitsverlust vereinfacht.

ПРЕОБРАЗОВАНИЕ БАЗЫ ДАННЫХ ДЛЯ РАСЧЕТА РАДИАЦИОННЫАХ ХАРАКТЕРИСТИК ВОДЯНОГО ПАРА

Аннотация—Первичные спектральные данные в виде массивов двух параметров модели узкой полосы спектра преобразуются в интегральные промежуточные величины. Пример преобразования дан для степени черноты в полном спектре. Достигнуто упрощение расчетов без существенной потери точности.