TAKING INTO ACCOUNT THE SPECTRA OF BODIES IN THERMAL
CALCULATIONS OF FURNACES

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For the example of water vapor, the application of a new method of calculating
radiant heat transfer, taking account of the line and continuous spectra of
bodies with multiple reflection and scattering of the energy fluxes, is shown.

Taking account of the spectra of bodies significantly increases the reliability of prac-
tical calculations of radiant heat transfer. Solutions for furnaces and occasionally for
kilns are found by the Hottel zonal method if the surface and suspended phase are gray. Heat
transfer with the lining and other heated surfaces may be distored here. In [1], the spectra
of the gas and the surfaces were taken into account by the multiple-reflection method, but
only for two surfaces. For the case of three surfaces, the calculations are extremely com-
plicated. Furnaces are sometimes divided into 180-240 zones. The number of different paths
of the fluxes in multiple reflection and scattering increases to billions or more before the
fluxes may be neglected. Systematic calculation of all the paths is possible but has yet to
be realized.

In fundamental theory, the spectral problem is formally solved on transition to mono-
chormatic radiation. The spectral absorption coefficients — Bouguer coefficients — depend
only on the local parameters of state of the medium. For the combustion products, hundreds
of thousands of lines must be calculated and their monochromatic contributions summed. So
far, calculations have been shown to be practical only for carbon monoxide [2]. The reli-
ability for triatomic gases is inadequate [3]. In numerical integration of the fluxes over
the spectrum, the interval must be no greater than 0.005 cm^{-1}. However, the system of heat-
transfer equations must be solved in each interval, and the volume of calculations is enormous.

The calculation is simplified when using models of the narrow spectral band. The width
of the integration interval is increased by more than three orders of magnitude — to 5-25
cm^{-1}. The volume of calculations is correspondingly reduced. However, other difficulties
arise. If the concept of absorption coefficients is introduced, the Bouguer properties are
lost. According to the Hood model, the coefficient takes the form (m^{-1})

$$(s/d)\, p/\sqrt{1 + (s/d)\, p l_\Sigma/(4b/d)},$$

where l_Σ is the sum of broken beam paths from emission to absorption through multiple re-
flection and scattering at elements of the system of bodies with respect to the real indices.
The complexity of taking account of the set of such elements was shown in [1] and earlier
works.

In 1954, Hottel represented the gas spectrum as a weighted sum of gray components. The
gray absorption coefficients take on Bouguer properties. They do not depend on the prior
form of the broken beam path. This is noted here, since the quality of the Hottel coefficients
is retained in the present method; its complication is justified to the extent that this is
possible. In practical calculations, the Hottel method has been the basic approach for a
long time, but it has the following deficiencies: 1) the rectangles of the transformed spec-
trum consist of elements with different coordinates at the axis of the spectrum and therefore
lose their overall relation to it; it is impossible to take correct account of the spectra of
the surfaces and the suspended phases; 2) the method includes the Hottel–Nevskii–Ivantsov
approximation, which sometimes gives a large error [4]; 3) the absorptive power of the gas is
found very approximately, with additional error. Only the first of these deficiencies cannot
be overcome within the framework of the method, and it is removed in the method of [5], in

TABLE 1. Fixing the Boundaries of the Bands of the Water-Vapor Spectrum at L = 8; in the Band [11,000; ∞], Absorption Is Negligibly Small

Bond number, l	1	2	3	4
Boundary, cm^{-1}	50—1150	1150—1600	1600—2600	2600—4600
Bond number, l	5	6	7	8
Boundary, cm^{-1}	4600—6000	6000—8000	8000—9300	9300—11000

which the spectrum is divided into nine intervals with averaging of the optical constants in each. However, within these very broad intervals, the spectra of the bodies are represented as gray, which is inapplicable for gases.

Attempts to resolve the contradictions of the Hottel method were made in [6]. The new approach, originally called the Hottel method within a narrow spectral interval, will be called the method of a sum of rectangles in the spectral interval (SRSI) here. The interval is regarded as arbitrary. In the limit of a small interval, the absorption coefficients over all the rectangles are equalized and become monochromatic. The "pure gas" disappears. In the limit of a large interval covering the whole spectrum, the method transforms to the Hottel method, with all its attendant deficiencies. In [6], the SRSI method was tested for the example of the Elsasser model; the error was found to be acceptable for the conditions of thermal-engineering problems. However, in view of the narrowness of the intervals, the volume of calculations is too large. In addition, other models of the spectral bands must be preferred.

In the present work, after an interval of more than ten years, the SRSI method is again considered, for the example of water vapor.

A new spectral data base for steam is used here [7]. The active part of the spectrum, up to 11,000 cm^{-1}, is divided into eight intervals, as shown in Table 1. With four rectangles, including the zero rectangle for pure gas within each interval, the system of heat-transfer equations must be solved 33 times, which is not beyond the capacity of computers. The emissivity is summed over L = 8 intervals

$$\varepsilon = \sum_{l=1}^{L} g_l \varepsilon_l, \quad g_l = \frac{\pi \Delta \omega}{\sigma T^4} \sum_{j=1}^{N_l} I_{0j}(T),$$

$$\varepsilon_l = \sum_{j=1}^{N_l} I_{0j}(T) \varepsilon_j(T; x) \Big/ \sum_{j=1}^{N_l} I_{0j}(T),$$

$$\varepsilon_j = 1 - \exp\left[-\frac{(s/d)x}{\sqrt{1 + (s/d)x/(4b/d)}} \right].$$

The emissivity in the l-th interval ε_l on the basis of the spectral data base is taken as the accurate value. The approximate value according to the SRSI method is

$$\tilde{\varepsilon}_l = \sum_{m=1}^{M} c_{lm} [1 - \exp(-K_{lm}x)], \quad c_{lm} = \sum_{\lambda=1}^{\lambda_0} b_{lm\lambda} T^{\lambda-1}. \tag{1}$$

The choice of K_{lm} and $b_{lm\lambda}$ is based on minimization of the difference between ε_l and $\tilde{\varepsilon}_l$. The minimum of the target function with linear constraints is found by the Davidson—Fletcher—Powell method [8]

$$\varphi = \sum_{z=1}^{Z} \sum_{v=1}^{V} (1 - \tilde{\varepsilon}_{vz}/\varepsilon_{vz})^2, \quad 0 \leqslant \sum_{\lambda=1}^{\lambda_0} b_\lambda T^{\lambda-1} \leqslant 1, \quad K_{lm} > 0,$$

TABLE 2. Mean Square Error of $\tilde{a}_\ell$, %, Calculated from Eq. (4) with SRSI Parameters M = 3, λ_0 = 4 (Normal Total Pressure; Vapor Infinitely Diluted with Nitrogen)

$\bar{x}$, cm·atm	Bond number l							Total spectrum	
	1	2	3	4	5	6	7	as a single band	with respect to sum for L = 8
3	4,15	2,01	3,05	1,90	1,93	3,55	3,44	22,07	1,75
30	3,87	1,99	3,63	1,55	1,91	2,65	3,44	11,95	1,54
50	4,15	1,99	2,55	1,53	1,90	2,48	3,44	11,10	1,51
100	4,64	1,98	2,60	1,60	1,89	2,35	3,44	12,00	1,49
300	5,42	1,99	3,38	1,94	1,89	2,56	3,43	16,68	1,54

where v and z are the temperature and optical-thickness indices; V and Z are their total numbers in the set of arguments. The values of ε_{vz} and $\tilde{\varepsilon}_{vz}$ are calculated for optical thicknesses of 0.1, 0.3, 0.5, 1, 3, 5, 10, 30, 50, 100, 300, 500, 1000 cm·atm and temperatures of 600, 800, 1000, 1200, 1400, 1600, 1800, 2000, 2200, 2400, 2600, 2800, and 3000 K. The constraints on this set of values of ε_{vz} and $\tilde{\varepsilon}_{vz}$ correspond to the result of [8], where insignificant increase in accuracy of the calculations was found with expansion of the smaple, involving considerable increase in machine time. Interpolation of the parameters of the narrow-band model with respect to the temperature is by the cubic-spline method with the calculation of the second derivative at the boundaries of the interpolational interval by the finite-difference formula using a four-point template, except for the bands from 9300 to 11,000 cm^{-1}, for which a three-point template is used.

The search for a local minimum of the target function with respect to the specified direction is by the quadratic-approximation method [9]. In the SRSE method, tables of coefficients $K_{\ell m}$ and $b_{\ell m \lambda}$ are obtained for each spectral interval ℓ; there is multiple increase in the mass of these coefficients. Their direct use is recommended in the Hottel method, but this is almost meaningless in the present case. The calculation is based on the spectral data base. Accordingly, the tables of coefficients are omitted.

For heat-transfer calculations, a formula more general than Eq. (1) for the absorptive power of the gas in the case of an incident flux with a black spectrum a_0 is required. In contrast to ε, b_0 depends on three variables — the depth x, surface temperature T_0, and the gas temperature $\bar{T}$ averaged over the depth x — and is not meaningless for an arbitrary temperature field. According to [10], a_0 is used for calculations of the intrinsic radiation of the gas volume at its boundary. In [10, 11], the simplest averaging was used: $\bar{T} = \int_0^1 T\, dv; \; v = x'/x$.

In the present method, the values obtained with respect to the new spectral data base are used as the standard of comparison

$$a_0 = \sum_{l=1}^{L} g_l(T_0)\, a_l(T_0; \; \bar{T}; \; x), \quad a_l = \sum_{j=1}^{N_l} I_{0j}(T_0)\, \varepsilon_j(\bar{T}; \; x) \Big/ \sum_{j=1}^{N_l} I_{0j}(T_0).$$

The approximate values according to the SRSI method are

$$\tilde{a}_0 = \sum_{l=1}^{L} g_l(T_0)\, \tilde{a}_l, \quad \tilde{a}_l = \sum_{m=1}^{M} c_{lm}^0(T_0; \; \bar{T})[1 - \exp(-K_{lm}x)]. \tag{2}$$

The absorption coefficients $K_{\ell m}$ are taken as in Eq. (1) for the emissivity. Then, when $a_0 = \tilde{a}_0$, the weights $c_{\ell m}^0(T_0; \; \bar{T})$ are unknown. The previous dependence $c_{lm} = \sum_{\lambda=1}^{\lambda_0} b_{lm\lambda} \bar{T}^{\lambda-1}$ may be extended, adding the new polynomials $b_{\ell m \lambda}(T_0)$ and finding the coefficients of the double polynomial. However, a more accurate but also more complex method using the spectral data base is preferable.

The following approximate expression is obtained from the identity $a_l = (a_l/\varepsilon_l)\varepsilon_l$:

$$\tilde{a}_l = \delta_l \tilde{\varepsilon}_l, \quad \delta_l = a_l(T_0;\ \bar{T})/\varepsilon_l(\bar{T}),$$

where $\tilde{\varepsilon}_l$ were defined in Eq. (1), and δ_l are calculated "accurately"

$$\delta_l = \frac{\sum\limits_{j=1}^{N_l} I_{0j}(\bar{T}) \left[\sum\limits_{j=1}^{N_l} I_{0j}(T_0)\varepsilon_j(\bar{T};\ \overline{x}) \right]}{\sum\limits_{j=1}^{N_l} I_{0j}(T_0) \left[\sum\limits_{j=1}^{N_l} I_{0j}(\bar{T})\varepsilon_j(\bar{T};\ \overline{x}) \right]} . \tag{3}$$

In the program bundle employed, the spectral data base from [7], interpolation of these data with respect to the temperature on the basis of spline functions [12], and calculations of the coefficients K_{lm} and $b_{lm\lambda}$ in Eq. (1) may be noted. The calculation of δ_l from Eq. (3) requires a special program; the first two are adequate.

In Eq. (3), $\overline{x}$ is some mean in the interval of x chosen on formulating the problem in the SRSI method. The averaging is necessary to eliminate the dependence of the weights c_{lm}^0 on x.

Table 2 gives the mean square error of $\tilde{a}_l$ for the first seven spectral intervals in Table 1

$$\sigma_l^2 = \sum_{x;\overline{T};T_0} (1 - \tilde{a}_l/a_l)^2/(N_x N_{\overline{T}} N_{T_0}). \tag{4}$$

The value of σ is expressed in percent. Here N_i is the number of discrete values of the arguments for which a_l and $\tilde{a}_l$ are calculated in the complete set of versions: x = 3, 10, 30, 100, 300 cm·atm; $\overline{T}$ = 1000, 1500, 2000, 2500, and T_0 = 1000, 1500, 2000, 2500 K. Thus, $N_x = 5$, $N_{\overline{T}} = N_{T_0} = 4$. In the penultimate column, the whole spectrum is considered as a single band; the corresponding error is large. In the last column, the result for the whole spectrum is summed over particular values of $\tilde{a}_l$. The error is less than for any particular interval, on account of partial compensation. The choice of $\overline{x} = 50$ cm·atm for Eq. (3) is confirmed by Table 2, which is the principal evaluation of the SRSI method in recommending its practical use.

Repetition of the investigation with increase in the parameters — M: 3 → 5; λ_0: 4 → 6 — does not yield significant reduction in the error, which is already very low and cannot be reduced to zero at such M and λ_0.

The system of heat-transfer equations is given as an illustration of the SRSI method, since it may be written in specific form. In [11], the heat-transfer problem in a plane layer with gray bodies was solved. The system of equations in [11] is taken as the starting point here. Its conversion for the SRSI method is simple.

The integral for the flux density of any form $q = \int_0^\infty q_\omega d\omega$ is approximated by the sum

$$q = \sum_{l=1}^{L} \sum_{m=1}^{M+1} q_{lm}.$$

The subscript lm is omitted below, but the discussion is only for q_{lm}. The density of the resulting flux for the m-th gray gas in the l-th spectral interval is equal to the difference of the forward and backward values

$$q_{\mathbf{r}} \equiv q = q_+ - q_-,$$

where at a depth τ_k

$$q_+(\tau_k) = q_{\mathrm{g1}} w_3(\tau_k) + \int_0^{\tau_k} B(\tau) w_2(\tau_k - \tau)\, d\tau,$$

TABLE 3. Error of the Mean Planck Absorption Coefficient $\Delta = \alpha_c - \tilde{\alpha}_c$, $(cm \cdot atm)^{-1}$, According to Eq. (5) for Water Vapor at Normal Pressure in a Mixture with Nitrogen at Infinite Dilution (Coefficients $c_{\ell m}$ and $K_{\ell m}$ Chosen on Segments x = 0.1-300 cm·atm; T = 1000-2600 K, for L = 8 (see Table 1); M, λ_0, Numbers of Gray Gases and Terms in Polynomial)

T, K	$\alpha_{c\ell}$ cm·atm^{-1}	When M is				
		3	3	4	5	5
		when λ_0 is				
		4	5	5	5	6
1073	4,866	0,443	0,397	0,240	0,187	0,184
1573	2,132	—0,069	—0,024	—0,033	—0,030	—0,029
2073	1,097	0,003	—0,008	—0,003	0	0,001
2573	0,636	—0,009	0	0,004	0,003	0,003

$$q_-(\tau_k) = q_{e2}w_3(\tau_0 - \tau_k) + \int_{\tau_k}^{\tau_0} B(\tau)w_2(\tau - \tau_k)\,d\tau,$$

$\tau = (pK + \alpha_V + \beta_V)\ell$ is the optical thickness with respect to the total attenuation coefficient; $K \equiv K_{\ell m}$; $w_n = 2E_n$; E_n is an integral exponential.

The effective flux densities q_{e1} and q_{e2} at the surfaces bounding the layer and the source function $B(\tau)$ are determined from three integral equations

$$q_{e1} = \frac{b_1 + b_2 d_1}{1 - d_1 d_2}, \quad q_{e2} = \frac{b_2 + b_1 d_1}{1 - d_1 d_2},$$

where

$$b_1 = (1 - R_1)\,g_1 c_1^0\,\theta_1^4 + R_1 \int_0^{\tau_0} B(\tau)w_2(\tau)\,d\tau,$$

$$b_2 = (1 - R_2)\,g_2 c_2^0\,\theta_2^4 + R_2 \int_0^{\tau_0} B(\tau)w_2(\tau_0 - \tau)\,d\tau,$$

and

$$B(\tau) = (1 - \Omega)\,g(\tau)c(\tau)\,\theta^4 + \Omega\theta_*^4; \quad g_i = \frac{\pi\Delta\omega}{\sigma T_i^4}\sum_{j=1}^{N_i} I_{0j}(T_i);$$

$$d_1 = R_1 w_3(\tau_0); \quad d_2 = R_2 w_3(\tau_0); \quad g \equiv g_i; \quad c \equiv c_{lm}; \quad \Omega = \beta_V/(pK + \alpha_V + \beta_V).$$

The dimensionless radiant temperature θ_* is calculated from the integral equation

$$4\theta_*^4 = q_{e1}w_2(\tau) + q_{e2}w_2(\tau_0 - \tau) + \int_0^{\tau_0} B(\tau')w_1|\tau - \tau'|\,d\tau'.$$

This system of integral equations is solved $L(M + 1) + 1$ times. The last time corresponds to the tail interval [11,000; ∞], cm^{-1}, beyond the limits of the active spectrum of water vapor. On taking account of the scattering anisotropy, the number of integral equations coupled in a single system rises [13], to an extent that increases with the complexity of the scattering index. The optical constants of the surfaces and suspended phases are averaged in each of the nine spectral intervals.

In the expressions for $b_i(\tau_0)$, the product $g_\ell c_\ell K_{\ell m}$, which is the intrinsic radiation of an element of volume of the m-th gray gas, is isolated from the factor $B(\tau)d\tau$ in the integrand. On summation over all the rectangles, the radiation coefficient in the total spectrum (the mean Planck absorption coefficient) is obtained. The "accurate" and approximate values take the form

$$\alpha_c = \sum_{l=1}^{L} g_l \alpha_{cl}, \quad \tilde{\alpha}_c = \sum_{l=1}^{L} g_l \tilde{\alpha}_{cl}, \tag{5}$$

where

$$\alpha_{cl} = \sum_{j=1}^{N_l} I_{0j} (s/d)_j \Big/ \sum_{j=1}^{N_l} I_{0j}; \quad \tilde{\alpha}_{cl} = \sum_{m=1}^{M} c_{lm} K_{lm}.$$

It is desirable to verify the products $c_{lm} K_{lm}$ because K_{lm} and $b_{lm\lambda}$ are determined on a finite segment of optical thicknesses $[x_{min}; x_{max}]$, where $x_{min} > 0$, whereas $\tilde{\alpha}_{cl}$ is extrapolated for $x \to 0$. The results in the total spectrum are shown in Table 3. It is evident that, with increase in M and λ_0, the error is reduced, but the economy of the calculations is also reduced with increase in M. Expansion of the segments of x and T is not considered here; it leads, as a rule, to large errors. The error also increases rapidly beyond the limits of the segments of x and T. The same calculations are undertaken in all eight spectral intervals for $\tilde{\alpha}_{cl}$. The relative error of these particular values is often higher than in Table 3, since the summation over the spectral intervals is accompanied by some compensation of the errors.

In future work, the SRSI method will be compared with others in solving heat-transfer problems.

NOTATION

a_0, absorptive power of gas for incident flux with black spectrum at temperature T_0, dimensionless; c_m, weight of gray gas, dimensionless; b, halfwidth of line, cm^{-1}; $b_{m\lambda}$, coefficient of polynomial for c_m; d, mean distance between lines, cm^{-1}; g_l, energetic fraction of l-th spectral interval, dimensionless; p, partial gas pressure, atm; q, heat flux density, W/m^2; s, integral intensity of line, $cm^{-1}/m \cdot atm$; $x = pl$, optical depth, $m \cdot atm$; B, source function, dimensionless; E_n, integral exponential; I_{0j}, Planck function in j-th spectral interval, $cm \cdot W/m^2 \cdot sr$; K_m, absorption coefficient of m-th gray gas, $(m \cdot atm)^{-1}$; R, reflective power; T, temperature, K; α_v, absorption coefficient of suspended phase, m^{-1}; β_v, scattering coefficient, m^{-1}; ε, emissivity of gas; τ, optical thickness with respect to attenuation coefficient, dimensionless; ω, wave number, cm^{-1}; Ω, albedo of elementary volume, dimensionless. Subscripts: 0, surface, standard value; j, number of elementary spectral interval; m, gray gas (M, total number of such gases); $\Theta = T/T_0$; $w_n \equiv 2E_n$; $\bar{q} \equiv q/\sigma T_0^4$.

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