ASSESSMENT OF PULVERIZED-COAL-FIRED COMBUSTOR PERFORMANCE

MODELS FOR COAL-COMBUSTOR PERFORMANCE

ANALYTICAL TOOL VERIFICATION

TOPICAL REPORT

W. Richter

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Energy and Environmental Research Corporation
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1.0 INTRODUCTION AND SELECTION OF ANALYTICAL TOOLS

The most important and initially unknown quantities in the performance of industrial furnaces and boiler combustion chambers are the overall heat transfer and the furnace outlet temperature on the one hand, and local heat flux distributions to furnace walls and other heat sinks together with local temperature distribution within the furnace on the other hand.

Due to the high temperature levels in fossil fuel fired combustion chambers (usually $> 1000^{\circ}\text{C}$), the dominant mode of heat transfer to the heat sinks is by thermal radiation. This is especially true when pulverized coal is fired, since here the emissivity of the furnace gas volume might be considerably increased by the presence of solids such as coal, char, ash, and soot particles.

Since the local emission of thermal radiation is limited by local black emissive power and local emissivity, heat which is locally released in flames is not completely radiated away but redistributed within the furnace by convection. Thus, the final temperature distribution which induces the heat fluxes is governed by local heat balances between convective and radiative fluxes and the local heat release.

An analysis of this complex heat transfer process requires some simplification of its physical description by means of "mathematical" models. According to the degree of this simplification, mathematical furnace models can loosely be grouped into

- pure heat transfer models (type I)
- coupled fluid flow, combustion, and heat transfer models (type II).

Pure heat transfer models require a priori description of the flow and heat release pattern in the furnace as input data. They enable flow and heat flux predictions by solving total energy balances for a certain number of volume zones. It is their relative simplicity which makes such models attractive for engineering analysis of furnace performance. Furthermore, the decoupling of the momentum and matter balances allows a more accurate evaluation of the important radiative heat exchange than is possible with type I models. However, a reasonable estimation of flow pattern and heat release zones is often difficult to obtain because of the mutual interaction of various transport and combustion processes.

In the coupled-heat transfer models of type II, the fluid flow and heat release pattern are computed instead of being empirically described. However, some empirical input data is still required, especially for modeling the burnout of gaseous and solid species with simple combustion models. Since the flow in most furnaces is elliptic, i.e. recirculating, expensive iterative methods have to be used in order to solve the finite-difference transport equations.

Considering the shortcomings of both principal approaches, it was decided (1) to select two models of type I and one model of type II as analytical tools for the present investigation.

The selected models of type I are based on a semi-stochastic zone method for evaluating radiative heat exchange in rectangular and cylindrical furnaces, respectively. The selected model of type II is a two-dimensional elliptic-flame model which includes a coal combustion model.

The following documentation contains a description of the three models together with some basic assumptions and sample problems which illustrate their major features and capabilities.

The three models were developed by the author of this report at Stuttgart University (West Germany). The 2D elliptic-flame model is well-documented elsewhere.^(2,3) The cylindrical furnace model was also documented^(4,5); however, no documentation was available of the recently developed rectangular furnace model. For this reason, the description of this model is more comprehensive than that of the other two.

2.0 RECTANGULAR FURNACE MODEL

2.1 Introduction

The rectangular furnace model, as well as the cylindrical furnace model described in section 3, is based on a zone method. The furnace volume is divided into a certain number of rectangular gas zones and into a corresponding number of surface zones. An example of such zonal arrangement is shown in Figure 1. It is assumed that temperatures and other relevant properties are uniformly distributed within each zone. The evaluation of heat transfer between the furnace zones is carried out in two parts.

Part one, which is called "Radiation Model," yields the radiative heat fluxes for actual or guessed temperatures and radiative properties of the furnace zones.

In part two, which will be called "Total Heat Transfer Model," total energy balances are set up for each zone with originally guessed temperatures. In these balances, the radiative heat fluxes obtained with the radiation model are equated to convective heat fluxes in and out of a zone and to the chemical heat release of the zone per-unit time. An improved set of zonal temperatures and temperature-dependent properties is obtained from a solution of the described balances. The new values are used to recalculate the radiative heat fluxes which then are used to obtain the next corrected set of temperatures and temperature-dependent properties, and so on, until a sufficiently converged solution is achieved.

2.2 Radiation Model

In order to model radiative heat transfer in such a complex system as a furnace, two major problems have to be solved; namely, the geometrical problem of radiative exchange and a suitable approximation of wavelength dependence of the radiative properties of combustion products and, eventually, of furnace walls. In the present radiation model, the former problem is separated from the latter by assuming, as a first step, that radiation is gray. The developed algorithm for the exchange of gray radiation is optionally extended in a second step to handle non-gray radiation exchange according to the chosen approximation of real radiative properties of the combustion products.

Figure 1. Example of Zone Arrangement in the Rectangular Heat Transfer Furnace Model.

2.2.1 Semi-stochastic Method of Radiative Exchange

The exchange of radiation between the furnace zones is evaluated with a semi-stochastic method. The emitted radiative energy of each furnace zone is distributed among a certain number of beams. The path of each beam is followed through the volume zones of the furnace taking reflection at surface zones into account. The tracing of a beam is terminated after its initial energy flux is reduced to a certain small reference flux by gas and surface absorption. During one gray radiation exchange calculation each zone is once regarded as emitter. In case of symmetry, the number of emitting zones is reduced by a factor of two for each symmetry plane of the furnace. The energy fluxes absorbed by the various volume and surface zones from all beams crossing or hitting them are accumulated in storages assigned to each zone. At the end of one calculation of radiative exchange, the total flux absorbed by each zone is subtracted from the total flux emitted by the zone in order to obtain the net heat flux from that zone.

This model of radiative exchange has some features of the Monte Carlo Method; however, contrary to the pure version of the latter method, several steps of the radiative transport process are evaluated deterministically as will be shown in more detail in the following sections.

2.2.1.1 Gas Zones as Emitters

The emitted energy $\dot{Q}_{e,I}$ of a finite volume zone V_I with uniform gray absorption coefficient $K_{a,I}$ and uniform temperature T_I is given by:

$$\dot{Q}_{e,I} = 4K_{a,I}\sigma T_I^4 V_I \quad (1)$$

This energy flux is distributed among a finite number n_I of "beams" with discrete starting points within the volume zone V_I . In the pure version of the Monte Carlo Method, the co-ordinates x_0, y_0 and z_0 of the starting point, as well as the direction of the beams specified by a polar angle ϕ^* and an azimuthal angle ψ^* (see Figure 2), are generated by random numbers. In the present model, however, x_0, y_0, z_0 , and the angles of direction are computed deterministically according to the following procedure.

The zone I with the volume V_I is further divided into $\Delta n_{V,I} = V_I/\Delta V_I$ equally-sized sub-elements ΔV_I , called cells, which emit $\Delta \dot{Q}_{e,I}$.

Figure 2. Volume-Cell-Oriented X^*, Y^*, Z^* Co-ordinate Frame and Definition of Beam Angles ϕ^* and ψ^* .

$$\Delta \dot{Q}_{e,I} = 4K_{a,I} \sigma T_I^4 \Delta V_I . \quad (2)$$

The cells are, if possible, cube-shaped and small enough so that they can be assumed to emit radiation almost isotropically over the solid angle 4π . Isotropic emission from the cells is then modeled by taking their geometric center as radiation source, i.e. as starting points of a bundle of "beams" and by spreading these beams as uniformly as possible over 4π . A beam associated with a solid angle of divergence $\Delta\Omega$ carries the initial energy flux

$$\Delta \dot{Q}_{I,o} = \Delta \dot{Q}_{e,I} \frac{\Delta\Omega}{4\pi} = K_{a,I} \frac{\sigma}{\pi} T_I^4 \Delta V_I \Delta\Omega . \quad (3)$$

$\Delta\Omega$ can be expressed in terms of the polar angle ϕ^* and the azimuthal angle ψ^* as $\Delta\Omega = \sin \phi^* \Delta\phi^* \Delta\psi^*$ with $\Delta\phi^*$ centered with respect to ϕ^* and being equal to $\Delta\psi^*$. This produces, however, a non-homogenous distribution of the number of beams over the solid angle 4π and also leads to non-conservation when the energy fluxes of the beams of one cell (eq.3) are added up in order to obtain the total cell emissive power $\Delta \dot{Q}_{e,I}$ (eq.2).

A better formulation for $\Delta\Omega$ is given by equations (4a) ÷ (4c):

$$\Delta\Omega = \left[\cos\left(\phi^* - \frac{\Delta\phi^*}{2}\right) - \cos\left(\phi^* + \frac{\Delta\phi^*}{2}\right) \right] \Delta\psi(\phi^*) , \quad (4a)$$

$$\Delta\phi^* = \frac{\pi}{n_\phi} , \quad (4b)$$

$$\Delta\psi(\phi^*) = \frac{2\pi}{n_\psi} = \frac{\pi}{2 \text{ INT } \left(\frac{\sin \phi^*}{2\Delta\phi^*} + 1 \right)} . \quad + \quad (4c)$$

n_ϕ is a chosen even number for sub-division of the range $0 < \phi^* < \pi$ into increments $\Delta\phi^*$ which are centered on ϕ^* . The orientation of ϕ^* with respect to a cellularly x^*, y^*, z^* fixed co-ordinate frame can be taken from Figure 2. ϕ^* is successively computed according to

$$\phi^* = -\frac{\Delta\phi^*}{2} + \ell \Delta\phi^* , \quad \ell = 1, n_\phi . \quad (5a)$$

For each ϕ^* the increment $\Delta\psi^*$ is evaluated from eq. (4c). The azimuthal angle ψ^* itself which, together with ϕ^* , finally fixes the orientation of a beam in the x^*, y^*, z^* frame is computed by

$$\psi^* = -\frac{\Delta\psi(\phi^*)}{2} + m \Delta\psi(\phi^*) , \quad m = 1, n_\psi \quad (5b)$$

+) The symbol INT means a truncation of the expression in brackets to an integer value.

with n_ψ taken from eq. (4c). The orientation of ψ^* with respect to the cellular cartesian co-ordinate frame is also seen in Figure 2.

The total number n_c of beams starting from a volume cell can be computed from (4b), (4c), and (5a). Values of n_c dependent on n_ϕ are listed in Table 1. The lowest possible number of beams from a volume cell is 8; i.e., one beam per octant.

Table 1. Total Number n_c of Beams Starting From a Volume Cell Dependent on Number n_ϕ of Polar Angle Increments Between 0 and π

Number n_ϕ of Polar Angle Increments Between $0 < \phi^* < \pi$	Number n_c of Beams Starting From a Volume Cell
2	8
4	24
6	56
8	96
10	144
12	200
14	264
16	360
18	448
20	544

2.2.1.2 Surface Zones as Emitter

The handling of surface zones as emitter is similar to the procedure used for volume zones. The emitted energy $\dot{Q}_{e,I}$ from a surface zone I with area A_I

$$\dot{Q}_{e,I} = \epsilon_I \sigma T_{s,I}^4 A_I \quad (6)$$

is distributed among $\Delta n_{s,I} = A_I / \Delta A_I$ equally-sized surface cells with area ΔA_I emitting the radiative heat flux

$$\Delta \dot{Q}_{e,I} = \epsilon_I \sigma T_{s,I}^4 \Delta A_I \quad (7)$$

It is assumed that the radiation source with a strength given by eq. (7) is concentrated in the geometric center of the surface cell. Provided the surface is gray and ideal diffuse radiating, beams of divergence $\Delta\Omega$ starting from the center point carry the initial energy flux:

$$\Delta\dot{Q}_{I,0} = \Delta\dot{Q}_{e,I} \cos \phi^* \frac{\Delta\Omega}{\pi} = \epsilon_{I\pi} \sigma T_{S,I}^4 \Delta A_I \cos \phi^* \Delta\Omega \quad (8)$$

The polar angle ϕ^* and the azimuthal angle ψ^* are related to a surface orientated x^*, y^*, z^* co-ordinate frame in the same way (Figure 3) as it was shown for volume cells.

In order to use the same spacing of the solid angle as for volume emitters, and in order to provide conservation, the expression $\cos \phi^* \Delta\Omega$ is computed in a special way similar to eq. (4a):

$$\cos \phi^* \Delta\Omega = \frac{1}{2} \left[\sin\left(\phi^* + \frac{\Delta\phi^*}{2}\right) - \sin\left(\phi^* - \frac{\Delta\phi^*}{2}\right) \right] \Delta\psi(\phi^*) \quad (9)$$

$\Delta\phi^*$ and $\Delta\psi^*$ are obtained from eqs. (4b) and (4c). Discrete values of the polar angle ϕ^* are calculated in the range $0 < \phi^* < \frac{\pi}{2}$ according to

$$\phi^* = -\frac{\Delta\phi^*}{2} + \ell\Delta\phi^*, \quad \ell = 1, \frac{n\phi}{2} \quad (10)$$

Discrete values of the azimuthal angle ψ^* are computed from eq. (5b).

The number of beams starting from a surface cell is exactly half the number of beams starting from a volume cell (see Table 1).

2.2.1.3 Transformation of Co-ordinates From Cell-Oriented Frames Into a Spatially-Fixed Frame

The directions of the beams calculated in terms of ϕ^* and ψ^* as shown above are initially related to the x^*, y^*, z^* co-ordinate system which is oriented with respect to the cells from which the beams start. However, the actual radiative exchange calculation, i.e., the tracing of the beams, is carried out for a spatially-fixed x, y, z co-ordinate frame which is oriented at the furnace as, for instance, shown in Figure 1. The direction angles of the beams ϕ and ψ in the x, y, z co-ordinate system are obtained by a transformation as explained in the following:

The angular orientation of the x^*, y^*, z^* co-ordinate frame with respect to the furnace oriented x, y, z system is described by the angles ϕ_r and ψ_r

Figure 3. Surface-Cell-Oriented X^*, Y^*, Z^* Co-ordinate Frame.

(Figure 4). ψ_r is that angle between the positive x and x^* directions, which is generated from congruent frames by clockwise rotation of the x^*, y^*, z^* frame around the positive z -direction ($0 \leq \psi_r \leq 2\pi$). ψ_r being defined in the foregoing manner, ϕ_r is the angle between the positive z and z^* directions which is produced by counterclockwise rotation of the x^*, y^*, z^* frame with respect to its x^* direction.

With the above definition, the beam angles ϕ and ψ in the furnace oriented co-ordinate system are calculated from ϕ^* and ψ^* (eqs. 5 and 10) by the following transformation formula (given here without proof):

$$\phi = \arccos (\cos \phi_r \cos \phi^* - \sin \phi_r \sin \phi^* \sin \psi^*) , \quad (11a)$$

$$\psi = \psi_r + \arctan \frac{\cos \phi_r \sin \phi^* \sin \psi^* + \sin \phi_r \cos \phi^*}{\sin \phi^* \cos \psi^*} . \quad (11b)$$

The value of the ambiguous function $\arctan$ in eq. (11b) is determined according to the signs of the numerator and denominator of the argument. The denominator being > 0 principal values between $-\pi/2$ and $+\pi/2$ have to be used. With the denominator and the numerator < 0 the next lower branch of the function between $-\pi$ and $-\pi/2$, with the denominator < 0 and the numerator > 0 the next upper branch between $\pi/2$ and π must be applied. This rule is implicitly followed in the computer code since use is made of the FORTRAN external function ATAN2. It is possible that the value of ψ computed with eq. (11b) as described above can be < 0 or $> 2\pi$. However, negative values of ψ correspond to $2\pi + \psi$ and values of $\psi > 2\pi$ correspond to $\psi - 2\pi$.

The transformation carried out through eqs. (11a) and (11b) is useful for several reasons:

- It allows to use the same code for describing the emission of beams regardless of the position of the emitting zone. This is especially useful for oblique surface zones for which the furnace program will be upgraded.
- Similarly, the reflection of beams at surface zones can be cast in the same code when the surface-oriented frame is used (see section 2.2.1.5).

Figure 4. Orientation of Arbitrary X^*, Y^*, Z^* Cell Co-ordinate Frame With Respect to X, Y, Z Furnace Co-ordinate Frame.

- The tracing of emitted or reflected beams (see section 2.2.1.4) through the furnace volume is carried out with the same routine despite different beam origins.
- Finally, the transformation allows a random rotation of each volume cell oriented co-ordinate frame and thus beam shifting can be carried out in order to improve the simulation of isotropic volume emission, especially when only a small number of beams per volume cell is considered (see section 2.2.1.10).

The z^* direction of a surface cell frame always coincides with a normal of the surface. The position of the x^*, y^* directions on the surface is somewhat arbitrary. However, in order to fix these directions, the above rules of generating ψ_r and ϕ_r were applied so that the requirements-- x^*, y^* axis lying in the surface plane and z^* axis being normal and directed into the furnace--were fulfilled in the shortest way starting with a frame orientation parallel and in direction of the furnace x, y, z frame (see Figure 4).

Angles ϕ_r and ψ_r which were determined in the described manner for x^*, y^*, z^* frames of the six surface planes of the rectangular furnace, are listed in Table 2.

Table 2. Angles of Orientation of Surface Cell Co-ordinate Frames With Respect to Furnace Co-ordinate Frame.

Surface Plane With Normal In Direction of	ϕ_r	ψ_r
Pos. x Axis	$\pi/2$	$3\pi/2$
Pos. y Axis	$\pi/2$	0
Pos. z Axis	0	0
Neg. x Axis	$\pi/2$	$\pi/2$
Neg. y Axis	$\pi/2$	π
Neg. z Axis	π	0

2.2.1.4 Tracing and Attenuation of Beams

The starting point of a beam is fixed by the co-ordinates x_0, y_0, z_0 of the geometric center of a volume or surface cell. The angles of direction ϕ and ψ of a starting beam are determined as described in the preceding section. Scattering being neglected, a beam follows a straight line until it hits a wall or until it is finally absorbed. Contrary to a pure Monte Carlo method, the absorption of a beam's initial energy $\Delta\dot{Q}_{I,0}$ given by eqs. (3) or (8) is also deterministically calculated. It is assumed that the attenuation of a beam along its path follows Beer's law. The attenuated energy flux $\Delta\dot{Q}_I$ of a beam at a volume zone boundary is given by

$$\Delta\dot{Q}_I = \Delta\dot{Q}_{I,0} e^{-\sum K_{a,J} \Delta s_J} \quad , \quad (12)$$

where the summation $\sum K_{a,J} \Delta s_J$ is implicitly carried out over all volume zones J which have been passed by the beam, including the emitting zone to account for self-absorption. The energy flux $\Delta\dot{Q}_{a,K}$ absorbed from the beam in the following volume zone K is computed according to

$$\Delta\dot{Q}_{a,K} = \Delta\dot{Q}_I (1 - e^{-K_{a,K} \Delta s_K}) \quad (13)$$

with $\Delta\dot{Q}_I$ taken from equation (12). This absorbed energy flux is accumulated in a storage assigned to the absorbing zone K in question.

The evaluation of the path lengths Δs_J or Δs_K of the beam in the volume zones J or K , respectively, is a pure geometrical problem and depends on the zone shape and the arrangement of the zones. For rectangular-shaped zones arranged in a mesh, the grid points of which coincide with constant cartesian co-ordinate lines, the following formulas are used (see Figure 5):

$$\cos \psi > 0: \quad \Delta s_x = \frac{x_p - x_0}{\sin \phi \cos \psi} \quad , \quad (14a)$$

$$\cos \psi < 0: \quad \Delta s_x = \frac{x_n - x_0}{\sin \phi \cos \psi} \quad , \quad (14b)$$

$$\sin \psi > 0: \quad \Delta s_y = \frac{y_p - y_0}{\sin \phi \sin \psi} \quad , \quad (14c)$$

$$\sin \psi < 0: \quad \Delta s_y = \frac{y_n - y_0}{\sin \phi \sin \psi} \quad , \quad (14d)$$

Figure 5. Path Length ΔS_J of a Beam Within a Rectangular, Volume Zone J .

$$\cos \phi > 0: \Delta s_z = \frac{z_p - z_o}{\cos \phi} , \quad (14e)$$

$$\cos \phi < 0: \Delta s_z = \frac{z_n - z_o}{\cos \phi} . \quad (14f)$$

x_o, y_o, z_o are either identical with the co-ordinates of the starting point of a beam within an emitting zone or with the co-ordinates of the beam entering the volume zone in question. $s_p, y_p, z_p = \text{const.}$ are the co-ordinates of the boundary planes of the volume zone with respect to positive co-ordinate directions, s_n, y_n, z_n are the corresponding boundary planes with respect to negative co-ordinate directions.

The actual path length Δs_J within a volume zone J, which is either an emitting zone or which is entered by the beam, is determined from

$$\Delta s_J = \min(\Delta s_x, \Delta s_y, \Delta s_z) . \quad (15)$$

The new co-ordinates of the beam leaving the volume zone are then calculated according to:

$$x = x_o + \Delta s_J \cdot \sin \phi \cos \psi , \quad (16a)$$

$$y = y_o + \Delta s_J \cdot \sin \phi \sin \psi , \quad (16b)$$

$$z = z_o + \Delta s_J \cdot \cos \phi . \quad (16c)$$

In the computing procedure, a volume zone J is associated with the indices i,j,k. The indices of a new volume zone entered by a beam are easily concluded from the minimum Δs of eq. (15) and from the sign of the denominator of its corresponding formula in eq. 14.

Whereas the code for the beam tracing in a cartesian alignment of rectangular volume zones is relatively simple, the tracing of beams in an arrangement of zones generated with an arbitrary grid requires a large computing effort.

Currently, a code is being developed which can handle beam tracing in a non-cartesian alignment of three-edged or four-edged prismatic zones. It is thought that such a zone arrangement can account for almost all combustion chamber geometries encountered in practice.

2.2.1.5 Absorption and Reflection at Surface Zones

Every time a beam leaves a volume zone it is checked whether the transversed boundary of the zone coincides with a surface zone. If this is true, the surface zone, say K, will absorb from the current energy flux of the beam given by eq. (12) the amount

$$\Delta\dot{Q}_{a,K} = \epsilon_K \Delta\dot{Q}_I \quad . \quad (17)$$

Similar to the absorption by a volume zone, $\Delta\dot{Q}_{a,K}$ is accumulated in a storage assigned to the absorbing surface zone.

If the surface zone is black ($\epsilon_K = 1$), the current beam is completely absorbed and the computation is continued with the next beam starting from the emitting zone considered. For $\epsilon_K < 1$ only a part of the current energy flux $\Delta\dot{Q}_I$ of the beam is absorbed, the rest of the energy flux is reflected according to:

$$\Delta\dot{Q}_{S,K} = (1 - \epsilon_K) \Delta\dot{Q}_I \quad . \quad (18)$$

Provided the surface zone is an ideal diffuse reflector (which is assumed at present), the reflected energy flux should be distributed over the whole hemisphere according to cosine law. This distribution could deterministically be modeled by ramifying the original single beam and treating the reflection in a similar way as the emission of beams from a surface cell. However, allowance of multiple ramification of beams under conditions of an optically thin furnace volume and highly-reflecting furnace walls, would lead to a too-large increase in computing time. Therefore, reflection is simulated with a stochastic model ("Monte Carlo approach") as follows.

The reflected energy flux (eq. 18) is assigned to one single beam starting at the interception point of the surface. The angles of direction ϕ^* and ψ^* of this beam with respect to the surface fixed x^*, y^*, z^* co-ordinate frame are determined from normalized random numbers R_m and R_{m+1} according to:

$$\phi^* = \arcsin \sqrt{R_m} \quad , \quad 0 \leq R_m < 1 \quad , \quad (19a)$$

$$\psi^* = 2\pi R_{m+1} \quad , \quad 0 \leq R_{m+1} \leq 1 \quad . \quad (19b)$$

The random numbers used to generate the polar angle ϕ^* are weighted by eq. (19a) in such a way that the energy flux distribution of a large assembly

of beams reflected at the surface element under consideration would approach the cosine weighted distribution of an ideal diffuse reflecting surface.

Finally, ϕ^* and ψ^* are transformed into the furnace-oriented co-ordinate frame by means of eqs. (11a) and (11b) and the beam tracing is resumed according to section 2.2.1.4.

2.2.1.6 Termination of Beam Tracing, Reference Beam

The tracing of a beam is terminated

- when a black surface zone is encountered, or
- when the energy flux of a beam leaving a zone has been reduced by attenuation to a value smaller than that of a certain reference flux $\Delta\dot{Q}_{\text{ref}}$.

In the latter case, the rest flux still carried by the beam is added to the fluxes absorbed by the zone where the latest attenuation of the beam occurred. This, together with the code for emission (see section 2.2.1.1 and 2.2.1.2) provides a fully conservative formulation of the radiative heat exchange.

The reference flux $\Delta\dot{Q}_{\text{ref}}$ for termination of tracing a beam can be defined in several ways. This definition influences somewhat the achievable accuracy for a given short computing time. However, by choosing the reference flux small enough (at the expense of computing time) the accuracy of the computations will become independent of how $\Delta\dot{Q}_{\text{ref}}$ is defined.

In the current model, the reference flux is determined in the following way.

Distinction is made between seven different furnace sections; i.e., the furnace volume, four furnace side walls, and bottom and top walls, the zones of which are successively regarded as emitter. For each section, an average intensity I_{ref} is computed from the emissive power of its zones.

The reference flux is calculated from the current maximum value $(I_{\text{ref}})_m$ of these average intensities according to eq. (20a) for beams starting from a volume zone and according to eq. (20b) for beams starting from a surface zone.

$$\Delta\dot{Q}_{\text{ref}} = a_o (I_{\text{ref}})_m \Delta\Omega \quad , \quad (20a)$$

$$\Delta\dot{Q}_{\text{ref}} = a_o (I_{\text{ref}})_m \cos \phi^* \Delta\Omega \quad . \quad (20b)$$

$\Delta\Omega$ and $\cos \phi^* \Delta\Omega$ are taken from (4a) and (9a), respectively. a_0 , which will be called "beam cutoff factor," is a constant less than 1. Reasonable values of a_0 lie in the range between 0.01 and 0.001 (see section 2.2.1.8). $(I_{\text{ref}})_m$ can change with the consecutive handling of the furnace sections, consecutive handling of the gray gas components in the model of the radiative properties (see section 2.2.2) or with changing temperature during the iterative solution of the total energy balances of the zones. However, because preceding $(I_{\text{ref}})_m$ values are always smaller, the intended level of accuracy is not diminished. The formulation (20b) for beams from surface zones is chosen in order to maintain a cosine distribution of the energy flux also for low accuracy levels.

2.2.1.7 Balances of Radiative Heat

During one radiative exchange calculation, each zone of the furnace once is regarded as emitter sending a certain number of beam as uniformly distributed as possible into the furnace volume. The energy fluxes absorbed by the various furnace zones from all the incident beams crossing or hitting them are accumulated in storages assigned to each zone. At the end of the calculation, the total absorbed flux in each zone is subtracted from the total flux emitted by the zone to obtain the net radiative heat flux out of that zone (eq. 21).

$$\dot{Q}_{r,I} = \dot{Q}_{e,I} - \sum_{\substack{\text{beams} \\ \text{incident on I}}} \Delta \dot{Q}_{a,I} \quad (21)$$

The net radiative heat flux $\dot{Q}_{r,I}$ from the zone I is one term of the total heat balance equation of that zone (see section 2.3). The net overall radiative heat transfer to all surface zones is easily computed by

$$\dot{Q}_{r,s} = \sum_{I=1}^{NS} \dot{Q}_{r,I} \quad (22)$$

where the summation is carried out for all NS surface zones.

Net fluxes to sections of the furnace walls or to other heat sinks exposed to the combustion chamber are obtained in a similar manner. It was mentioned earlier, that the code for the radiative heat exchange is strictly conservative; i.e.,

$$\sum_I \dot{Q}_{e,I} = \sum_I \sum_{\substack{\text{beams} \\ \text{incident on I}}} \Delta \dot{Q}_{a,I} \quad (23)$$

At present, furnace openings are handled like "pseudo"-surface zones the emission and absorption of which are included in eq. (23). The only difference between the left- and right-hand side of (23) is caused by the round-off error of the computer. A typical order of magnitude for this difference is 10^{-12} (ca. 13000 beams, CDC 7600, single-precision).

2.2.1.8 Influence of Beam Number, Beam Distributing Parameters, and Beam Cutoff Factor on the Accuracy of Calculated Overall Heat Transfer

For a prescribed zone arrangement of a furnace, the accuracy of the calculated radiative heat fluxes depends on the total number of beams, their distribution, and the earlier-defined "beam cutoff" factor a_0 .

The total number n of beams is related by eq. (24) to the numbers n_v of volume cells and n_s of surface cells and to the numbers n_c and $n_c/2$ of beams starting from a volume cell and a surface cell, respectively.

$$\begin{aligned} n &= n_c n_v + \frac{n_c}{2} n_s, \\ &= n_c \sum_{I=1}^{NV} \frac{V_I}{\Delta V_I} + \frac{n_c}{2} \sum_{I=1}^{NS} \frac{A_I}{\Delta A_I}. \end{aligned} \quad (24)$$

NV in (24) is the number of volume zones and NS the number of surface zones. n_c is a function of the number n_ϕ of increments of the polar angle as described in section 2.2.1.1 and shown in Table 1.

In the present code, a constant value of n_c is used throughout the furnace. Similarly, the volume cells ΔV_I are, if possible, equally sized. the total number n_v of volume cells is then linked to the uniform cell volume ΔV and the total furnace volume V by

$$n_v = \sum_{I=1}^{NV} \frac{V_I}{\Delta V_I} = \frac{V}{\Delta V}. \quad (25)$$

Since the size of a surface cell corresponds to the size of the neighboring volume cell, n_s is depending on n_v . This fact, together with the preceding ones, allows that the distribution of a fixed number n of beams can solely be described by the two parameters n_c and n_v . A variation of this distribution is achieved by different weighting of these parameters with respect to n .

In this section, some results of a study are presented which was carried out in order to assess the impact of n , n_c and n_v , as well as of a_0 , on the accuracy of predictions of overall radiative heat transfer and in order to establish reasonable values of these parameters. In the next section, the influence of n , n_c and n_v on local heat fluxes will be shown for the same example.

The boundary conditions and input data of the test example were chosen similar to that of a large, gas-fired boiler combustion chamber, which will be investigated later (see 2.4) and which also served as an example elsewhere (ref. 6). For the radiative exchange calculations discussed in this section, the data listed in Table 3 were used.

Table 3. Input Data of Test Example to Study the Effect of n , n_c , n_v , and a_0 on Accuracy of Computed Radiative Transfer

Furnace Geometry	: 5*5*15 m
Surface Temperature of the Walls (completely enclosing the furnace volume)	: $T_s = 700$ K
Well-Stirred Temperature of Radiating Gas Volume	: $T = 1631.1$ K
Gray Absorption Coefficient	: $K_a = 0.1$ 1/m
Emissivity of Surfaces	: $\epsilon = 0.8$

For that part of the study which was carried out to investigate the effect of n_c and n_v , a_0 was held constant at the low value of 0.001.

The influence of n_c on the computed radiative heat transfer was investigated using the values 8, 24, 96, 360 corresponding to n_ϕ 's of 2, 4, 8, and 16 (see also Table 1).

The number n_v of cube-shaped volume cells was varied between 1 and 5184 for the six different values 1, 3, 24, 192, 1536, 5184. Computations for $n_v = 1, 3$, or 24 were carried out with the furnace volume as a single zone, for the values ≥ 24 , the 2*2*6 zone arrangement shown in Figure 1 was used. In this case, $n_v = 24$ corresponds to one cell per volume zone, 192 to 2*2*2 cells, 1536 to 4*4*4 cells; and, finally, 5184 to 6*6*6 cells per one volume zone.

Since the furnace volume is assumed to be isothermal with a uniform absorption coefficient and to be enclosed by walls of constant surface temperature and emissivity (see Table 3), the predictions of the overall heat transfer should be not dependent on the zoning. For example, the predictions should be the same whether they are carried out for one volume zone and $2*2*6$ volume cells or for $2*2*6$ zones and 1 volume cell per zone. This has been verified for $n_v = 24$; however, the finer zoning allows a better resolution of local radiant heat fluxes.

The finer $2*2*6$ zoning also allows to apply a special algorithm written for symmetrical zones with respect to 1, 2, or 3 cartesian symmetry planes of the furnace. This part of the code was checked by comparing symmetrical and non-symmetrical computations produced with otherwise identical input data. Agreement was found with exception of slight differences due to the statistical error introduced by the random approach of wall reflection.

Since symmetry is threefold in the present example, only three of the $2*2*6$ zones are scanned as emitting zones as indicated by the bold broken line zones in Figure 1. Thus, the number of beams actually traced is reduced by a factor of 8. However, for reasons of comparison, the following results are interpreted in terms of the total number of beams which would have been traced without considering symmetry.

In Figure 6, the execution times (CDC 7600, FTN4 compiler, opt = 1) of each run of the present study are plotted versus the corresponding total number of beams. Curve a refers to the non-symmetric runs with one volume zone and curve b to the symmetric runs for the arrangement of $2*2*6$ zones. Curve c, finally, shows the projected execution times if the computations of the $2*2*6$ zone arrangement had been carried out without considering symmetry.

The total number of beams encountered for the investigated values of n_c and n_v ranged from 32 ($n_c = 8$, $n_v = 1$) up to 714 240 ($n_c = 360$, $n_v = 1536$). Figure 6 reveals that, above $n > 10000$, the execution time of the radiation exchange program is almost proportional to the total number of beams despite different weighting of n_c and n_v . The deviation from proportionality for $n < 10000$ is due to some overhead routines performed before and after the beam tracing. For the same total number of beams, the non-symmetric computations in the $2*2*6$ zone arrangement (curve c) are slightly higher than those

Figure 6. Program Execution Times Dependent on Total Number of Beams
(CDC 7600, 7TN4, opt = 1; $a_0 = 0.001$)

for one volume zone (curve a), since in the former case, more zone boundaries are encountered during the beam tracing.

The overall radiative heat transfer from the isothermal furnace volume to the surrounding walls of uniform temperature and of surface area A_s can be expressed in terms of a total emissivity

$$\epsilon_t = \frac{\dot{Q}_{r,s}}{A_s(\sigma T^4 - \sigma T_s^4)} \equiv \frac{\overline{GS}}{A_s} \quad (26)$$

with $\dot{Q}_{r,s}$ obtained from eq. (22). Figure 7 shows how this computed ϵ_t , which may also be related to a total exchange area $\overline{GS}$ (7), varies with the total number of beams for different values of the distribution parameters n_c and n_v . For large values of n_c and n_v corresponding to a large number of beams, the computations obviously approach a limiting value of $\epsilon_t = 0.301$. This value was obtained for $n_c = 24$ and $n_v = 5184$ corresponding to a total number of beams $n = 148608$. Provided 0.301 is the true value, Figure 8 shows the percentage error of the predicted ϵ_t (i.e., of the overall heat transfer) for lower total beam numbers. It can clearly be seen from Figures 7 and 8 that the parameter n_v , the number of volume cells, is of more importance for the accuracy of the prediction of overall radiative heat transfer than the parameter n_c , the number of beams per volume cell.

Figures 7 and 8 also contain values of ϵ_t and its percentage error which were evaluated using charts of direct exchange areas in ref. 7 and ref. 8, respectively, in order to determine the emissivity ϵ_g of the furnace volume, and by applying eq. (27)

$$\epsilon_t = \frac{1}{1/\epsilon_g + 1/\epsilon - 1} \quad (27)$$

where ϵ is the surface emissivity. Since the direct exchange areas in ref. 7 and ref. 8 are based on the same source,⁽⁹⁾ the small difference between the cited ϵ_t 's is due to a reading error. Compared to the value of this study the total emissivities determined from the refs. 7 and 8 are lower by 2.2 percent and 2.5 percent, respectively.

Figure 8 further shows that, for the chosen example, a prediction of total radiative heat transfer, which is accurate within 1 percent can already be obtained with $n_c = 8$ and $n_v = 192$ corresponding to a total number of beams

Figure 7. Computed Total Emissivities Dependent on Total Number, n , of Beams and on Beam Distribution Parameters, n_v and n_c ($a_0 = 0.001$).

Figure 8. Error in Computed Overall Radiative Heat Transfer Dependent on Beam Number ($a_0 = 0.001$).

$n = 2432$ and 3 percent of the execution time needed to compute the reference value.

The effect of the beam cutoff factor a_0 on the execution time (Figure 9) and on the accurate predictions of the total radiative heat transfer (Figure 10) is not so dramatic as is the total number of beams.

Decreasing a_0 by an order of magnitude only causes an increase in execution time of about 30 percent, whereas a change of the number of beams by one order of magnitude leads to a 100 percent increase in execution time. Choosing again the value $\epsilon_t = 0.301$ obtained with $n_c = 24$, $n_v = 5184$, and $a_0 = 0.001$ as reference value, it can be seen from Figure 10 that no essential gain of accuracy can be achieved for values of a_0 lower than 0.01.

Since the program code uses absolute values of physical properties, the preceding radiative exchange calculations were carried out with the actual gas and surface temperatures listed in Table 3. However, the presented results do not depend on temperature apart from a slight influence introduced by the special definition of the reference beam flux. This influence was eliminated by choosing a low value for a_0 (when n_c and n_v were varied).

On the other hand, the above results certainly depend on the value of the absorption coefficient K_a which was 0.1 1/m in the present case. It can be expected that, with the same total beam number, the overall radiative heat transfer will be less accurately predicted for increasing optical thickness. However, the relative influence of the various parameters should be similar to the current study.

2.2.1.9 Influence of Beam Number and Beam Distributing Parameters on Local Heat Flux Distributions

Although the gas volume in the test example is assumed to be isothermal ("well-stirred") and the furnace walls are assumed to have uniform temperature, the radiative heat flux distributions are not uniform because of the corner influence. Figure 11 shows the flux distribution computed for the 2*2*6 zoning of Figure 1 at the furnace side walls. The maximum heat flux density is found at the side wall zones $k = 3$ and $k = 4$.

Vertical symmetries were considered; however, angular symmetries were not. Therefore, one set of fluxes is computed for each of the two perpendicular rows of side wall zones $k=1 \div k=3$ in the planes $x=0$ and $y=0$. These fluxes

Figure 9. Program Execution Times Dependent on Beam Cutoff Factor a_0 (CDC 7600, FTN4, opt = 1).

Figure 10. Error in Computed Overall Heat Transfer Dependent on Beam Cutoff Factor for Different Beam Distribution Parameters, n_c and n_v .

Figure 11. Distribution of Heat Flux Density at Furnace Side Walls (computed with $n_c=96$, $n_v=5184$, $a_0 = 0.001$).

should be identical; however, differences as indicated in Figure 11 arise due to numerical errors which will be discussed later.

The computed maximum heat flux density is, like the predicted overall heat transfer, a function of the total number of beams and of the distribution parameters n_c and n_v . The dependency obtained for the investigated example is plotted in Figure 12. The maximum heat flux density approaches a limiting value of about 126 kW/m^2 for higher beam numbers. Contrary to the total heat flux predictions, the (local) maximum heat flux density is more influenced by the number n_c of beams per volume cell, especially for low n_c , and not so strongly by the number of cells itself.

A dramatic influence of n_c was detected for the computed net fluxes to the bottom (top) walls which are plotted as a function of the total beam number in Figure 13. The limiting value of the corresponding heat flux density, which is about 110 kW/m^2 , is approached at a rather large beam number.

The pronounced influence of n_c on local heat fluxes was studied in more detail. This study led to an upgrading of the code which is described in the following section.

2.2.1.10 Random Orientation of the Volume Cell Reference Frame for Counting Beam Angles

Numerical errors of the present code are of systematic and of random nature. Since randomness is only introduced by modeling the wall reflection, and since the surface emissivity is high in the present example, the statistical error is small. The lower accuracy at lower beam numbers is predominantly caused by systematic numerical errors. This is also obvious from some clear dependencies between accuracy and distribution parameters shown in the two preceding sections.

The poor accuracy of predicted local heat fluxes for low n_c is caused by the following systematic errors.

The geometry and zone arrangement of the present example, in combination with the spatially-fixed angular distribution of beams, would effect that a certain number of beams precisely hits the side edge of the furnace. The ratio between this number and the total number of beams increases with decreasing n_c . In order to avoid beam splitting in that case, all beams were uniformly shifted in the same rotational sense by a very small amount

Figure 12. Computed Maximum Radiative Heat Flux Density at Side Wall Zones Dependent on Total Number of Beams and Beam Distribution Parameters n_v and n_c ($a_0 = 0.001$).

Figure 13. Computed Radiative Heat Flux Density at Bottom Wall Dependent on Total Number of Beams and Beam Distribution Parameters n_v and n_c ($a_0 = 0.001$).

so that always only one corner surface is intercepting. This fact, together with the handling of symmetry, caused maximum heat fluxes to be overpredicted at lower n_c (Figure 12).

The poor heat flux predictions at the bottom walls for lower n_c (Figure 13) originated from the prescribed angular distribution of beams, too. This can most easily be demonstrated for $n_c = 8$ and $n_v = 24$, the lowest possible values of the 2*2*6 zone arrangement. In that case, all the beams of the volume zones are emitted in their vertical diagonal planes with a polar angle ϕ of $\pm 45^\circ$ and $\pm 135^\circ$. None of the beams emitted by the $k = 1$ volume zones directly hits the neighboring side wall zones; thus, because of conservation, a too large energy flux is directed through the $z = \text{const.}$ boundaries of the volume zones. That also means that the surface zones of the bottom (top) walls intercept too much radiation. The described effect only gradually vanishes with increasing n_c .

A large reduction of the systematic numerical error connected with the fixed angular distribution of beams could be achieved by random orientation of the volume cell co-ordinate frame, from which the beam angles ϕ^* and ψ^* are counted (see sections 2.2.1.1 and 2.2.1.3). This random orientation is carried out for each volume cell individually according to

$$\phi_r = \frac{\pi}{2} R_m, \quad 0 \leq R_m \leq 1, \quad (28a)$$

$$\psi_r = \frac{\pi}{2} R_{m+1}, \quad 0 \leq R_{m+1} \leq 1, \quad (28b)$$

with R as random number uniformly distributed between 0 and 1. The factor $\pi/2$ in (28a) and (28b) is arbitrary; however, this factor should be larger than $\Delta\phi^*$ and $\Delta\psi^*$, respectively. The beam angles ϕ^* and ψ^* , consecutively counted from the volume-cell-oriented frame, are transformed into the furnace-oriented frame with eqs. (11a) and (11b). It must be emphasized that, in spite of the random choice of the reference frame of each volume cell, deterministic simulation of isotropic emission of volume radiation; i.e., uniform angular spreading of beams, is maintained--thus, the statistical error of local heat flux predictions remains small except for very low beam numbers.

The considerable gain in accuracy using random orientation of the reference frames of the volume cells can be seen in Figure 14. In this figure,

Figure 14. Effect of Random Orientation of Beam Angle Reference Frame on Computed Radiative Heat Flux Density at Bottom Wall.

heat flux densities at the bottom (top) zones computed with the new method are compared to those of Figure 13, which were computed with fixed orientation of the reference frames for the beam angles.

2.2.1.11 Some Conclusions Concerning the Semi-stochastic Method

Although there is no explicit proof, it can be said that the present semi-stochastic method for computation of radiation exchange is superior to pure Monte Carlo methods since the statistical error is reduced by reinforcing isotropic distribution of emitted beams and by deterministic computation of absorption. Some systematic directional errors connected with the simulation of isotropic emission could be reduced by allowance for a restricted random shifting of each bundle of starting beams which otherwise remain uniformly spread over the solid angle 4π .

A sufficient accuracy of predicted total and local heat fluxes could already be achieved for total beam numbers lower than 10000. In case of symmetry, the actual beam number is even more reduced, namely by a factor of 2, for each symmetry plane of the furnace. This should be compared to pure Monte Carlo Methods for which several ten thousands of beams are usually said to be necessary in order to obtain a representative solution.

It is expected that the accuracy of local heat flux predictions will decrease when the same furnace geometry is investigated with the same number of beams, however with finer zoning. Such a study will be carried out in the near future.

2.2.2 Modeling the Exchange of Non-gray Radiation

The semi-stochastic radiation model described in the preceding sections was developed, at first, to evaluate the exchange of gray radiation.

The method can easily be modified to handle the exchange of monochromatic radiation. For this purpose, the emissive power σT^4 of all volume and surface zones has to be replaced by their spectral emissive power E_λ given by Plank's law. Further, the gray absorption coefficients K_a and the total surface emissivities ϵ of the zones must be replaced by the spectral values $K_{a,\lambda}$ and ϵ_λ , respectively, corresponding to the radiative properties of the media constituting the zones.

Provided the properties $K_{a,\lambda}$ and ϵ_λ of the media in the zones are known over the whole spectrum, the exchange of non-gray radiation could principally be simulated with the present code in the following way: At first, the spectrum is stepwise divided into n_λ small wavelength regions $\Delta\lambda = \lambda_2 - \lambda_1$ of approximate constant properties $K_{a,\Delta\lambda}$ or $\epsilon_{\Delta\lambda}$. Then, similar to the handling of monochromatic radiation, the black total emissive power of the zones is replaced by

$$\Delta E(T) = \int_{\lambda_1}^{\lambda_2} E_\lambda(T) d\lambda \quad (29)$$

With these quantities, the above-documented computation of radiative transfer is carried out consecutively for each of the n_λ wavelength regions. The absorbed energy fluxes are accumulated in one storage place for each zone like before; thus, no change of the code for beam tracing is necessary. The totally absorbed fluxes in a zone I are finally subtracted from the zone's totally emitted flux leading to the net radiative outward flux. This is shown in eq. (30) for a volume zone.

$$\dot{Q}_{r,I} = \sum_{n_\lambda} 4K_{a,\lambda,I} \Delta E_I V_I - \sum_{n_\lambda} \sum_{\substack{\text{beams} \\ \text{incident on I}}} \Delta \dot{Q}_{a,I} \quad (30)$$

The described coupling of the radiative exchange model with band models requires large computing times and will only be applied in order to test simpler approximations of the emission/absorption characteristics of non-gray media.

Such a simple approach is the representation of non-gray volume radiation by the sum of weighted contributions of several gray gas components⁽⁷⁾. This approach is generally formulated in terms of an emissivity of a real gas layer of thickness s according to:

$$\epsilon_g = \sum_{\ell=1}^{n_g} a_\ell(T) (1 - e^{-K_{a,\ell}s}) \quad (31)$$

with the weighting factors $a_\ell(T)$ given as a function of T in polynomial form

$$a_\ell(T) = \sum_m b_{m,\ell} T^{m-1} \quad (32)$$

The coefficients $b_{m,\ell}$ in (32) are subjected to the condition that

$$\sum_{\ell=1}^{n_\ell} a_\ell(T) = 1 \quad (33)$$

Absorption coefficients $K_{a,\ell}$ of the fictional n_ℓ gray gas components may be expressed in the following way:

$$K_{a,\ell} = K_{g,\ell}(p_{H_2O} + p_{CO_2} + p_{CO}) + K_{soot,\ell} C_{soot} + \sum K_{gray} C_{gray} \quad (34)$$

$K_{g,\ell}$ is a specific absorption coefficient (1/m bar) of the mixture of combustion gases H_2O , CO_2 and CO assigned to the ℓ th fictional gray radiating gas component. Similarly, $K_{soot,\ell}$ is the specific absorption coefficient (1/(m · kg/m³)) of a cloud of suspended soot particles assigned to the same fictional gray component (for more details see ref. 10). Finally, $\sum K_{gray} C_{gray}$ represents the contribution of actually-supposed gray radiating species to $K_{a,\ell}$ (coal/char particles, ≈ ash particles). Obviously, the K_{gray} 's of each of the actual gray radiating species do not depend on ℓ .

The foregoing approximation can also be interpreted as a model in which n_λ bands or wavelength regions of equal spectral absorption coefficients $K_{a,\lambda} = K_{a,\ell}$ are contracted to a ℓ th range. The black emissive power of that range is then given by

$$E_\ell = \sum_{n_\lambda} \int_{\lambda_i}^{\lambda_j} E_\lambda d\lambda = a_\ell(T) \sigma T^4 \quad (35)$$

From the above-described coupling of a band model with the radiative exchange model and from eq. (35) it is easy to see how the weighted gray-gas approach of non-gray radiation is (optionally) incorporated in the present code. The absorption coefficient K_a of gray radiation is replaced by $K_{a,\ell}$ and the calculation of the radiative exchange is consecutively carried out in the n_ℓ ranges. The initial energy flux in beams starting from zones I in the ℓ th range is weighted with $a_\ell(T_I)$ according to

$$\dot{Q}_{I,\ell,0} = a_\ell(T_I) K_{a,\ell} \frac{\sigma}{\pi} T_I^4 \Delta V_I \Delta \Omega \quad (36a)$$

$$\dot{Q}_{I,\ell,0} = a_{\ell}(T_I) \epsilon_I \frac{\sigma}{\pi} T_{s,I}^4 \Delta A_I \cos \phi^* \Delta \Omega, \quad (36b)$$

where eq. (36a) is related to beams starting from volume zones and eq. (36b) to beams from surface zones with a gray emissivity of $\epsilon_I = \epsilon_{I,\ell}$. During the scanning of the n_{ℓ} ranges absorbed fluxes are again accumulated in zonal storage places. The end balance of radiative transfer for a zone is carried out by summing its emitted fluxes over the n_{ℓ} ranges and then subtracting its accumulated absorbed fluxes.

The way the weighted gray gas approach is embodied in the present program indirectly includes the assumption that the absorbtivity of a volume zone layer (with fixed value of the product : concentration * layer width) equals its emissivity calculated at the temperature of the radiation source; that is, of the emitting zone.

Actual test calculations were carried out with an approach of three weighted gray gases. The coefficients $b_{m,\ell}$, $K_{g,\ell}$, and $K_{soot,\ell}$ are currently taken from ref. 10. They are listed in Table 4. Values of K_{gray} (for coal/char ash particles) are not recorded here because it is rather the aim of the present project to establish such values. However, K_{gray} is generally the product of a so-called efficiency factor for absorption and a specific surface area; which, in turn, depends on the size distribution of the considered particle types and their density. It has also to be mentioned that the values of Table 4, as well as the approach with three weighted gray gases, are not thought to be absolutely ideal. Better approximations will eventually be the outcome of the present study. It may be possible that a temperature dependency will be introduced for some of the specific absorption coefficients. Contrary to the zone method of ref. 7, the present radiation exchange model can consider such a dependency.

Table 4. Constants of a Three-Weighted Gray Gas Approach for Combined Gas and Soot Radiation (ref. 10)

ℓ	$b_{1,\ell}$ -	$b_{2,\ell}$ 1/K	$K_{g,\ell}$ 1/m · bar	$K_{soot,\ell}$ 1/m kg/m ³
1	0.130	+0.000265	0	3460
2	0.595	-0.000150	0.835	960
3	0.275	-0.000115	26.25	960

2.3 Model of Total Heat Transfer

The computation of radiative heat exchange described in the preceding section 2.2 is based on specified temperatures and on specified absorption coefficients and surface emissivities, respectively, for each zone. Whereas the surface emissivities only depend on the optical properties of the surface material, the absorption coefficients of volume zones depend as well on the optical properties of the radiating species as on the species concentration. Both, optical properties of the radiating media and species concentration, might also be temperature dependent.

In general, the furnace zones are initially unknown. However, they can be run from the solution of total heat balances set up for each zone with unknown temperature as described in the following.

2.3.1 Total Heat Balance for Volume Zones

In total heat balances for volume zones, the net heat fluxes of sensible heat $\dot{Q}_{s,I}$ and radiative heat $\dot{Q}_{r,I}$ from the zone I are equated to the release of chemically bound heat $\dot{Q}_{ch,I}$ in that zone:

$$\dot{Q}_{s,I} + \dot{Q}_{r,I} - \dot{Q}_{ch,I} = 0 \quad (37)$$

$\dot{Q}_{s,I}$ is further split into a net convective heat flux $\dot{Q}_{c,I}$ and a net diffusional heat flux $\dot{Q}_{d,I}$ from the zone

$$\dot{Q}_{c,I} + \dot{Q}_{d,I} + \dot{Q}_{r,I} - \dot{Q}_{ch,I} = 0 \quad (38)$$

The radiation term $\dot{Q}_{r,I}$ in the balance equation (38) is identical with the result of the radiative exchange calculation given by equation (21).

The term $\dot{Q}_{c,I}$ in eq. (38) is coded for a general three-dimensional (3D) cartesian alignment of a rectangular zone cluster in the following way (Figure 15):

$$\begin{aligned} \dot{Q}_{c,I} = & \dot{M}_{i-\frac{1}{2},j,k}^+(c_p T)_{i-1,j,k} + \dot{M}_{i,j-\frac{1}{2},k}^+(c_p T)_{i,j-1,k} + \dot{M}_{i,j,k-\frac{1}{2}}^+(c_p T)_{i,j,k-1} \\ & + \dot{M}_{i+\frac{1}{2},j,k}^-(c_p T)_{i+1,j,k} + \dot{M}_{i,j+\frac{1}{2},k}^-(c_p T)_{i,j+1,k} + \dot{M}_{i,j,k+\frac{1}{2}}^-(c_p T)_{i,j,k+1} \\ & - (\dot{M}_{i-\frac{1}{2},j,k}^+ + \dot{M}_{i,j-\frac{1}{2},k}^+ + \dot{M}_{i,j,k-\frac{1}{2}}^+ + \dot{M}_{i+\frac{1}{2},j,k}^- + \dot{M}_{i,j+\frac{1}{2},k}^- + \dot{M}_{i,j,k+\frac{1}{2}}^-) \\ & (c_p T)_{i,j,k} \quad (39) \end{aligned}$$

The zone I for which the balance (35) is written is identified by the indices i, j, k . The half valued indices refer to the zone's boundaries; i.e., to grid planes of the zone arrangement. $\dot{M}^+$ and $\dot{M}^-$ are total mass fluxes (kg/s) over the zone boundaries (or grid planes) in positive and negative co-ordinate directions (see Figure 15). These total mass fluxes (always $0 \leq \dot{M}$) have to be prescribed as input data from an estimated flow pattern of the investigated furnace.

The first two lines of eq. (39) represent the convective flux of sensible heat into the zone under consideration. It can be seen that a complete "upwind" formulation of these fluxes is applied. The outward flux of sensible heat is given by the third line of eq. (39). It is assumed that the zone has no mass source.

All temperatures in eq. (39) are generally supposed to be identical with the radiation temperature of the corresponding zones, which means that the zones are perfectly stirred. However, following a suggestion in ref. 7, it can optionally be differed between the radiating and the exit temperature of a zone. In that case, the T 's in eq. (39) are identical with a zone's exit temperature, and the effective radiation temperature is determined by an empirical weighting between the adiabatic temperature of the zone and its exit temperature.

The specific heats in eq. (39) are composite values computed from zonal concentrations of the furnace fluid (see section 2.3.4) and from interpolation formulas⁽¹¹⁾ for the temperature dependence of individual $c_{p,j}$'s of the various species j .

Internal diffusional (conductive) fluxes over the boundaries of neighboring volume zones are so far neglected. However, turbulent interchange of sensible heat between neighboring volume zones can principally be simulated by specifying forward as well as backward convective mass flow's $\dot{M}^+$ and $\dot{M}^-$ over the same zone boundaries.

The diffusional heat flux from a volume zone to a neighboring surface zone is currently formulated by

$$\dot{Q}_{d,I} = \sum_m A_m \alpha (T_{i,j,k} - T_{s,m}) \quad (40)$$

Figure 15. Notation for Total Mass Flows Across the Boundaries of a Zone.

α is a specified overall convective heat transfer coefficient. The summation is carried out for all m surface zones of area A_m adjacent to the volume zone I .

The final form in eq. (38b) which has to be specified is the release of chemically-bound heat $\dot{Q}_{ch,I}$ in each volume zone. This is done by prescribing the fuel flows $\dot{M}_f$ in kg/s over the boundaries of each volume zone as input data. $\dot{Q}_{ch,I}$ is then computed by eq. (40):

$$\begin{aligned} \dot{Q}_{ch,I} = & (\dot{M}_{f,i-\frac{1}{2},j,k} + \dot{M}_{f,i,j-\frac{1}{2},k} + \dot{M}_{f,i,j,k-\frac{1}{2}} \\ & - \dot{M}_{f,i+\frac{1}{2},j,k} - \dot{M}_{f,i,j+\frac{1}{2},k} - \dot{M}_{f,i,j,k+\frac{1}{2}}) \cdot H_u \end{aligned} \quad (40)$$

H_u is the lower calorific value of the fuel in KJ/Kg. Contrary to the total mass flow, the fuel mass flows $\dot{M}_f$ can have a positive or negative sign. The sign is positive with the fuel flow in positive co-ordinate directions and negative with the flow in negative co-ordinate directions.

2.3.2 Total Heat Balances for Surface Zones

In several practical cases (e.g., refractory walls, deposit layer on tube walls) the temperature of the surface zones are also originally unknown. However, analogous to the procedure for volume zones, total energy balances are set up for these zones and solved for the surface temperatures. In these balances convective and radiative heat fluxes $-\dot{Q}_{d,I}$ and $-\dot{Q}_{r,I}$ toward these zones I are equated to the heat $\dot{Q}_{w,I}$ conducted through the corresponding wall or surface layers.

$$-\dot{Q}_{d,I} - \dot{Q}_{r,I} - \dot{Q}_{w,I} = 0 \quad (41)$$

$\dot{Q}_{r,I}$ is again expressed by eq. (21). The convective (diffusional) flux $-\dot{Q}_{d,I}$

$$-\dot{Q}_{d,I} = A_I \alpha (T_{i,j,k} - T_{s,I}) \quad (42)$$

with $T_{i,j,k}$ being the temperature of the neighboring volume zone. $\dot{Q}_{w,I}$ is currently modeled in a very simple way

$$-\dot{Q}_{w,I} = A_I \frac{\lambda_I}{\Delta w_I} (T_{s,I} - T_{o,I}) \quad (43)$$

λ_I is the thermal conductivity of the wall layer of width Δw_I and $T_{o,I}$ is the outer temperature of this layer. In principle, eq. (43) can be replaced

by more sophisticated approaches; e.g., for ash deposits with layers of different width and composition.

2.3.3 Iterative Solution of the Total Energy Balances

With n_z zones of unknown temperatures, the total energy balances yield n_z algebraic equations. These equations are non-linear in the zonal temperature T_I . This is caused by the radiation term $\dot{Q}_{r,I}$ and the temperature dependency of the specific heat; furthermore, the equations are linked, and this linkage is of elliptic nature since radiation is directed in upstream directions. The elliptic characteristic is increased when a recirculating flow pattern is considered. Therefore, a solution of the equation system can only iteratively be obtained. In the present program, an algorithm is applied which is based on a combined Newton-Raphson and Gauss-Seidel iterative solution technique. The algorithm includes the following steps:

Using prescribed temperatures on the one hand, or guessed temperatures for all zones with unknown temperatures on the other hand, the semi-stochastic method is applied to compute the radiation terms $\dot{Q}_{r,I}$. During this first step, the contributions of zones with constant temperature to all $\dot{Q}_{r,I}$'s are stored. The computed radiation terms $\dot{Q}_{r,I}$ are then used to obtain a set of improved zonal temperatures. Following a Newton-Raphson technique, an improved value for the temperature of a volume zone is found by

$$T_{I,new} = T_I - \frac{\dot{Q}_{c,I} + \dot{Q}_{d,I} + \dot{Q}_{r,I} - \dot{Q}_{ch,I}}{\frac{\partial}{\partial T_I}(\dot{Q}_{c,I} + \dot{Q}_{d,I} + \dot{Q}_{r,I})} \quad (44a)$$

Improved surface zone temperatures are similarly computed:

$$T_{s,I,new} = T_{s,I} - \frac{-\dot{Q}_{d,I} - \dot{Q}_{r,I} - \dot{Q}_{w,I}}{\frac{\partial}{\partial T_{s,I}}(-\dot{Q}_{d,I} - \dot{Q}_{r,I} - \dot{Q}_{w,I})} \quad (44b)$$

It is sufficient to evaluate the derivatives with respect to the zone temperature of the terms in parentheses in eqs. (44a) and (44b) only for the strongest dependencies of these terms on T_I or $T_{s,I}$; for instance, in evaluating $\partial \dot{Q}_{r,I} / \partial T_I$ reflection can be neglected.

During the computation of improved zonal temperatures, the convective and diffusional fluxes $\dot{Q}_{c,I}$ are determined either from old zone temperatures or

new corrected zone temperatures. The latter are used as soon as they are available (e.g., from "upstream" zones). This is basically a Gauss Seidel approach.

After improved temperature values are found for all zones of unknown temperature, the radiative exchange calculation is repeated with these zones as emitter. The corresponding absorbed fluxes are augmented by stored amounts originating from zones with constant temperatures[†] and improved values of $\dot{Q}_{r,I}$ are formed.

The new values of $\dot{Q}_{r,I}$ are then used in a second cycle for further improvement of the zonal temperatures with eq. (44a) and (44b), and so on.

The iteration process is carried out until the differences of zonal temperatures or local fluxes of two consecutive iteration cycles are reduced to small fluctuating values, unavoidable because of the stochastic nature of the radiative exchange calculation.

The whole iteration procedure is, at least for the coarse zone arrangements studied so far, remarkably fast and stable. This can also be seen from Figure 16, where maximum values of the relative residua of volume zone temperatures are plotted versus the number of iterations. The three different curves in Figure 16 refer to the sample problem presented in section 2.4. It has to be pointed out that the stochastic fluctuations of the residua for higher iteration numbers correspond to temperature fluctuations of less than 0.5 K.

2.3.4 Specification of Species Concentration in Volume Zones

A specification of species concentration in the various volume zones is necessary for the evaluation of zonal absorption coefficients and for the evaluation of the bulk specific heat of a zone. Since combustion is not modeled at present, species concentrations have to be supplied as input data.

For gaseous species j , it is often sufficient to assume that they are equally distributed throughout the furnace volume. The corresponding concentrations p_j (supplied in bar) are determined for complete combustion. However, it is optionally possible to specify $p_{j,I}$ zonewise from measured or estimated combustion patterns.

[†]The use of stored values for fluxes absorbed from zones with constant temperatures is only allowed when the absorption coefficients are temperature independent. If this is not true, the exchange calculation has to be repeated for all zones.

Figure 16. Maximal Relative Residuum of Volume Zone Temperature Depending on Number of Iterations.

Concentrations of solid particles k are either a priori specified as $c_{k,I}$ in kg_k/m^3 (at actual temperatures) for each volume zone or they are given as $m_{k,I}$ in kg_k/kg as the ratio between the mass of these particles and the total mass M in the volume zone.

$m_{k,I}$ may be constant throughout the furnace which is, for instance, a reasonable assumption for the distribution of ash particles (submicron particles excluded).

With different values of $m_{k,I}$ in the various volume zones or at zone boundaries, formation/destruction or segregation of particles can be simulated. Simple codes for describing inhomogenous particle mass concentrations (e.g., for char particles, soot particles) will be developed.

In order to evaluate the absorption coefficient of the radiating suspension with eq. (34) or similar equations particle concentrations m_k in kg_k/kg have to be converted into concentrations c_k in kg/m^3 :

$$c_{k,I} = \frac{m_{k,I}}{1 - \sum m_{\text{solid},I}} \frac{1}{RT_I} \sum_{\text{gas}} M_j p_j \quad (45)$$

In (45), R is the universal gas constant, and M_j the molecular weight of the gaseous species. The concentration $c_{k,I}$ depends on the zone temperature, and it follows from eq. (34) that the absorption coefficients $K_{a,\ell,I}$ of a zone will vary with temperature if particles are present. Therefore, when total heat balances are solved in that case, new values of the absorption coefficients are computed prior to the radiative exchange calculation of each iteration cycle.

2.4 Application of the Rectangular Furnace Model to a Gas-Fired Boiler Combustion Chamber

The following sample problem shows how the rectangular furnace model is applied in order to predict heat transfer and furnace temperatures in an idealized gas-fired combustion chamber of a utility boiler. This problem is similar to an example studied with a well-stirred approach by Sarofim and Hottel (ref. 6).

2.4.1 Input Data

The necessary input data to prepare and run the mathematical furnace model may be classified into five groups; namely, into

- data of combustion chamber design and actual operating conditions of the investigated furnace,
- model data concerning the zoning of the furnace,
- estimated field data and zonal average values
- data of radiative and thermodynamic properties of volume and surface media of the furnace, and
- data for numerical parameters influencing accuracy.

According to the classification, the input data of the sample problem is summarized in the following:

2.4.1.1 Inlet and Boundary Conditions Based on Design and Operating Condition of the Investigated Furnace

- Geometrical Data

Furnace shape	: rectangular
Furnace dimensions	: 5*5*15m
Smooth surface walls completely enclosing the furnace volume	

- Fuel Data

Fuel type	: gas
Fuel composition	: CH ₄ , saturated at 289 K
Lower calorific value H_v	: 49961.6 kJ/kg _{dry}

- Furnace Operational Data

Combustion chamber pressure	: 1 bar
Thermal input	: 117 MW
Total fuel mass flow $\dot{M}_{f,0}$ corresponding to thermal input	: 2.34 kg _{dry} /s
Fuel temperature	: 298 K
Excess air	: 30%, half-saturated at 289 K
Total mass flow $\dot{M}_0$ corresponding to fuel mass and excess air	: 54.44 kg/s
Air temperature	: 298 K
Ambient temperature T_0	: 298 K
Uniform temperatures $T_s = T_{s,I}$ of inner surfaces of furnace walls	: 700 K

2.4.1.2 Zoning of the Furnace

- Well-Stirred Approach (see 2.4.1.3)

Shape of volume zone	: rectangular
Number of volume zones	: 1
Number of surface zones	: 6
Considered symmetry planes of furnace	: none

- Other Approaches (see 2.4.1.3)

Shape of volume zones	: cubic
Zone arrangement (see Figure 1)	: 2*2*6
Number of volume zones	: 24
Number of surface zones	: 56
Considered symmetry planes of furnace	: 2

2.4.1.3 Estimated Field Data in Combustion Chamber and Zonal Average Values

- Flow Pattern (convective flow across volume zone boundaries)

<u>Well-stirred approach</u>	: Case A, Fig. 17
<u>Plug flow approach</u>	: Case C, Fig. 17
Total mass introduced into	: bottom volumes zones $k = 1$
Total mass extracted from	: top volume zones $k = 6$
<u>Combined recirculating flow/ plug flow</u>	: Case D, Fig. 17
Total mass introduced into	: volume zones $k = 2$
Total mass extracted from	: top volume zones $k = 6$
Recirculation between	: volume zones $k = 2$ and bottom volume zones $k = 1$
Ratio of recirculating mass flow $\dot{M}_r$ to total mass flow $\dot{M}_0$	: 1

Figure 17. Total Mass and Fuel Mass Flows at Volume Zone Boundaries for Investigated Flow and Heat Release Pattern.

- Heat Release Pattern (fuel mass flow)

Well-stirred approach : Case A, Fig. 17
 Total heat release : uniform over furnace volume

However, radiating gas temperature is weighted with $(1-a)^*$ pseudo-adiabatic zone temperature and a^* exit temperature according to ref. 6)

Weighting factor a : 0.75

Plug flow approach : Case C, Fig. 17

Total heat release in : bottom volume zones
 $k = 1$

Combined recirculating flow/
 plug flow

: Case D, Fig. 17
 Total heat release in : volume zones $k = 2$

- Concentration of Species

Uniform distribution at values corresponding to complete

combustion p_{CO_2} : 0.074 bar

$p_{\text{H}_2\text{O}}$: 0.157 bar

p_{N_2} : 0.725 bar

p_{O_2} : 0.044 bar

- Transport Coefficients

Convective heat transfer coefficient at furnace walls (corresponding to ref. 6):

$$\alpha_I^* = \alpha \frac{2(T_I^2 + T_{s,I}^2)}{(T_I + T_{s,I})^2} \quad \text{with } \alpha : 0.0058 \text{ kW/m}^2\text{K}$$

2.4.1.4 Radiative Properties

- Radiative Properties of Wall Zones

Uniform total emissivity ϵ_I : 0.8

1 gray gas approach with uniform
 absorption coefficient K_a : 0.0893 1/m
 K_a corresponding to mean beam
 length L_m : 3.835 m
 and given gas composition at : 1631 K

2.4.1.5 Input Data Influencing Numerical Accuracy

● Beam Distribution Parameters

Total number n_v of volume cells : 192
 Number n_c of beams starting from
 volume cells : 96
 Total beam number n corresponding
 to n_v and n_c : 29184

● Beam Cutoff Factor a_0 : 0.001

2.4.2 Heat Transfer Predictions for the Sample Problem

The heat transfer calculations for the gas-fired furnace specified in 2.4.1 were carried out, all other input data being the same with three different approaches for the basic flow and heat release pattern; namely, a well-stirred approach, a plug flow approach, and a combined recirculating-flow/plug-flow approach. The latter approach was thought to be the most realistic one for the investigated boiler combustion chamber.

Figure 18 reveals the influence of the flow and heat-release pattern on the heat flux density computed for the furnace side walls. The straight line a corresponds to the present well-stirred analysis. This flux density compares well with the average heat flux density taken from the well-stirred analysis in ref. 6 for the same case (line b). Curve c represents the flux density for plug flow along the furnace and heat release in the bottom zones. Curve d, finally, shows the flux distribution for the most realistic case with a recirculating flow in the furnace bottom and heat release in the second lowest volume zone layer $k = 2$.

The corresponding computed distribution of volume zone temperatures are shown in Figure 19. A good agreement, expected from Figure 18, is found between the well-stirred gas temperature of the present analysis and the one taken from 6 (difference 3 K). Whereas the flux densities for the different

Figure 18. Influence of Flow and Heat Release Pattern on the Heat Flux Distribution at the Side Wall of a Methane Fired Boiler Combustion Chamber.

Temperature of
Volume Zones

Figure 19. Influence of Flow and Heat Release Pattern on the Temperature in a Methane-Fired Boiler Combustion Chamber.

flow pattern of Cases C and D have about the same peak value, the peak temperature of both cases differ by 70 K. The lower temperature peak for the recirculating flow (curve d) occurring in the heat-release zones $k = 2$ is obviously caused by the additional backflow of sensible heat into the bottom zones where it is partially radiated to the walls. In spite of the lower peak temperature, the furnace outlet temperature in Case D with recirculation has a higher value than in Case D with pure plug flow. This is not unexpected, since it is known, that the plug flow pattern, combined with heat release in the very beginning of a furnace, yields an upper limit of attainable furnace efficiency. The furnace efficiency η is closely related to the furnace outlet temperatures. Provided combustion is complete, η is given by

$$\eta = 1 - \frac{(\dot{M}_o c_p T)_{ex}}{\dot{Q}_o} \quad (46)$$

Values of η computed for the investigated cases are listed in Table 5.

Table 5. Furnace Efficiencies Computed with Different Assumptions of Flow Pattern

Case	Furnace Efficiency η
A Present well-stirred analysis	0.3034
B Value of well-stirred analysis in ref. 6	0.3005
C Pure plug flow	0.3184
D Combined recirculating flow/plug flow	0.3079

The relatively high value of η for the well-stirred assumption is due to the introduction of a effective radiating gas temperature as a weighted mean of the exit temperature (0.75) and a "pseudo" adiabatic flame temperature (0.25). The weighting factors 0.75 and 0.25, respectively, are suggested in ref. 6 for boiler combustion chambers.

3.0 CYLINDRICAL FURNACE MODEL

3.1 Introduction

With the exception of axisymmetric geometry, the cylindrical furnace model chosen as the second analytical tool is based on the same physical principles and model features as the rectangular furnace model described in the preceding chapter. At the current stage of development, only the main part, which handles the exchange of gray or non-gray radiation, is coded. However, the second part of the model, which delivers temperature distributions by means of total energy balances of a certain number of furnace zones, will be coded in close analogy to the rectangular counterpart.

3.2 Computation of Radiative Exchange in the Cylindrical Furnace with Special Regard of Axisymmetry

Because of the similarity between the radiation models for the rectangular furnace (see section 2.2) and for the cylindrical furnace--the latter one being also documented in^(4,5)--only the basic differences between the two models due to different geometric configuration or different stage of development are mentioned in the following.

The zones of the cylindrical furnace for which the radiative exchange calculation is carried out, are arranged in a cylindric polar co-ordinate system as, for instance, shown in Figure 20. The zones are annular in shape (Figure 21), the cross-sections of volume zones in the axial planes are rectangular. A constricted furnace outlet can be considered. The cartesian grid by which the zones are generated may be non-equidistant.

The radiative exchange between the ring zones is evaluated by the semi-stochastic method described in 2.2.1.

A ring zone is divided into nearly equally-sized segments or cells. In long furnaces, these cells are rather rectangular than cubic shaped. The center of the cells, defined as the geometric center of the cross-section in their axial symmetry plane, is chosen as the starting points of beams, the sum of which carry the energy flux initially emitted by the zone. The beams of each starting point are uniformly spread over the solid angle 4π for volume emission, or 2π for surface emission, according to the same formulae given in 2.2.1. However, because of axisymmetry, only a certain number of these beams has to be traced; namely, only beams from cells with center

Figure 20. Example of Zone Arrangement for the Cylindrical Furnace (sample problem 3.3.2).

Figure 21. Division of a Volume Zone Into Cells and Definition of Beam Angles in Furnace-Oriented z, r, θ Frame.

points in one r, z plane and from these, only the beams directed into one half of the furnace volume $\frac{\pi}{2} < \psi < \frac{3}{2}\pi$ as indicated in Figure 21. Symmetry is then accounted for by multiplying the initial energy fluxes of the traced beams by a factor $(2\pi/\Delta\theta) \cdot 2$, in which the term $(2\pi/\Delta)$ represents the number of cell segments along the perimeter with radius r_0 given by the cell center points. For instance, the energy flux of a beam starting from a volume cell has, according to eq. (3), originally the energy flux

$$(\Delta\dot{Q}_{e,I})_{\text{no sym}} = K_{a,I} \frac{\sigma}{\pi} T_I^4 \Delta z \Delta r r_0 \Delta\theta \Delta\Omega \quad (47)$$

with $\Delta z \Delta r_0 \Delta\theta$ as cell volume. However, because of symmetry considerations this energy flux is replaced by

$$\begin{aligned} \Delta\dot{Q}_{e,I} &= \frac{2\pi}{\Delta\theta} \cdot 2 \cdot (\Delta\dot{Q}_{e,I})_{\text{no sym}} \\ &= 4K_a \sigma T_I^4 \Delta z \Delta r r_0 \Delta\Omega, \end{aligned} \quad (48)$$

and only beams starting from one z, r plane into one half of the cylindrical furnace are considered. The handling of axisymmetry for beams starting from surface cells is similar.

The transformation of beam angles from a cell frame into a furnace-oriented frame is carried out in a similar way as in the rectangular case. Beam tracing itself, however, is more complicated since direct self-absorption can occur twice because of the annular zone shape. The path length Δs_J through the volume zone J is evaluated with the help of the following formulae (see also Figure 22):

$$\sin \psi > 0: \Delta s_z = \frac{z_p - z_0}{\sin \phi \sin \psi}, \quad (49a)$$

$$\sin \psi < 0: \Delta s_z = \frac{z_n - z_0}{\sin \phi \sin \psi}, \quad (49b)$$

$$\cos \phi > 0: \Delta s_r = \frac{-r_0 \cos \phi + \sqrt{r_0^2 \cos^2 \phi + (1 - \sin^2 \phi \sin^2 \psi)(r_p^2 - r_0^2)}}{1 - \sin^2 \phi \sin^2 \psi}, \quad (49c)$$

$$\cos \phi < 0: \Delta s_r = \frac{-r_0 \cos \phi - \sqrt{r_0^2 \cos^2 \phi + (1 - \sin^2 \phi \sin^2 \psi)(r_n^2 - r_0^2)}}{1 - \sin^2 \phi \sin^2 \psi}. \quad (49d)$$

z_0, r_0 are the co-ordinates of the starting point of a beam within an emitting zone or, alternatively, the co-ordinates of the beam entering the zone

Figure 22. Path Length ΔS_J of a Beam Within an Annular Volume Zone J

in question. z_p and z_n are the plane radial boundaries of the zone in positive and negative z -direction; similarly, r_p and r_n are the upper and lower cylindrical boundaries. The beam length Δs_J within the zone J is determined from:

$$\Delta s_J = \min(\Delta s_z, \Delta s_r) \quad . \quad (50)$$

From eqs. (49) and (50), indices of the newly entered zone are concluded. It has to be mentioned that the actual programming of beam tracing in the cylindric case differs from that in the rectangular case due to the convex curvature of the zones in the former case. However, each code is thought to have a good efficiency for the particular case.

Reflection of beams at surface zones is stochastically handled as described in Chapter 2. However, axisymmetry is considered by revolving the starting point of the reflected beams around the z -axis onto the z, r plane from which all beams are initially emitted.

The criterium for termination of beam tracing, embodied in the current program version, is very simple. The energy flux of a beam is neglected when it is reduced by attenuation to a certain fraction of its initial value. This criterium is non-conservative, and also not the most efficient one, since beams with low initial energy fluxes, which are unimportant for the radiative exchange, are traced with the same accuracy as high-energetic beams. Therefore, in future computations beam termination will be handled in a similar manner as described in Chapter 2.

One other major difference between both radiation models is that the cylindric model version does not make use of random shifting of volume-cell-oriented frames, a method which was used in Chapter 2 in order to reduce the systematic directional error in predicting total fluxes. However, this option can also be easily embodied in the current code.

As in the rectangular furnace, the computation of radiative exchange in the cylindric enclosure can alternatively be carried out for gray and non-gray radiation. In the latter case, the radiation characteristic is approximated by the sum of three weighted gray gases. Applications of the code, to a gray and a non-gray case are demonstrated in the next section.

3.3 Application of the Axisymmetric Radiation Model

As stated earlier, the cylindrical furnace model does not yet include total heat balances for the zones; thus, the following examples were carried out with prescribed zonal temperatures and represent, above all, verifications of the basic axisymmetric radiative exchange model.

3.3.1 Test Example for computation of Gray Radiation Exchange in a Long Cylindrical Furnace With Idealized Temperature Distribution

The input data for the test calculations are summarized below.

- Geometrical Data
 - Furnace shape : cylindrical
 - Furnace length : 10.5 m
 - Furnace diameter : 1.69 m
- Wall Temperature : 500°C
- Zoning of the Furnace : see Fig. 23
- Field Data
 - Prescribed gray gas temperature distribution : see Fig. 23
- Radiative Properties
 - Total emissivity ϵ of surface zones,
Cases A, B, C : 1.0
 - Case D : 0.5
 - Gray absorption coefficient K_a
of volume zones : 0.25 1/m
- Beam distribution parameters
 - Beams neglected when attenuated down to : 5%
 - Number of volume cells emitting from
z,r plane Cases A,B,C,D : 336 (56*6)
 - Number of beams emitted per volume
cell into one half of the furnace,
Cases A,D : 9 ($n_\phi=3, n_\psi/2=3$)[†]

[†]This differs from eq. (4), since $\Delta\Omega = \sin\phi\Delta\phi^*\Delta\psi^*$ with $\Delta\psi^* = \text{const}$ was used. Also, n_ψ for wall cells is computed from $n\psi/2 = \text{INT}(n\phi/2)$.

Figure 23. Zone Arrangement and Idealized Temperature Distribution of Test Example for Axisymmetric Radiation Model.

Case B	:	49 ($n_\phi=7, n_\psi/2=7$)
Case C	:	121 ($n_\phi=11, n_\psi/2=11$)
— Corresponding total number of traced beams, Cases A,D	:	3228
Case B	:	17892
Case C	:	44396

Heat flux predictions for the above idealized furnace, the temperature distribution in which coarsely resembles a long flame burning on the axis, are plotted in Figures 24 and 25. Figure 24 shows normalized heat flux densities computed at the circumferential furnace wall for three different total numbers of beams traced. The predictions are compared to results of another code of radiative exchange independently developed and based on so-called radiative exchange coefficients.⁽¹²⁾ It can be seen that, above a beam number of 18000, no essential gain in accuracy can be achieved any more. A beam number as small as 3000 already enables flux predictions with 90 percent accuracy. However, for more inhomogenous temperature distributions, an accurate resolution of the peak flux distribution might require the use of larger beam numbers.

In Figure 25, those computations are compared which were carried out for the two different surface emissivities $\epsilon = 1.0$ and $\epsilon = 0.5$. The differences between the predictions of the current code and those of ref. 12 are mainly due to the relatively small beam number in the former case (compare with Figure 24). The overall accuracy of the present heat flux predictions is higher in case of the lower emissivity $\epsilon = 0.5$ since here the systematic numerical error produced by discrete starting points and beam directions becomes less important. However, the stochastic handling of wall reflection causes some perceivable unevenness in the local flux distribution which was smooth for $\epsilon = 1$.

3.3.2 Computation of Radiative Transfer in a Cylindrical Furnace Fired With Heavy Fuel Oil.

The model input data for this case are based on boundary and inlet conditions of a flame trial carried out in an experimental, cylindrical, vertical, 1-MW furnace, operated at Stuttgart University.⁽⁵⁾

● Geometrical Data

Figure 24. Dependence of Predicted Heat Flux Distributions on Total Beam Number for Idealized Gray Axisymmetric Test Example.

Figure 25. Heat Flux Distribution Predicted With Different Surface Emissivities for Idealized Gray Axisymmetric Test Example.

- Furnace shape : cylindrical
- Furnace dimension
 - Diameter of combustion chamber : 1m
 - Length of cylindrical section of combustion chamber : 4m
- Smooth surface walls
- Fuel Type : heavy fuel oil
- Furnace Operational Data
 - Combustion chamber pressure : 1 bar
 - (— Thermal input : 0.8 MW)[†]
 - (— Fuel mass flow : 63 kg/h)
 - (— Excess air : 5%)
 - (— No air preheat)
 - Assumed temperature T_s of inner surface of water-cooled circumferential walls : 318 K
 - Temperature of front wall : 613 K
- Zoning of the Furnace : Fig. 20
 - Number of volume zones : 136
 - Number of surface zones : 34
- Field Data

The field data necessary for the radiative exchange calculation was taken from measurements. The representative value for the zone center point was won by interpolation; in regions near the burner, where no measurements were possible, zonal values were extrapolated from data.

 - Measured temperature field : Fig. 26a
 - Concentration of solids : Fig. 26b
 - H_2O , CO_2 , CO concentrations : see ref. 5

[†]Data in parentheses were not necessary for present radiation exchange calculation.

a) Measured Temperature Distribution (K)

b) Measured Concentration of Solids (mg/m^3 , wet)

Figure 26. Field Data Used for Radiative Exchange Calculation in Oil-Fired Furnace.

H ₂ O chamber outlet value	:	0.114 bar
CO ₂ chamber outlet value	:	0.130 bar

- Radiative Properties

- Emissivity of water-cooled surfaces and outlet zones : 0.95
- Emissivity of burner wall : 0.6
- Gas-soot radiation computed with approval of three weighted gray gases, coefficient of the approach according to : Table 4

- Beam distribution parameters :

- Total number n_v of volume cells : 36 ($n\phi=8$)[†]
- Number $n_c/2$ of beams emitted per volume cell into one half of the furnace : 540 (54*10)
- Corresponding total number of beams traced in three gray ranges : 3*20772
- Beams neglected when attenuated down to : 0.25%

Results of the radiative heat transfer computations carried out with the above input data are shown in Figure 27. The computed radiative heat fluxes incident at the circumferential sink walls (curve A) are compared with fluxes measured by an ellipsoidal radiometer and extrapolated to cool, clean inner surface conditions. (circles). Also shown in Figure 27 are the net heat flux densities measured calorimetrically in the twelve water-cooled sections (squares). Assuming cool inner surfaces and neglecting the small reflected fluxes, the difference between net heat fluxes and incident radiant fluxes are the convective heat fluxes. These fluxes, not accounted for by the current radiative exchange calculation, seem to have a maximum at a position of about 1.5m from the burner wall, which corresponds to the stagnation point of the outer recirculating flow in the experimental furnace.

[†] $n_{\psi}/2$ was computed from $n\psi/2(\phi^*) = 2 \text{INT } 0.5 \text{ INT } (\pi/\sin\phi^* \Delta\phi^*)$.

Figure 27. Heat Flux Distribution at the Circumferential Sink Walls of the Oil-Fired Combustion Chamber.

In order to investigate the importance of soot for the radiation from luminous oil flames, heat fluxes at the circumference were also calculated neglecting soot, all other conditions being the same (Figure 27, curve B). The maximum contribution of soot to the radiative transfer is found between 0.5 and 1m from the burner and amounts to 50 percent of the whole radiative flux at that position. Naturally, this value is only valid for the present study and it can be expected to vary in other cases depending on fuel type, furnace geometry, and operating conditions.

4.0 TWO-DIMENSIONAL FLAME MODEL

4.1 Introduction

A flame is defined as that part of a gas or furnace volume in which reactions between fuel and oxygen are taking place. The flame envelope which may be fluctuating and also torn is approximately given by the locations where rapid flame reactions are practically completed with release of most of the chemically-bound heat. One task of the present project is to determine how exact this flame geometry and local temperature and concentration distributions have to be specified in order to allow reasonable assessment of overall and local heat transfer in industrial furnaces.

In order to solve this problem, the furnace models of the preceding sections could be applied with increasing fineness of zones and with zonal flow and concentration data taken from estimated or measured patterns. However, despite the fact that a large amount of specially-prepared input data is necessary, measured full-scale data are seldom available, and the finer the zoning, the more uncertain the estimation of zonal values.

For this reason, use will also be made of a mathematical flame model which allows generation of local flow and concentration data from first principles with a limited number of input data corresponding to actual boundary conditions of a furnace. The flame model is restricted to axi-symmetry. Thus, it will be coupled, first of all, with the cylindrical furnace model.

Despite the restriction to axi-symmetry, the chosen flame model is, like the chemical reaction and physical transport processes in a real flame, very complex and is constructed from a number of various interacting sub-models. Because of this complexity the following description of the flame model, which is also documented elsewhere^(2,3,13-15), is by no means comprehensive. However, in addition to the description, a new application of the model to a recent coal flame trial⁽¹⁶⁾ will be shown, which allows a better assessment of the capabilities and shortcomings of the model.

4.2 Description of the Flame Model

The most important sub-models of the model, which is primarily developed for predictions of pulverized-fuel flames, are:

- A model of convective transport including approaches of turbulent exchange and two-phase flow.

- Models for homogenous and heterogeneous flame reactions with a particle combustion model.
- A radiative exchange model with approximation of particle and gas radiation.
- Model of boundary conditions of actually operated furnaces.

4.2.1 Model of Convective Transport

The model of convective transport in the flame is based on the laws of conservation of mass, momentum, matter and energy. The laws are applied to non-moving differential control volumes ("Eulerian approach") and result in a system of so-called convective transport equations. The assumed axis-symmetry allows the use of a stream-function ψ and the vorticity component ω_θ as dependent variables. Other variables of the transport equations are mass concentrations m_j of chemical species j , properties related to m_j (e.g., mixture fraction f , etc.), bulk enthalpy h and turbulent properties of the flow like the turbulent kinetic energy k and the square of vorticity fluctuations W . In principle, the tangential velocity v_θ can also be a dependent variable; however, applications of the model to p.f. flames are at present restricted to non-swirling cases.

The transport equations are written for the steady state and cast in the general form of eq. (51):

$$a_\phi \left[\frac{\partial}{\partial z} \left(\phi \frac{\partial \psi}{\partial r} \right) - \frac{\partial}{\partial r} \left(\phi \frac{\partial \psi}{\partial z} \right) \right] - \frac{\partial}{\partial z} \left[r b_\phi \frac{\partial}{\partial z} (c_\phi \phi) \right] - \frac{\partial}{\partial r} \left[r b_\phi \frac{\partial}{\partial r} (c_\phi \phi) \right] - r d_\phi = 0 \quad (51)$$

ϕ is any of the above mentioned dependent variables (however, in case of ω_θ : $\phi \equiv \omega_\theta/r$, and in case of v_θ : $\phi \equiv v_\theta r$), which is transported by convection and diffusion. a_ϕ , b_ϕ , and c_ϕ are the corresponding transport coefficients. The last term in eq. 51, namely, d_ϕ represents the source of the property ϕ . The transport equations are written in the fully-elliptic form, thus they account for flow recirculation which is found for almost all practical flame/furnace configurations.

Because of this elliptic nature, the finite difference solution of the transport equations (51) has to be carried out iteratively. The solution

algorithm adopted for the present model was elaborated by Spalding and co-workers⁽¹⁷⁾ and is basically a Gauss-Seidel method with under-relaxation of some of the dependent variables and transport coefficients.

The dependent flame variables mentioned above are understood as time-averaged quantities. However, in a turbulent flow field, which is common for all industrial furnaces, the local distribution of time averaged variables is strongly influenced by turbulence itself. Turbulence acts on the mean quantities like additional diffusional fluxes. In the present model, these turbulent fluxes are, in analogy to the laminar case, related to gradients of the mean values of the variables. As a constant of proportionality of turbulent momentum exchange, a turbulent viscosity η_t is introduced and other turbulent exchange coefficients are deducted from η_t by means of turbulent Schmidt-Prandtl numbers. The assessment of η_t itself is carried out with a two-equation model of turbulence, namely, the so-called k-W model⁽¹⁸⁾ according to eq. 51:

$$\eta_t = \rho k W^{-1/2} \quad (52)$$

k is the time-averaged value of the specific kinetic turbulence energy, and W is the mean value of the square of vorticity fluctuations. For both k and W, approximate transport equations of form of eq. (51) are simultaneously solved together with the other transport equations. The use of the turbulence model requires input of some empirical constants, namely, turbulent Prandtl-Schmidt numbers and four constants associated with generation and dissipation of k and W. The constants currently used were checked by comparison with experimental data from enclosed air jets and have been proved to produce reliable predictions for a variety of non-swirling flows.⁽¹⁹⁾

When pulverized fuel flames are investigated, two-phase flow has to be considered. A detailed mathematical model of that flow should include momentum balances of both phases linked by drag forces at the particles. However, the assumption is made that there is no relative convective velocity between solids and gases at every point in the flow field. This greatly facilitates the computation, since, by assigning turbulent exchange coefficients to them, particle mass concentrations can be evaluated with an Eulerian approach in the same manner as mass concentrations of gaseous species. The main difference between single- and two-phase flow computation is that in the latter

case, the gas density ρ_g is replaced by the mixture density ρ_m in all transport equations. ρ_m is calculated from eq. (53).

$$\rho_m = \rho_g + \rho_s = \frac{p}{RT \sum_g \frac{m_{j,g}}{M_j}} \quad (53)$$

ρ_s is the density of the particle cloud. The summation in (53) is carried out for all gaseous components of the mixture.

4.2.2 Combustion Model for High-Volatile Coal Flames

The combustion models which were tested with earlier-developed versions of the flame program were related to

- mixing controlled turbulent gas flames, and
- predominantly kinetically-controlled anthracite p.f. flames.

These model versions are documented elsewhere.⁽³⁾ In the following, a more recently developed combustion model for high-volatile coal flames⁽¹⁵⁾ will be described, which originated from a coupling of the two codes mentioned above.

The combustion of the high-volatile coal is assumed to take place in the five global reaction steps listed below:

The first reaction (eq. 54-1) of this scheme describes the finite rate decomposition process of the coal into fixed carbon and volatiles. The latter are presumed to be composed of C_nH_m , CO, H_2O , CO_2 , and N_2 . The actual composition of the volatiles, i.e., the stoichiometric coefficients in (54-1), are taken from available measurements (e.g., ref. 20) and are made consistent with the proximate and ultimate analyses of the investigated coals.

The second equation of the above scheme is the heterogeneous char reaction with oxygen from the combustion air. This reaction has a finite rate, too. The hydrocarbons of the volatiles are supposed to react partially to CO and H_2O at an infinite rate (eq. 54-3), whereas the following oxidation of CO which also originates from char burning has again a finite rate. Finally, it is assumed that water-gas equilibrium, according to eq. (54-5), is encountered throughout the flame.

In order to combine the reaction scheme given by eq. (54) with a physical model of particle devolatilization and burn-out it is, first of all, assumed that coal and mineral particles are always separate (i.e., no inclusion of mineral matter in a coal particle).

The devolatilization process itself is modeled in a simple, but very abstract way. Provided its devolatilization is initialized, each single coal particle is instantaneously converted into a char particle with release of its volatiles as expressed by eq. (54-1). However, if the cloud of particles initiating devolatilization shall occur for different particles at different times in such way that the mass conversion rate (devolatilization rate) of coal particles is of first order with respect to the mass of non-decomposed particles:

$$\frac{dm_{\text{Coal}}}{dt} = -k_1 \left[m_{\text{Coal}} - C_1 (m_{\text{Coal}})_p f \right] \quad \text{with } k_1 = A_1 \exp(-E_1/RT_s) \quad (55)$$

The temperature dependence of the rate coefficient is formulated by an Arrhenius type expression. The second term in eq. (55) accounts for the fact that, depending on the coefficient C_1 , the final decomposition is not complete, even at the end of a flame. With exception of C_1 , currently chosen values for the rate constants A_1 and E_1 for devolatilization are those recommended by Field et al.⁽²⁰⁾ (see also section 4.3).

Since it is assumed that the decomposition rate (eq. 55) does not depend on size, the coal particles are not classified and the mass concentration m_{coal} is evaluated by one equation only.

However, char particles generated by decomposition are distributed among five diameter classes according to the initial size distribution. Principally, at this step swelling could be considered, but it is neglected at present. The burning rate of the char particles in the five size classes is supposed to be of first order with respect to O_2 according to:

$$r_s = k_2 p_{O_2} = 1 / \left[1/k_s + 1/k_d(x_\ell) \right] p_{O_2} \quad \text{kg}_c/\text{m}^2\text{s} \quad (56)$$

with $k_s = A_2 \exp(-E_2/RT_s)$.

r_s is referred to the outer surface area of the ℓ th size fraction. It can be seen from eq. (56) that this rate can either be controlled by chemical surface reaction or by diffusion of oxygen through the boundary layer around the particle. The diffusional rate coefficient k_d depends on the class diameter x_ℓ . Values chosen for surface reaction rate coefficients of char burning are also those of ref. 20. Although there is a program option for computing char particle temperatures T_s from a heat balance at a particle of mean size, the sample problem shown later was obtained with the assumption that T_s everywhere equals the gas temperature.

In order to evaluate the decrease of mass in a size class due to burning (eq. 56) the surface area of that class must be determined. For this purpose, it is assumed that the particles burn at constant density with decreasing diameter. In modeling this burning mechanism, particles are allowed to change from one size class into the next lower one.

The expression for the overall reaction rate of CO-oxidation, which is also dependent on H_2O , is taken from ref. 21. However, the value chosen for the frequency factor is smaller than that in ref. 21. Thus, unmixedness, otherwise neglected, is roughly taken into account.

The reaction model described above requires mass balances of 13 different species, including char species of five diameter classes and one inert fraction of mineral matter. The corresponding number of differential equations of type of eq. 51 to be solved would be 12. However, since it is assumed that the turbulent Schmidt numbers of all species are equal, and since two of the reactions are purely mixing controlled, this number was reduced to 8 by introducing combined variables such as the mixture fraction f (for more detail, see refs. 3 and 15). Thereby, a saving of computing time and increase in stability of the solution algorithm could be achieved.

4.2.3 Computation of Flame Radiation

The radiative transport in the flame and to the furnace walls is approximated either by a 4-flux model or alternatively by a combination of a 2-flux model for the radial directions and a diffusion approach for the axial exchange.

The flux models are based on the assumption that the angular distribution of the radiant intensity is constant for parts of the solid angle associated with the positive and negative co-ordinate directions. The integration of the transport equation of directional intensity over these solid angles leads to ordinary differential equations for the radiative heat flux densities in the specified directions. The flux equations are solved grid-linewise by a matrix inversion technique. The resulting heat flux densities are used to evaluate the radiative source term in the convective transport equation of enthalpy. New radiative heat fluxes are computed for each iteration cycle of the Gauss-Seidel algorithm of convective transport.

In an optical thick medium (i.e., for large values of the product : concentration x path length), radiation exchange can at best be expressed as a diffusion process as shown for axial exchange in eq. (57).

$$\dot{p}_z = -(4/3) \frac{1}{K_a} \frac{dE}{dz} \quad (57)$$

K_a in (57) is the absorption coefficient and E the local black emissive power. High optical thickness is found in axial directions in the beginning of a pulverized fuel jet. Since radiative exchange in this part is important for ignition the axial diffusion approximation was chosen, although, in other furnace regions, this approach is more approximate than a flux model.

The radiative properties of the suspension are modeled in the following way. The radiation of coal, char, and ash particles is assumed to be gray. A uniform value of 0.85 is assigned to the absorption efficiency factor of these particles. Scattering in all except forward directions is neglected. Since it is uncertain how the specific surface area of ash particles depends on burn-out, this area is assumed to be constant and it is specified as input data.

Recently, soot radiation was also included in the heat transfer model. For a given temperature, this radiation is presumed to be gray. The soot concentration, necessary to evaluate the corresponding absorption coefficient, is correlated to the CO formation from partially burnt hydrocarbons of the volatiles according to an empirical relationship found for heavy fuel oil flames.

The radiation of the combustion gases CO_2 and H_2O is modeled with the weighted sum of one gray and one "clear" gas. However, since the radiation of solids exceeds the gas radiation, the computation of radiative exchange is simplified by supposing that the gaseous components absorb radiation in the whole frequency spectrum. Furthermore, local gas and particle temperatures are considered to be the same, at least for the sample problem shown below.

4.2.4 Modeling of Heat Transfer Boundary Conditions

In the past, the mathematical flame model was mainly applied to pilot-scale flames produced in experimental furnaces of the International Flame Research Foundation (IFRF). The flames of the sample problem in section 4.3 were also investigated in one of the furnaces. From the modeling point of view, the IFRF furnaces display complicated boundary conditions, especially when a 2D model like the present one is used to predict their performance. Difficulties arise for three reasons:

- The IFRF furnaces do not have a circular cross-section.
- The main heat sinks are water-cooled tubes introduced in front of refractory walls.
- The arrangement of heat sinks is non-symmetrical with respect to the furnace axis.

A considerable part of the flame program is spent for a reasonable modeling of boundary conditions for radiative and convective heat transfer under these circumstances.

The real combustion chamber is replaced by an equivalent cylinder of the same mean radiation beam length, which by coincidence, yields a diameter close to the hydraulic one. The calculation of heat transfer to the non-symmetrical heat sinks of complicated configuration is approximated by

effective wall temperatures for radiation and convection, effective emissivities and effective heat transfer coefficients (see also ref. 22).

The model of heat transfer to the heat sinks allows to predict the inner surface temperatures of the refractory walls. Besides this, it can be used to investigate the effect of ash deposit layers covering the cooling tubes on the overall and local heat transfer in the furnace and on the flame behavior.

4.3 Application of the Flame Model to Two Long p.f. Flames

The flame model was recently applied to predict two flames of a pulverized-coal trial (LCF trial) carried out by the IFRF for EPA under subcontract from EER.⁽¹⁶⁾ The main purpose of the trial was to supply detailed data of long, non-swirling p.f. flames for the characterization of pollutant formation. The investigated flames were produced with a double concentric burner. The fuel was a high-volatile bituminous coal, each flame had a total thermal input of about 2.1 MW and the nominal excess air was 10 percent. The two flames for which the following predictions were carried out differed by the ratio v_s/v_p of secondary air to primary transport air velocity and by the primary air amount, i.e., the particle loading of the fuel jet. One flame, flame A1, had a velocity ratio of 1.15 and a primary air amount of 11 percent; the other flame, B1, was produced with a velocity ratio of 0.24 and a primary air amount of 18.6 percent.

4.3.1 Important input Data

The most important data used to prepare and run the flame program for the mentioned flames are listed below.

● Geometrical Data

- Furnace dimensions : $\approx 2 \times 2 \times 6.25\text{m}$
- Furnace cross-section : 3.85m^2
- Burner diameters

	Primary m	Inner Sec. m	Outer Sec. m
Flame A1	0.0703	0.0763	0.260
Flame B1	0.0703	0.0763	0.399
- Arrangement of water-cooled tubes (see also ref. 16)

First half of furnace	: 6 tubes on roof, 6 tubes on bottom
Second half	: 6 double loops around cross-section
— Outer diameter of tubes	: 0.033m
● Fuel Data	: Bituminous coal
— Proximate analysis	
Fixed C (+S)	: 0.6537 kg/kg _{daf}
Volatile matter	: 0.3463 "
Ash	: 0.0823 "
Moisture	: 0.0221 "
— Modeled composition of volatiles	
"CH _{3.38} "	: 0.1823 "
CO	: 0.0372 "
H ₂ O	: 0.0948 "
CO ₂	: 0.0199 "
N ₂	: 0.0121 "
— Lower calorific value	
Fixed carbon (+S)	: 33587 kJ/kg _{C+S}
"CH _{3.38} "	: 61545 kJ/kg _{CH3.38}
CO	: 10130 kJ/kg _{CO}
Total	: 33550 kJ/kg _{daf}
— Size distribution of coal particles (ash free)	:
1 - 3 μm	: 0.022 kg/kg
3 - 10 "	: 0.070 "
10 - 31 "	: 0.220 "
31 - 96 "	: 0.458 "
96 - 300 "	: 0.230 "
— Spec. surface area of ash particles assumed:	: 375 m ² /kg
● Furnace Operational Data	A1 B1
— Coal mass flow (kg _{dry} /h)	: 207.8 207.8

●	Furnace Operational Data (Continued)	A1	B1
—	Primary air (half-sat. at 10°C) + fuel moisture (kg _{wet} /h)	: 260.2	439.9
—	Secondary air (half-sat. at 10°C) (kg _{wet} /h)	: 2072.0	1907.4
—	Primary temperature (°C)	: 150	190
—	Secondary temperature (°C)	: 490	500
—	Total heat extraction deducted from chimney gas temperature (ca. 3% unburnt) (kW)	: 1025	1032
—	Tube deposit layer surface tempera- ture to match total heat extraction	: 700	500
—	Static pressure	: 1 bar	
●	Convective Heat Transfer Coefficients		
—	Refractories (assumed)	: 0.0058 kW/m ²	
—	Tubes (extrapolated from model measure- ments)	: Varying along the/ furnace from 0.015 kW/m ² tube surface to 0.030 kW/m ²	
●	<u>Assumed Heat Sink Properties</u>		
—	Conductivity of refractories/ wall thickness λ/s	: 0.0020 kW/m ²	
—	Emissivity of refractory surface	: 0.5	
—	Emissivity of surface of tube deposits	: 0.5	
●	Some Important Physical Parameters of Field Calculations		
—	Constants of turbulence model	: From Roberts, cited in ref. 19	
—	Turbulent Schmidt number	: 1.0	
—	Turbulent Prandtl numbers	: 0.7	
—	Density of coal material (ash free)	: 1300 kg/m ³	
—	Density of char material	: 900 kg/m ³ +	

[†]The exact value corresponding to density of coal, proximate analysis, complete devolatilization, and no change in size would be 850 kg/m³.

- Reaction rate coefficients
 - Devolatilization (eq. 54-1) : $E_1 = 73160 \text{ kJ/kmole}$
 $A_1 = 1.15 \cdot 10^5 \text{ 1/s}$
 $C_1 = 0.01$
 - Surface reaction of char (eq. 54-2) : $E_2 = 149900 \text{ kJ/kmole}$
 $A_2 = 8.71 \cdot 10^4 \text{ kg}_c/\text{m}^2 \text{ bar}_{\text{O}_2}$
 - CO-oxidation (eq. 54-4) : See ref. 21; however,
 $A_{f,4} = 0.4 \cdot 10^{10} (\text{m}^3\text{K/kmole})^{0.75} \text{ 1/s}$
- Grid for Finite-Difference Computation : 20*20 perpendicular non-equidistant grid-lines

4.3.2 Results of Flame Modeling

In Figures 28-33, flame variables predicted with the above input data are compared to corresponding measured values obtained in a horizontal plane through the flame axis.

The flow pattern of flame A1 is plotted in Figure 28. The recirculation zone extends along the whole furnace. Computed and measured position and strength of the core of this zone are in good agreement. The measured distortion of the flow pattern near the burner wall is probably due to 3D effects (buoyancy, secondary flow).

Overall fair agreement is also found, when calculated and measured isotherms of the investigated flames are compared (Figure 29-30). However, a closer study of the temperature distribution and other variables reveals, for each flame, special differences between predicted and experimental values.

The real flame A1 showed a stronger mixing in the burner region than the modeled one. Further, ignition was observed to occur in a thin fluctuating layer at the edge of the primary pipe. Both strong mixing and earlier ignition are responsible that the actual temperature increase of the double-concentric jet exceeds the predicted one (Figure 29). Too weak mixing is probably computed for two reasons:

- Too low values assigned to unknown turbulent quantities (turbulent kinetic energy, mixing length) at the burner inlet.

Figure 28. Comparison of Calculated and Measured Stream-Lines for Flame A1 of the LCF Trials.

Figure 29. Comparison of Calculated and Measured Isotherms ($^{\circ}\text{C}$) for Flame A1 of the LCF Trials.

Figure 30. Comparison of Calculated and Measured Isotherms ($^{\circ}\text{C}$) for Flame B1 of the LCF Trials.

Figure 31

Flame A1
Burnout of Solids on Flame Axis

Figure 32

Figure 33

- A too-small number of radial grid-lines to account for flow separation at the primary nozzle edge.

With respect to flame B1, differences in the temperature distribution arise from the observed fact that the low momentum secondary air jet is partially deflected into the recirculation zone by "3D" aerodynamic or buoyancy forces, thus cooling this region down (Figure 30). The predicted higher temperature of the recirculating zone causes earlier ignition of the model flame. Similar to the measurements, the numerical experiment showed that the position of the ignition zone of flame B1 was very sensitive to the recirculating gas and adjacent wall temperatures. The ignition zone moved downstream when these temperatures were lowered.

The predictions reflect one principal difference of the measured behavior of flames A1 and B1 correctly; namely, that ignition of the higher loaded fuel jet A1 occurs at the jet edges, whereas fuel jet B1 ignites on the axis. This can clearly be seen from a comparison of the radial temperature profiles of both flames at the same axial distance 1.5m (Figure 31).

Figure 32 and 33, finally, show the progress of devolatilization (curves a), heterogeneous reaction (curves c) and removal of total combustibles from solids (curve b) along the flame axis.

Predicted poor mixing in flame A1 is responsible for the fact that O_2 supply on the axis of the model flame is restricted. The available oxygen is consumed by the rapid burning of volatiles. The consequent lack of oxygen delays the heterogeneous reaction considerably in comparison to the measurements (Figure 32).

For flame B1, the predicted burnout of solids starts too early corresponding to the shorter ignition distance which was also observed from the temperature field (Figure 33). However, the general agreement between predicted and measured axial burnout is better than for flame A1, since the predictions do not show a lack of O_2 in the B1 case.

The predicted devolatilization rate in both flames seems too high after a certain amount of volatiles has been released. The model can surely be improved by a two-step decomposition with the second step slow. This would also lower the predicted peak temperatures which at present and in earlier flame computations were found to exceed the measured ones by about $150^{\circ}C$. Consideration of unmixedness is further envisaged as model improvement.

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