MODELLING THE COMBUSTION CHAMBER OF AN ALUMINIUM CASTING FURNACE: A METHODOLOGY

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Abstract

Mathematical modelling of the phenomena occurring in a combustion chamber is a very difficult task. Recently, computational methods have been developed allowing the simulation of all the processes involved in a more elaborate and reliable manner than ever before. These methods however often present weaknesses originating from their lack of generality and prohibitive computation time. Our aim was to come up with a technique that could be applied to rectangular furnaces of any size and characteristics, and that would require a reasonable computation time. The technique is based on combining the PHOENICS code (used for velocity and combustion fields) with a new radiation method, the so-called imaginary planes method. Results are presented for an aluminium melter/holder furnace. Comparison between the imaginary planes method and the zone method illustrates the excellent agreement obtained for the radiative transfer. The technique used for the coupling of PHOENICS with the radiative part is explained. Provisions are made to take care of the unsteady state regime often encountered in such furnaces where several different operations are performed in a row. The simulation of a transient operation is presented and it is found that a single determination of the velocity pattern on the basis of a steady state assumption is sufficient to simulate adequately time dependent gas temperature and heat flux distributions.

Introduction

The efficiency of an aluminium casting furnace of the melter/holder type is generally very low (~30%) and quite a few plants have turned to mathematical modelling in an attempt to find the best operating conditions or even the best geometry. These furnaces have essentially two parts: a combustion chamber and a bottom section where the metal melts or is simply kept at the liquid state. A well structured mathematical model should be able to simulate adequately the behaviour of each of these parts as well as the link between them. This is a difficult task since both parts are highly complex. In the combustion chamber, kinetics of the combustion reaction, velocity distribution and radiation heat transfer are to be coupled, whereas, in the metal part, melting of the solid, conduction heat transfer, natural and forced convection and velocity distribution are to be solved simultaneously. Once these are adequately simulated, one still has to devise a convenient interface between the gas and the solid. Moreover, since steady state is very seldom encountered in these types

of furnaces, owing to the numerous operational procedures to be performed (alloying, skimming, high fire heating, low fire heating, mixing, fluxing) transient numerical procedures are to be used.

All these phenomena can nowadays be modelled interactively with up-to-date numerical techniques. However, one has to bear in mind that the computation time is a very important variable and that it can rapidly become prohibitive. For instance, methods to solve the melting of a solid associated with natural convection in the melt are known but they are very time-consuming (Voller, 1987). The same can be said about the phenomena which occur in the combustion chamber. Radiation for example is a very complex heat transfer mode and, when coupled with the solution of motion and combustion kinetics equations, it can become very demanding in computation time, especially in transient processes when the coupled code is called for again and again. This is a very accurate problem and it stresses the necessity of working out simplified methods.

This paper will focus on the combustion chamber of a melter/holder furnace. It is part of an ongoing project aimed at developing a general mathematical model of such a furnace. The work is conducted in cooperation with Alcan International Ltd. A *3D* version of the so-called imaginary planes method for radiative transfer will first be presented. The technique previously applied for *2D* problems (CHARETTE et al., 1988) is being extended to a more general case. The reduced computation time associated with this method allows complex problems to be treated without affecting the accuracy of the results compared to the zone method. Results obtained by coupling this new technique with the commercial code PHOENICS (for the solution of the Navier-Stokes and combustion equations) will then be presented and discussed for the case of a transient process.

The 3D imaginary planes method (IPM)

Various numerical methods have been traditionally used to describe radiation in furnaces. Among others, zone, Monte Carlo, flux and discrete transfer methods may be cited (KOCAEFE et al., 1987b). A new technique, the imaginary planes method, has drawn attention recently owing to its very interesting features (LAROUCHE et al., 1986). The original idea was set forth by STRÖM (1980). The method combines reliability and low computation time. As in most of the other techniques, the furnace is divided into volume and surface zones, however the particularity of the IPM lies in the fact that each volume zone has a direct view only of its own boundaries, thus being, in a sense, self-confined. This aspect is the main feature of the method since it reduces considerably the number of interchange areas to be calculated. The

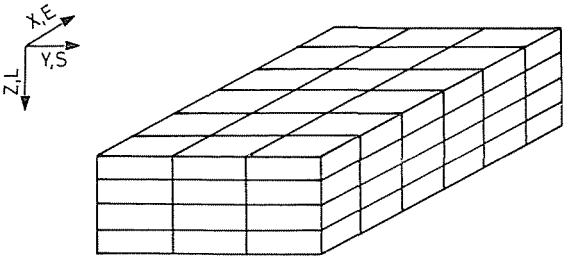

Fig. 1. Subdivided schematic combustion chamber

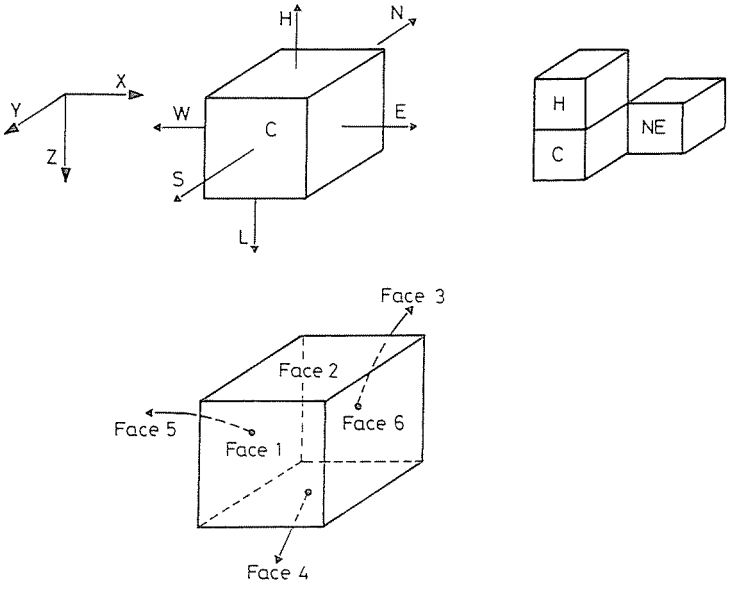

Fig. 2. Identification of the boundaries and immediate neighbours of a given volume zone C

boundaries are of two types: (a) those which are part of the chamber wall (referred to as real surfaces), and (b) imaginary planes which separate the volume zones. The adjacent volume zones are linked through radiative heat fluxes crossing the imaginary planes, providing an indirect interaction between all the zones as opposed to the direct interaction in the zone method.

Let Figure 1 represent an idealized rectangular furnace that has to be modelled in *3D* for radiative exchange. The identification of the boundaries (by numbers) and immediate neighbours (by letters) for a given volume zone *C* is given in Figure 2. If zone *C* is surrounded by immediate neighbours that are all volume zones, all its boundaries are imaginary planes for which the

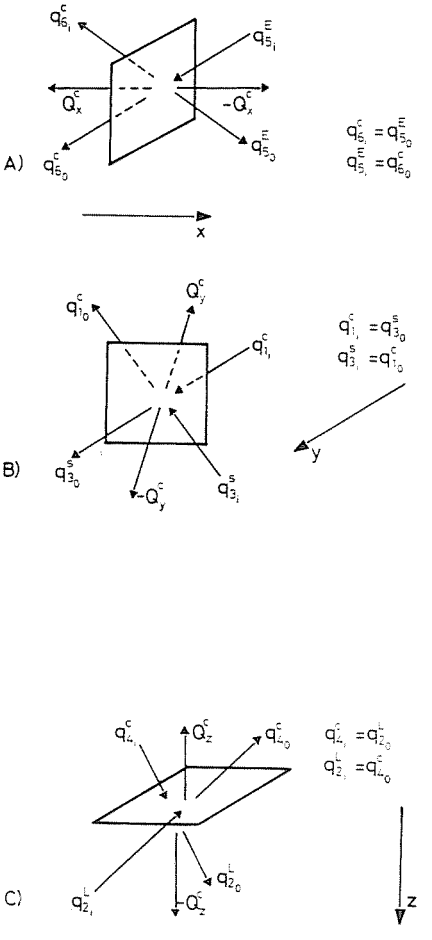

Fig. 3. Heat balances on imaginary planes in X, U and Z directions

representative heat balances are explained in Figure 3. The subscripts i and o stand respectively for incident and emerging, Q is the net heat (in watts) taken as positive in the inward direction of zone C. The linking principle between adjacent volume zones is that incident flux on a given imaginary plane coming from volume C is equal to the emerging flux from that same plane but directed towards the neighbouring volume (see Fig. 3). Because of space limitations, only the basic mathematical development will be given here. A more detailed presentation will appear in LAROUCHE (1988).

For a given imaginary plane k, the heat balance takes the form:

$$Q_k^C = (q_{k_o}^C - q_{k_i}^C)A_k^C \tag{1}$$

where $q^C_{k_o}$ is the outflowing flux emerging from imaginary plane k into volume zone C [W/m²]

$q^C_{k_i}$ is the inflowing flux impinging on imaginary plane k from volume zone C [W/m²]

A_k is the area of the given imaginary plane [m²].

By applying the fundamental equations of radiation heat transfer to a one-zone volume, the following relations can be found for imaginary and real surfaces if the gas medium is gray:

$$\sum_{j=1}^{6} b_{kj} q_{j_o} = D_k \quad k = 1, \ldots, 6 \quad \text{(six boundary surfaces)} \tag{2}$$

where b_{kj} and D_k are defined as follows:

$$b_{kj} = \begin{cases} \delta_{kj} - (1 - \varepsilon_k)\, \overline{s_j s_k}/A_k & \text{for a real surface} \\ \delta_{kj} - \overline{s_j s_k}/A_k & \text{for an imaginary plane} \end{cases} \tag{3}$$

$$D_k = \begin{cases} \varepsilon_k E_k + (1 - \varepsilon_k)\, E_g \overline{g s_k}/A_k & \text{for a real surface} \\ Q_k/A_k + E_g \overline{g s_k}/A_k & \text{for an imaginary plane} \end{cases} \tag{4}$$

δ being the Kronecker delta, ε_k the emissivity of surface k, $\overline{s_j s_k}$ the direct interchange area between real surfaces j and k, E_g and E_k the black emissive powers of the gas and surface k respectively, $\overline{g s_k}$ the direct interchange area between the gas and surface k.

The inversion of equation system (2) gives:

$$q_{k_o} = \sum_{j=1}^{6} B_{kj} D_j \quad k = 1, \ldots, 6 \tag{5}$$

where $B = b^{-1}$.

Equation (5) cannot be used directly since D is a function of the net heat Q which is sought for. The missing link is found through Equation (1) combined with the coupling equations between adjacent volumes given on Figure 3. One can obtain for the three coordinate directions:

$$\frac{Q^C_x}{A^C_x} = q^C_{6_o} - q^E_{5_o} \tag{6}$$

$$\frac{Q^C_y}{A^C_y} = q^C_{1_o} - q^S_{3_o} \tag{7}$$

$$\frac{Q^C_z}{A^C_z} = q^C_{4_o} - q^L_{2_o}. \tag{8}$$

By introducing (5) into (6), the following equation is obtained for the X-direction:

$$\frac{1}{A_x}[Q_x^W(B_{65}^C) + Q_x^C(1 - B_{66}^C - B_{55}^E) + Q_x^E(B_{56}^E)] +$$
$$+ \frac{1}{A_y}[Q_y^N(B_{63}^C) + Q_y^C(-B_{61}^C) + Q_y^{NE}(-B_{53}^E) + Q_y^E(B_{51}^E)] +$$
$$+ \frac{1}{A_z}[Q_Z^H(B_{62}^C) + Q_Z^C(-B_{64}^C) + Q_Z^{HE}(-B_{52}^E) + Q_Z^E(B_{54}^E)] =$$
$$= \sum_{j=1}^{6} B_{6j}^C\left(\varepsilon_j E_j^C + \frac{(1-\varepsilon_j)E_g\overline{gs}_j^C}{A_j}\right) -$$
$$- \sum_{j=1}^{6} B_{5j}^E\left(\varepsilon_j E_j^E + \frac{(1-\varepsilon_j)E_g\overline{gs}_j^E}{A_j}\right). \tag{9}$$

Similar equations are obtained for the Y and Z directions by introducing (5) into (7) and (8).

Let L, M and N be the number of volume zones in directions X, Y and Z respectively. Then the total number of imaginary planes [equal to the total of unknowns in equations of type (9)] is equal to:

$$(L-1)MN + (M-1)LN + (N-1)LM$$

and the Q values are found through a banded matrix system of that dimension represented by:

$$[\mathbb{BM}]\{Q\} = \{\mathbb{C}\} \tag{10}$$

where matrix $[\mathbb{BM}]$ contains the interchange areas and vector $\{\mathbb{C}\}$ the emissive powers of gases and surfaces. It is to be noted here that Equation (9) is written in a general form where a given volume zone C might be surrounded by either six volume zones or six surface zones. In programming, some of the terms are dropped according to the particular locations of the zones. Once the Q's are known, these can be introduced into (5) to yield the emergent fluxes at real surfaces k which in turn are used to calculate the net fluxes at the same real surfaces by:

$$q_k = \frac{\varepsilon_k}{1-\varepsilon_k}(E_k - q_{k_0}). \tag{11}$$

If the temperature field is unknown a priori, then heat balances are written for both the volume and the surface zones:

for a gas zone:

$$Q_{COMB}^C + \sum_{\substack{\text{real}\\ \text{surfaces}}} A_k q_k^C + h_{CONV}^C A_k(T_k^C - T_g^C) + (Q_x^C - Q_x^W) +$$
$$+ (Q_y^C - Q_y^N) + (Q_Z^C - Q_Z^H) + \Delta H_{ga}^C = 0 \tag{12}$$

where Q^C_{COMB}: the heat generated by combustion in volume C

h^C_{CONV}: the heat transfer coefficient between real surface k (of temperature T^C_k) and the adjacent volume zone C (of temperature T^C_g).

ΔH^C_{gas}: the enthalpy variation of the gas through the given volume zone C.

$$A_k q^C_k + h^C_{CONV} A_k (T^C_k - T^C_g) + U A_k (T^C_k - T_{AMB}) = 0 \tag{13}$$

where U: the overall heat transfer coefficient between surface temperature T^C_k and ambient temperature T^C_{AMB}.

An iterative procedure is started by assuming a temperature field which enables to solve successively Equations (10), (5) and (11). Nonlinear equations (12) and (13) are then solved by the Newton—Raphson multivariable technique. The method yields values of ΔT which are then used to update the temperature field and the iterative loop is resumed until successive values of the temperature field fall into an acceptable margin:

$$\{\Delta \mathbf{T}\} = [J]^{-1}\{-\mathbf{F}\} \tag{14}$$

where $\{\Delta \mathbf{T}\}$: the temperature correction vector sought for.

$\{\mathbf{F}\}$: the function vector resulting from a first order multivariable Taylor series expansion about assumed temperature values T^*. This vector is in fact the right hand term of Equations (12) and (13) which are set equal to F and become ~0 upon convergence.

$[J]$: The Jacobian of functions F, containing the partial derivatives.

The partial derivatives can be evaluated numerically by resuming the calculations for $T^* - \varepsilon$ and $T^* + \varepsilon$. However, for *3D* applications, it is much more economical to find them analytically and this is the approach we have chosen.

In the case of real gases, the direct interchange areas in Equations (3) and (4) are replaced by the directed interchange areas $\overrightarrow{s_j s_k}$ and $\overrightarrow{g s_k}$ which can be expressed as a weighted sum of the direct interchange areas of a number of gray gases:

$$\overrightarrow{s_j s_k} = \sum_{n=1}^{4} a_n(T_j, T_g)(\overrightarrow{s_j s_k})_n \tag{15a}$$

$$\overrightarrow{g s_k} = \sum_{n=1}^{3} a'_n(T_g)(\overrightarrow{g s_k})_n \tag{15b}$$

where a_n and a'_n are the weighting coefficients. The summation is shown here for three gray gases and one clear gas (window). It is limited to $n = 3$ in Equation (15b) because the clear gas does not contribute to the total emission. The

weighted sums are applied here to the direct interchange areas as opposed to the total interchange areas for the original method presented by HOTTEL (1967). The rest of the mathematical development in the IPM method is changed accordingly. The evaluation of the partial derivatives for the Newton—Raphson method is however more complicated in this case since Equation (10) is no longer linear, the matrix [**BM**] being now dependent on temperature.

Assessment of the method

The results yielded by IPM are compared firstly with those of the method of zones (ZONE) for a typical combustion chamber of a melter/holder furnace sketched on Figure 4a. A grid of 36 volume zones was used ($6 \times 3 \times 2$). For the purpose of comparison a total combustion heat release of 4213 kW (natural gas) was uniformly distributed over the first eight central volume zones (covering 4/6 of the furnace length), the flow-rate of fuel was 450 m³/h STP

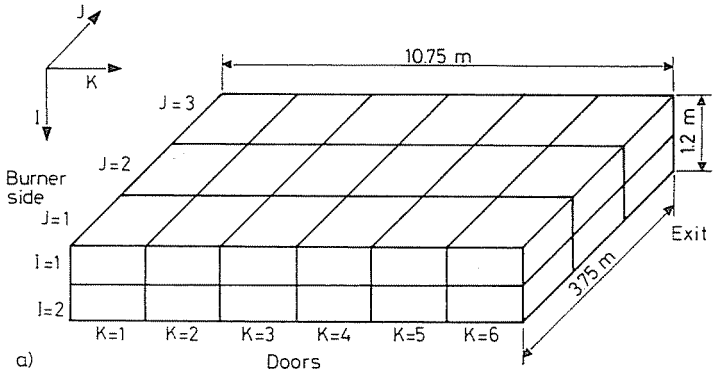

Fig. 4a. Furnace and grid chosen for the first assessment of IPM

and an excess air of 7.3% was imposed. Surface emissivities of floor (interface gas/liquid metal) and refractories were set at 0.5 and 0.7 respectively and floor was assigned a constant temperature of 1033 K. Appropriate convective and overall heat transfer coefficients were chosen for side walls, roof, metal surface, doors and end walls. A plug flow pattern was used for the longitudinal direction and a simple oscillating up-and-down pattern was imposed along the height, as illustrated on Figure 4b. The version of the zone method used is explained in KOCAEFE (1987a). Figure 5 shows good agreement between the two methods for both gas temperatures and heat fluxes. Parts a) and b) were found for the furnace described above in the case of real gases, whereas part c) and d) refer to a modified furnace in which a gray gas ($K = 0.175\ \text{m}^{-1}$) was used. In this latter case the following modified characteristics have been used: square

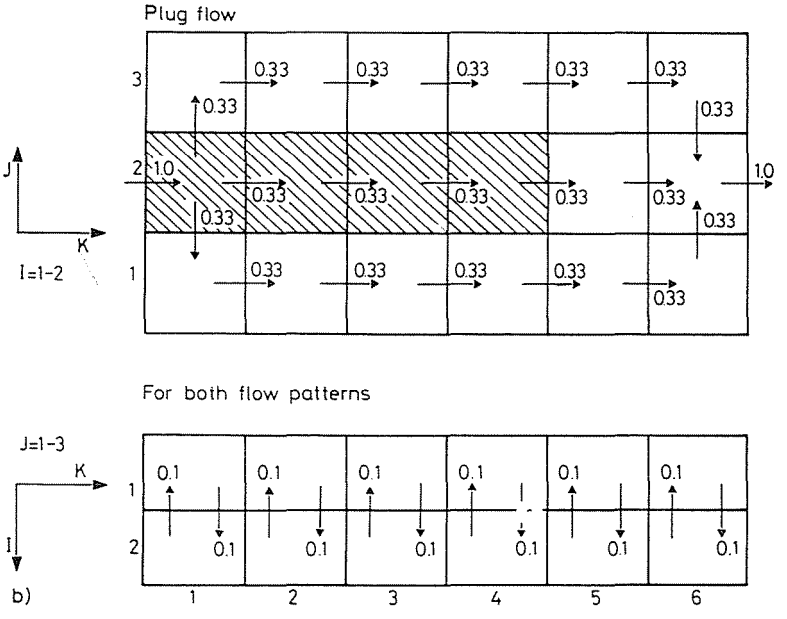

Fig. 4b. Flow pattern chosen in conjunction with the grid of Figure 4a

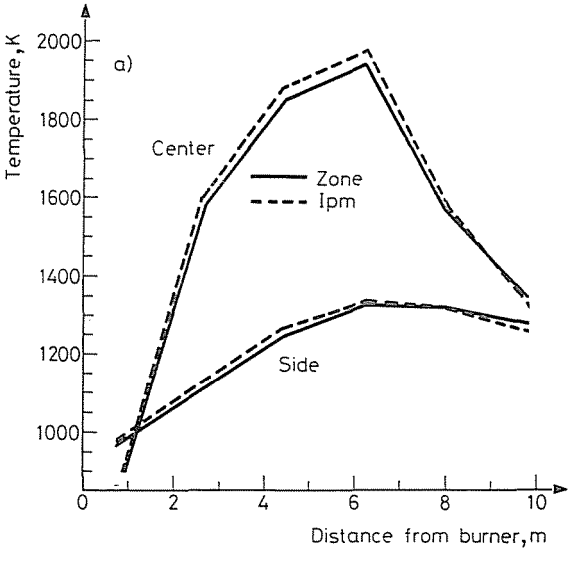

Fig. 5a. Validation of IPM against ZONE for the furnace of Figure 4 (temperature)

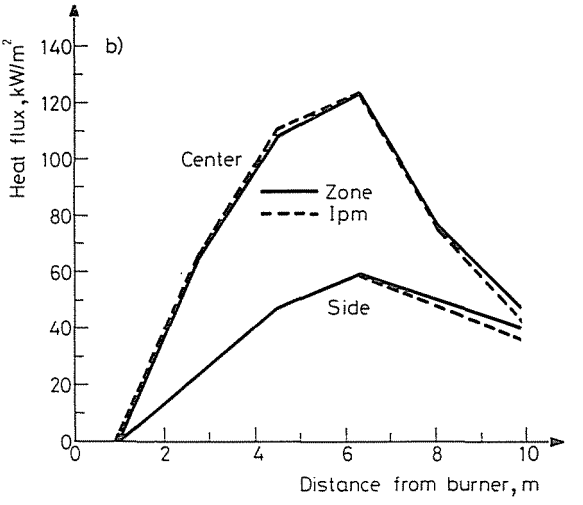

Fig. 5b. Validation of IPM against ZONE for the furnace of Figure 4 (heat flux)

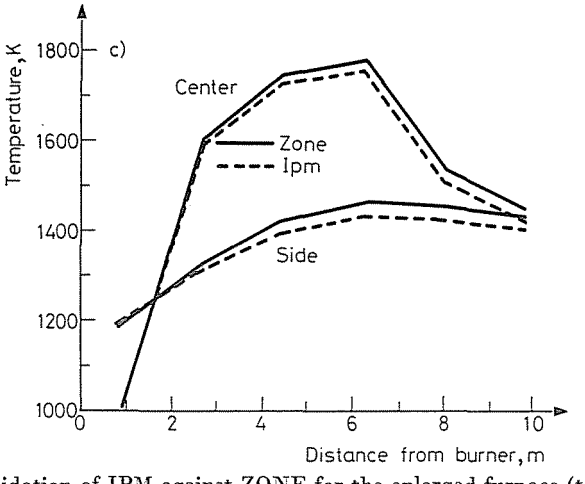

Fig. 5c. Validation of IPM against ZONE for the enlarged furnace (temperature)

section of 5×5 m, total inlet mass flow of 3.5 kg/s (instead of 1.75), total heat release of 8426 kW. Computation times are given in Table 1 for both cases. The new method shows a definite advantage in this respect. Computation reduction factors of 20 and 10 are noted for real and gray gases respectively.

This comparison is a first confirmation of the validity of the IPM. More tests are actually being carried out to assess the generality of the method. The code is capable of handling non-uniform absorption coefficients in the gas, non-uniform grids and rectangular furnaces of any relative dimensions (since the interchange areas are obtained by a Monte Carlo technique).

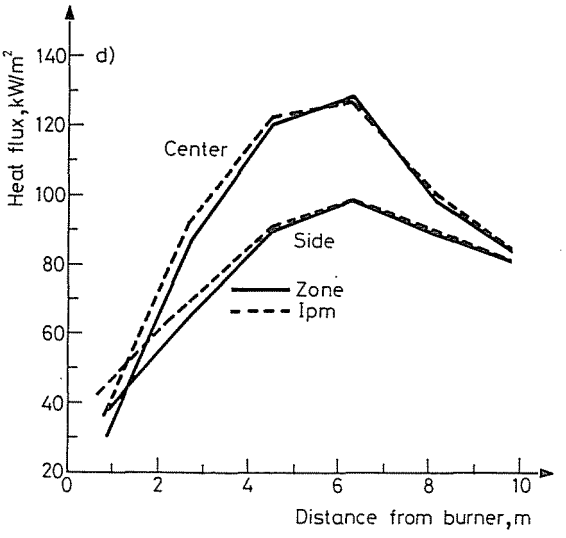

Fig. 5d. Validation of IPM against ZONE for the enlarged furnace (heat flux)

Table 1

Computation times (s) (on VAX-785)

Case	Interchange areas*	Convergence from iterative calculations	Total
Figures 5.a and b			
ZONE	1278	1419	2697
IPM	66	64	130
Figures 5.c and d			
ZONE	480	258	738
IPM	21	42	63

* Computation time required by the Monte Carlo method used.

Coupling IPM/PHOENICS

A complete modelling of a combustion chamber can be achieved only if a given radiation method is combined with the solution of motion and combustion equations (MCE). While flux methods have been combined with MCE for some time, it was only recently that this combination was obtained for the zone method (KOCAEFE 1983, POST 1987, TRIVIC 1987). We feel that

the proposed coupling with IPM will have the advantage of combining reliable results and low computation time.

For the MCE part, we have chosen to use the commercial code PHOENICS which is one of the most powerful means to solve the generalized conservation equation and is well known for its reliability. It offers the possibility of linking to it personal codes through a source term. The coupling IPM/PHOENICS can be done in a number of ways. A possible way is to have the energy equation solved by IPM which will feed the temperature field into PHOENICS to update the velocity and species fields, these new values being then picked up by IPM to recalculate new temperatures and the loop is resumed until convergence. However, better results are obtained if the transfer from IPM to PHOENICS is done on the basis of the radiation sources instead of the temperatures, letting the energy equation be solved by PHOENICS. The chosen scheme is illustrated in Figure 6.

PHOENICS is based on a similar algorithm to the SIMPLE algorithm which is detailed in PATANKAR (1980). This technique approaches the solution in an interactive way. For instance, for a first assumed temperature field, PHOENICS calculates iteratively the velocity field which is then updated by the input of S_{rad} from IPM until convergence is obtained. This procedure works well for steady state problems but, when transient physical processes are being investigated, repetition of the entire scheme over and over can become very cumbersome and computationally expensive. Thus, a simplified method for transient cases is sought for and this is explained in the next section.

Analysis of a transient process

As stated earlier, the numerous operations performed in a melter/holder furnace mean that, for long periods, adequate simulation of such a furnace has to take care of transient phenomena. The process chosen here is the open-fire heating following a casting operation. In this case, the transient state is induced mainly by the thermal inertia of the refractories. Therefore, dealing with such a problem implies that the IPM is to be modified in order to cope with different boundary conditions. The transient nature of the refractories forces the use of a trial and error technique (for every time step) which is explained in Figure 7. The idea is to compute and compare the heat transfer Q_{IN} between the gas and the refractories both by IPM and a 1–D transient conduction model, the loop being resumed if a large discrepancy is noted. Attention must be drawn here on the fact that the loop is imbedded into PHOENICS in the sense that it takes information from it at the beginning and sends information to it at the end. This procedure indeed consumes a lot of computation time if both the velocity and combustion fields are being

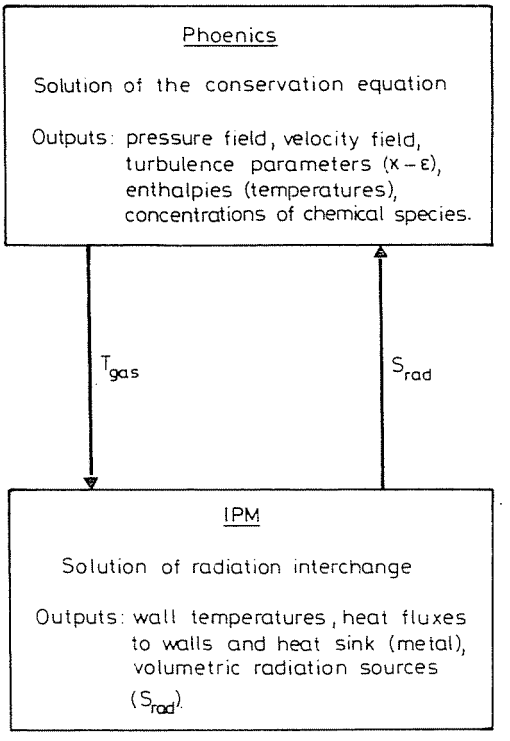

Fig. 6. Interaction IPM/PHOENICS

updated at every time step. Therefore, we have tested the validity of a semi-interactive procedure which is similar to the totally interactive procedure except that only enthalpies and chemical species concentrations are being re-evaluated by PHOENICS. The velocity field (this includes the pressure, the three components of velocity and the turbulence parameters) is computed only once by assuming steady state. We have then compared the results of this simplified version with the more rigorous totally interactive version. The calculations were performed on the same furnace as described before (Figure 4) with the following modifications in input data: 3×10^6 J/kg total enthalpy inlet, 8.7 m/s velocity inlet, no excess air, 0.6 refractory emissivity. Initial values were set at: $T_{gas} = 450$ °C, internal and external wall temperatures: 427 and 100 °C respectively, arbitrary profile in wall between 427 and 100 °C. The grid used for IPM was the one illustrated in Figure 4 except that four divisions were used along the height (instead of two), making it $6 \times 3 \times 4$ (see Figure 1); for PHOENICS, we have chosen a $12 \times 9 \times 8$ grid. Figure 8 shows very interesting results: the simplified procedure yields nearly exact

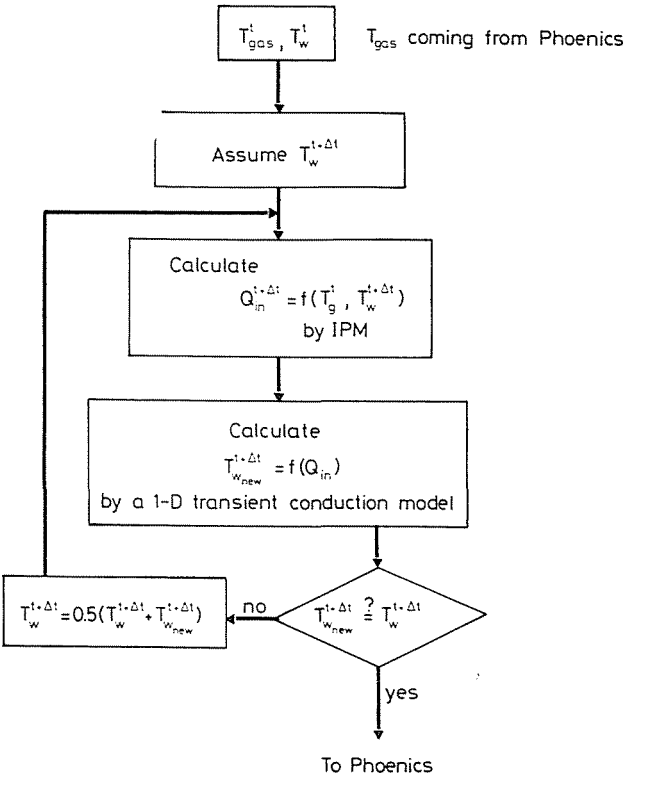

Fig. 7. Iterative procedure for the calculation of time-dependent wall temperature T_w

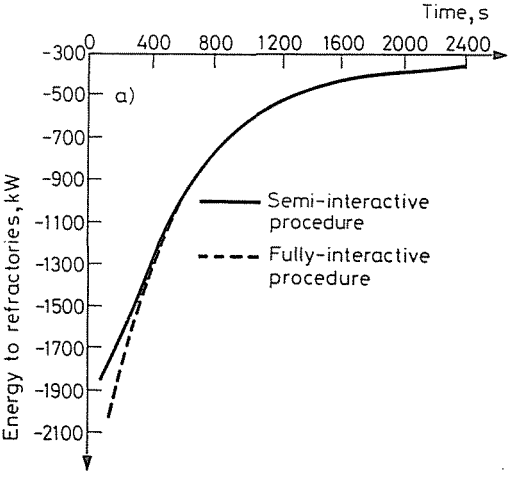

Fig. 8a. Transient results for energy to the refractories

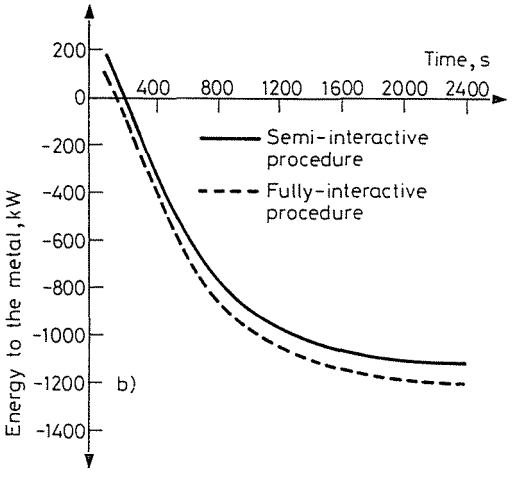

Fig. 8b. Transient results for energy to the metal

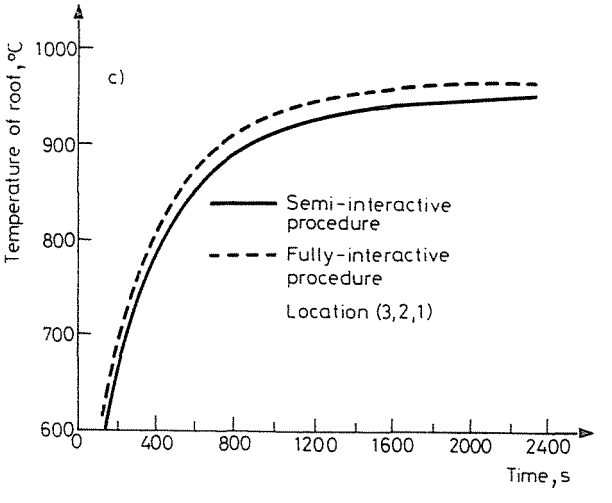

Fig. 8c. Transient results for roof temperature

results for the energy to the refractories (part a) and a maximum discrepancy of 8% is noted for the energy to the metal (part b); part c) exhibits also good agreement between results for the roof. Even more interesting is that the simplified procedure reduces significantly the computation time, the reduction factor standing between 5 and 10 depending on the simulation parameters.

This can be explained by the fact that the velocity field is responsible for six of the variables calculated by PHOENICS (out of nine). By-passing this part is thus of great advantage as far as cpu time is concerned.

Conclusion

The 3-D imaginary planes method in rectangular coordinates appears to be a very promising method for the calculation of radiative transfer in combustion chambers. For the cases studied, it combines accuracy and computational efficiency. A more complete assessment is actually being made, especially for different sizes of furnaces, non-uniform concentration distribution and different medium opacities. A 3-D cylindrical version will be investigated in the near future.

The method was then applied to the combustion chamber of a typical aluminium melter/holder furnace. The proposed coupling with PHOENICS opens the door to all sorts of simulation possibilities, including furnaces fired with several burners. The combined package was namely used to simulate an open-fire heating in transient regime and the results obtained lead to the conclusion that gas temperature and heat flux distributions are little affected by the changing velocity pattern. From now on, simulating complex transient problems becomes accessible in a simplified manner without sacrificing too much on the accuracy.

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