Computational modelling of turbulent flow, combustion and heat transfer in glass furnaces

C J HOOGENDOORN, C L KOSTER and J A WIERINGA

J M Burgers Centre for Fluid Mechanics, Lorentzweg 1, 2628 CJ Delft, The Netherlands

Abstract. For the combustion of natural gas in high temperature glass furnaces a computational model “Furnace” has been developed. It includes 3-D turbulent flow, flame chemistry, radiative heat transfer and the formation of soot and of the pollutant NO. Turbulent fluctuations have been taken into account, and are shown to have a large effect on thermal radiation and NO-formation. Spectral behaviour of gas radiation results in changes of heat transfer efficiency up to 5%, depending on refractory emissivity.

The model has been employed to predict NO formation for different burner geometries. In general, a decrease in mixing of gas and air results in a reduction of 1600 to 400 ppm in flue gas NO concentration. Except for some of the low mixing flames, however, they lead to a lower burnout and a very high CO level in the flue gas. A comparison with semi-technical furnace tests shows that the model can predict NO formation reasonably well. With this computational model the designer of furnaces and burners can study further possibilities for increased furnace performance and low NO emissions.

Keywords. Turbulent combustion; computational heat transfer; radiative heat transfer; NO_x formation; glass furnaces.

1. Introduction

Owing to the increasing costs of energy, the higher demands on the quality of glass and the need to decrease NO_x emission, the glass-industry needs more detailed information concerning the processes in glass-melting furnaces. Experimental investigations of glass-furnaces are difficult and expensive because of the high temperatures involved, typically 2000 K in the combustion chamber, so the use of models is useful. Often physical flow models have been used (Günther 1973; Gustafson 1980; Gustafson *et al* 1981, pp. 16–20). More recently also computational models have been considered (Gosman *et al* 1980; Ungan 1985). A complete description of the glass melting process requires a model for the laminar glass flow and a model for the turbulent gas flow in the combustion chamber. While the cooperating groups of Simonis *et al* (1986, 1993) and Muysenberg *et al* (1993) modelled the glass-flow,

we have concentrated on the processes in the combustion chamber for the case of natural gas-fired glass furnaces. Due to the high flame temperatures we can expect a high level of NO_x formation in such a furnace.

The use of advanced mathematical simulation models for glass furnaces have been recently reported by Gosman *et al* (1980), Carvalho *et al* (1987) Carvalho & Nogueira (1990), Ugan & Viskanta (1987). They describe the heat transfer from the flame. However, Ugan & Viskanta (1987) also give a modelling of the 3-D flow in the glass melt. A similar 3-D glass-melt model has been reported by Simonis *et al* (1986), whereas Horvath & Hilbig (1988) reported on a 2-D model coupled to a simplified flame-radiation model.

In this paper a complete model of 3-D flow and combustion, as well as of radiative heat transfer and of NO_x formation for gas-fired glass furnaces will be presented. For the 3-D turbulent flow a standard $k-\epsilon$ model has been used. Combustion is incorporated through a simple model, using the transport equation for fuel fraction. The heat of combustion is incorporated in the energy equation. In this equation the radiative heat transfer term is also included in the source term. A problem in radiation modelling is that it essentially requires the solution of an integral equation, whereas all other equations are partial differential equations typical for transport of mass, heat and momentum. This means that the radiation term needs a separate solution procedure. Two methods will be discussed: the Hottel zone and the discrete transfer methods. Spectral radiative effects for the typical gas emission of the flue gases will be shown. In standard $k-\epsilon$ turbulence modelling only the Reynolds averaged or Favre averaged values of transport quantities is used. However, in nonlinear source terms, as for instance radiation or chemical reactions (combustion), the fluctuating character of the turbulent fields has to be accounted for. This has been done by using an assumed shape for the probability density function of the turbulent fluctuating quantities involved. A transport equation for the variance of these fluctuations is solved to obtain quantitative results. The importance of the fluctuations will be shown for the radiative source term as well as for the combustion reactions. For the formation of NO a separate post-processor has been developed. It contains a transport equation for NO, with the thermal NO reaction as source term, via the Zel'dovich mechanism.

Computational results will be compared to experimental results obtained in a semi-technical furnace at the International Flame Research Foundation (IFRF) at Ijmuiden, The Netherlands.

2. The simulation model

2.1 Furnace code

A complete computational model for the simulation of a natural gas-fired furnace should contain all physical factors contributing to furnace performance. This means that it should contain model-flame chemistry, turbulent flow and mixing as well as heat transfer. Figure 1 shows the total scheme of the "Furnace" code of this study. The different factors interact and determine local field quantities like temperature, velocities and chemical composition of the gases. From the results the heat transfer to the glass, the emission of pollutants like NO_x and CO can be found.

Figure 1. Simulation of flow, combustion and heat transfer for natural gas flames.

2.2 The flow model

The flow model of the combustion chamber uses a numerical method to solve the continuity equation and the three-dimensional Navier–Stokes equations for a steady state case. The effect of turbulence on the flow has also to be modelled. This has been done by Launder & Spalding (1980) using a standard k – ϵ model with wall functions. As a result a set of six coupled equations is obtained from which the three velocity components can be found, and the two variables of the turbulence model, the turbulent kinetic energy k and the dissipation of the turbulent energy ϵ . The general transport equation for each of these variables can be written as,

$$\text{div}(\rho \mathbf{v} \phi) = \text{div}(D_\phi \text{grad}(\phi)) + S_\phi, \quad (1)$$

where ρ = density and D_ϕ = diffusivity. Here ϕ stands successively for the three velocity components of the vector $\mathbf{v}$ and for k and ϵ . With $\phi = 1$ one has the continuity equation. The first term gives the convective effects ($\text{div}(\rho \mathbf{v} \phi)$), the second, the diffusion effects ($\text{div}(D_\phi \text{grad}(\phi))$), and the last (S_ϕ) is a source term.

2.3 The energy equation

The energy (enthalpy) equation has also to be solved to obtain the temperature field. This equation has the same form as (1). The source term in it comes from the enthalpy of combustion and radiative energy exchange.

2.4 The combustion model

When modelling combustion of natural gas a rather complex flame chemistry is involved. Very often it is sufficient for heat transfer and flow modelling to use reduced chemical reaction schemes. Also depending on reaction rate and mixing rate time scales an equilibrium model or a full kinetic model has to be used. For large furnaces at high temperatures an equilibrium or flame sheet model can be used; except for the formation of NO_x , which is reaction rate limited. In the "Furnace" code a simple one-step, a two-step and a constrained equilibrium model (Bilger & Stårner 1983) for CH_4 combustion has been included as computational options.

When modelling the turbulent combustion in the natural gas/air mixture with a one-step model the following assumptions have been made:

(a) The reaction is expressed as

where s is the stoichiometric mass ratio oxidant/fuel.

(b) The reaction is infinitely fast, consequently the reaction rate is determined by the turbulent mixing of fuel and oxidant.

(c) The fuel and oxidant may coexist at the same place, but at different times (intermittency). This is due to concentration fluctuations caused by turbulence. They are accounted for by means of a probability density function. Here the probability density function is represented by a combination of two Dirac delta functions.

In the model the following five species are considered: fuel, O_2 , N_2 , H_2O , CO_2 . The composition of a fluid element can be expressed in terms of a mixture fraction f . The mixture fraction gives the concentration of the fuel relative to its initial concentration. For stoichiometric conditions in the present case $f = 0.0612$, whereas $f = 0.0$ for air and $f = 1.0$ for the fuel. Applying the above-mentioned assumptions one can find a transport equation again of the form of (1) for the mixture fraction f . In the two-step combustion model the reaction has been split at first into oxidation of CH_4 to CO and H_2O and a later oxidation of CO to CO_2 , when all CH_4 has been converted.

Turbulent fluctuations of the mixture function f have been taken into account by a method as described by Khalil (1982), a probability density approach. In this approach one considers the probability density function ($P(f)$) for the fluctuations of f for a location in the furnace. If we have a quantity $\Phi(f)$ depending on f , we will have to find the average of Φ from:

$$\bar{\Phi} = \int_0^1 \Phi(f) P(f) df, \quad (3)$$

which in case of a nonlinear relation $\Phi(f)$ gives a value differing from $\Phi(\bar{f})$. Examples

of nonlinear behaviour are the emissive radiative power (T^4) or the formation rate of NO_x in a furnace. Good predictions of these quantities require the use of $P(f)$. For the turbulent fluctuations of f we can introduce a fluctuation function g by,

$$g = (f' - \bar{f})^2, \quad (4)$$

with f' the fluctuating value of f . For this function g , Khalil (1982) also derived a transport equation like (1). For the entire set of equations see table 1. For the PDF one has to assume a shape of the function to give a good prediction. If one assumes intermittency, this function $P(f)$ reduces to a double delta function, symmetric or clipped around $\bar{f}$. In the mixing zone of the flame this gives an adequate description for the combustion model. For NO_x formation also taking place downstream of the initial mixing a top hat distribution has been used in the "Furnace"-code.

Table 1. Transport equations used in "Furnace" code.

$$\frac{\partial}{\partial x_j}(\bar{\rho} \bar{u}_j) = 0$$

$$\frac{\partial}{\partial x_j}(\bar{\rho} \bar{u}_j \bar{u}_i) = -\frac{\partial \bar{\rho}}{\partial x_i} - \frac{\partial}{\partial x_j}(\bar{\tau}_{ij}) + \bar{\rho} g_i$$

$$\tau_{ij} = -(\mu + \mu_t) \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) + \frac{2}{3} (\mu + \mu_t) \frac{\partial \bar{u}_k}{\partial x_j} \delta_{kj} + \frac{2}{3} \bar{\rho} k \delta_{ij}$$

$$k = \frac{1}{2} \overline{u'_i \cdot u'_i}, \mu_t = C_\mu \bar{\rho} k^2 / \varepsilon, \varepsilon = \frac{\mu}{\bar{\rho}} \left(\frac{\partial u'_i}{\partial x_j} \cdot \frac{\partial u'_i}{\partial x_j} \right)$$

$$\frac{\partial}{\partial x_j}(\bar{\rho} \bar{u}_j k) = \frac{\partial}{\partial x_j} \left(\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right) - \bar{\rho} (G + \varepsilon)$$

$$\frac{\partial}{\partial x_j}(\bar{\rho} \bar{u}_j \varepsilon) = \frac{\partial}{\partial x_j} \left(\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right) - \bar{\rho} \left((\rho_{1\varepsilon} G + \rho_{2\varepsilon} \varepsilon) \frac{\varepsilon}{k} \right)$$

$$\bar{\rho} G = \left(\mu_t \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{2}{3} \bar{\rho} k \delta_{ij} \right) \frac{\partial \bar{u}_i}{\partial x_j}$$

$$\frac{\partial}{\partial x_j}(\bar{\rho} \bar{u}_j H) = \frac{\partial}{\partial x_j} \left(\frac{x}{C_p} + \frac{\mu_t}{\sigma_H} \right) \frac{\partial \bar{H}}{\partial x_j} + \bar{S}_{rad}$$

$$\frac{\partial}{\partial x_j}(\bar{\rho} \bar{u}_j \bar{Y}_i) = \frac{\partial}{\partial x_j} \left(D_i + \frac{\mu_t}{\sigma_i} \right) \frac{\partial \bar{Y}_i}{\partial x_j} + \bar{S}_i$$

$$\frac{\partial}{\partial x_j}(\bar{\rho} \bar{u}_j f) = \frac{\partial}{\partial x_j} \left(\Gamma_f \frac{\partial \bar{f}}{\partial x_j} \right)$$

$$\frac{\partial}{\partial x_j}(\bar{\rho} \bar{u}_j \bar{g}) = \frac{\partial}{\partial x_j} \left(\Gamma_g \frac{\partial \bar{g}}{\partial x_j} \right) + C_{1g} \mu + \frac{\partial \bar{f}}{\partial x_j} \frac{\partial \bar{f}}{\partial x_j} - C_{2g} \bar{\rho}^g \varepsilon k$$

with $C_\mu = 0.09$, $C_{1\varepsilon} = 1.44$ and $C_{2\varepsilon} = 1.92$; $\sigma_k = 1.0$, $\sigma_\varepsilon = 1.3$, $\sigma_H = 0.9$ and $\sigma_i = 0.9$; $C_{1g} = 2.8$, $C_{2g} = 2.0$, $\Gamma_f = \Gamma_g = \mu_t / \sigma_f$ and $\sigma_f = 0.9$; H is the enthalpy and Y_i the concentration of species i .

2.5 Radiative modelling

In order to evaluate the source term in the energy equation the radiative heat exchange must be modelled. One of the models used is the well-known Hottel zone method derived by Hottel & Sarofin (1967). One of the main reasons for choosing this method is the fact that in the present study the heat flux to the relatively cold and strongly absorbing glass surface is an important quantity. For this case the zone method gives very reliable results.

In the Hottel zone method one divides the combustion space into a number of equal-sized volume zones (parallelopipeds), surrounded by surface zones along the glass bath and roof. The three-dimensional space has to be divided in the model in n_i by n_j by n_k volume zones (flame length, width, height direction, respectively). The modelling consists of half the combustion chamber, using symmetry conditions along the mid-plane through the flame.

In the Hottel zone method one has to evaluate the radiation exchange factors: $\overline{s_i s_j}$, $\overline{s_i g_k}$, $\overline{g_m g_k}$. They represent the surface to surface, the surface to gas volume and volume to volume exchanges, respectively. With these factors evaluated beforehand and a calculated temperature field, one obtains for the net heat exchanges for surface zones:

$$Q_{n,j} = \sum_{i=1}^N \overline{s_i s_j} q_i^- + \sum_{k=1}^K \overline{s_i g_k} E_k - A_j q_j^-, \quad (5)$$

with q_i^- and q_j^- = leaving fluxes from areas A_i and A_j , E_k = emitted flux from volume zone k , and for volume zones:

$$Q_{n,k} = \sum_{j=1}^N \overline{s_j g_k} q_j^- + \sum_{m=1}^K \overline{g_m g_k} E_m - 4k_k V_k E_k, \quad (6)$$

with k_k = absorption coefficient of volume V_k .

Calculation of the $\overline{g_m g_k}$ factors is especially cumbersome as they contain a six-fold space integration. Therefore, use was made of an algorithm from Siddal (1986) for the exchange factors. Up to now the full zone method was only applied for one gray gas with a constant absorption coefficient k . For the latter a value of $k = 0.12 \text{ m}^{-1}$ has been taken as a good average value for the whole space. This has been done on basis of a literature review for natural gas flames by Post (1988). In this reference it has also been shown that the results are not very sensitive to k in the range of 0.08 to 0.15.

Next to the Hottel method, a second radiative model has been included in the "Furnace" code as a computational option. The Discrete Transfer Method (DTM) solves the equation of radiative transfer in a different way. A detailed transcription of the DTM can be found in Lockwood & Shah (1981) and Wieringa (1992). The enclosure that is studied is divided into a number of volume and surface elements, as in the zone method. In each surface element a number of beam directions is chosen. From here each beam is traced towards the other side of the enclosure from where the beam is thought to emerge with an energy dependent on the boundary conditions. Then the beam is followed back and the intensity is determined in each volume that it passes, until the beam has reached the surface element. A major problem with the

Figure 2. The two gas spectra.

DTM is the fact that a heat balance over the complete enclosure is not automatically satisfied, it requires a sufficient number of beam directions (16 or 32).

The DTM has the advantage, compared to the Hottel zone method, that the absorption coefficient can easily be made position-dependent. Hence, it is possible to take into account the effect of soot on heat transfer by radiation. The disadvantage is that the computational time per radiation iteration is higher than with the Hottel zone method.

In a few detailed studies also the spectral character of gas radiation for the combustion gases (CO_2 and H_2O) have been taken into account. Two gas spectra have been used, figure 2. The first has been taken from an earlier study by Alexander *et al* (1988) on the spectral effects in furnaces. It consists of 15 wavelength bands, of which 7 are perfectly transparent. It was computed according to data from Edwards (1960) for a somewhat smaller furnace and for gas of lower temperature. It has been used to show the influence of the combustion profile on the spectral effects, using the Hottel zone method. At 2000 K the total emissivity of the 15 band spectrum is 0.14.

The second spectrum has been computed according to the statistical narrow band model by Goody (1964). This states that the mean gas emissivity of a narrow spectral band at wave number ν can be written as:

$$\epsilon_{\text{gas}, \nu} = 1 - \exp(-\bar{W}/\delta) \quad (7)$$

where $\bar{W}$ is the so-called equivalent width of a spectral line, averaged over a distribution of line strengths and δ is the mean line spacing. An exponential-tailed inverse distribution has been taken for the probability density function of line strength. Soufiani *et al* (1986) showed that this distribution gives very accurate results for spectral lines having a Lorentz profile. Ludwig *et al* (1973) give approximations for

the emissivity using various line shapes and probability density functions, and tables of experimental values for several variables in wave number intervals of 25 cm^{-1} . This way a spectrum has been obtained by using 372 intervals that are believed to reproduce the form of the spectrum accurately. It is shown in figure 2 for a mean beam length of 2.83 m and partial pressures of CO_2 and H_2O of 0.08 and 0.15 atm, respectively. This spectrum yields a total emissivity of 0.23 at 2000 K.

The apparent differences between the two gas spectra can be explained from the different geometries, gas temperatures and possibly also gas compositions, and also from the fact that the 15-band spectrum has been calculated using a wide band model. It should be noticed that the maximum of the Planck curve at high temperatures in the furnace lies at about $1.5\text{ }\mu\text{m}$. This makes large differences, at high wavelengths, relatively unimportant.

2.6 Modelling of turbulence–radiation interaction

Due to turbulent fluctuations of chemical composition (CO_2 , H_2O -concentration) and of temperature, the transmissivity (absorptivity) and emissivity in a grid cell will fluctuate as well. Due to nonlinear behaviour of gas-radiation simple average values can give less accurate results. This effect has been investigated for a number of typical radiation beams for a converged Furnace-code (including grey-gas radiation) computational result using the following method.

In order to find the spectral, directional radiative flux in a point, one beam of radiation is followed in a certain direction. In the first place, we determine the volumes that are run through, and the corresponding distances. In each volume the chemical composition and temperature are determined. Then the radiative transfer equation has to be solved, which is given by:

$$L_\omega(x) = L_\omega(0)\tau_\omega(0, x) + \int_0^x e_{b,\omega}(x') \frac{\partial \tau_\omega(x', x)}{\partial x'} dx' \quad (8)$$

or in discretized form:

$$L_\omega(n) = L_\omega(0)\tau_\omega(0, n) + \sum_{m=1}^n e_{b,\omega}(m)(\tau_\omega(m, n) - \tau_\omega(m-1, n)). \quad (9)$$

Here ω is wave number ($1/\lambda$), L_ω is spectral luminance, τ_ω is transmissivity and $e_{b,\omega}$ is directional black body emissive power, given by the Planck function. Further, x is the coordinate in the given direction and n and m are volume numbers. Transmissivities from the point of observation are calculated making use of the narrow band model as described above using 372 wave number intervals of 25 cm^{-1} .

Chemical composition and temperature in a volume are found from local values of mixture fraction (f), mixture fraction variance (g), enthalpy (h) and temperature (T). Now the radiative fluxes from the turbulent flame can be modelled in three ways.

(1) Method 1 makes use of mean values for the partial pressures and temperature. Thus, the emissive power in each volume is calculated as:

$$e_{b\omega} = e_{b,\omega}(\bar{T}). \quad (10)$$

This method clearly underestimates the emission of the gas, because of the nonlinearity of emissive power with temperature.

(2) A better way is therefore method 2, which uses pdf-averaged values for the emissive power in each volume:

$$e_{b,\omega} = \int_0^1 e_{b,\omega}(T(f))P(f)df. \quad (11)$$

This method neglects, however, the correlation between emissivity (or τ) and (black body) emissive power. When the instantaneous value of f is near the stoichiometric value (f_{st}), the concentrations of H_2O and CO_2 and the temperature will be high, so that at the same time emissivity and emissive power will be high. When f is far from f_{st} , the reverse is the case. In this method, however, transmissivity is calculated from mean properties, and the correlation is lost.

(3) Drawbacks of method 2 are avoided when an ensemble average is calculated of the spectral flux, using a large number of instantaneous (spatial) distributions of f along the optical path. With the double-delta pdf, it is possible to evaluate every possible f -distribution, but it appears to be more convenient when these are generated statistically. Then each instantaneous value of f in a volume is determined by a random number. The pdf prescribes the relation of f with the random number R ,

$$f = P_c^{inv}(R), \quad (12)$$

here P_c is the cumulative distribution function of f ,

$$P_c(f) = \int_0^1 P(f')df'. \quad (13)$$

Taking a large enough number of beams will give a small statistical error in the solution. In practice 250 beams were enough to obtain a standard deviation in the total flux of less than 1%. This stochastic procedure is also described by Faeth *et al* (1989, pp. 1–38).

2.7 NO_x formation model

A thermal NO formation model has been added to the combustion model. Thermal NO formation occurs via the so-called Zel'dovich mechanism (Zel'dovich 1946):

where k_i is the Arrhenius constant of reaction i .

Reaction scheme 1 results in the following production equation:

$$\frac{d[NO]}{dt} = \frac{2[O]}{k_2[O_2] + k_3[NO]} [k_1 k_2 [N_2][O_2] - k_3 k_4 [NO]^2]. \quad (15)$$

The Arrhenius constants used for all reactions were obtained from Warnatz (1983) and Hanson & Salimian (1984) and are given in table 2. For the O-atom concentration

Table 2. Arrhenius constants of the reaction of the Zel'dovich mechanism. $k_i = A \cdot T^n \exp(-E/RT)$.

	A ($\text{m}^3/\text{kmol s}$)	n ($-$)	E (kJ/kmol)
k_1	$1.8 \cdot 10^{11}$	$-$	$3.19 \cdot 10^5$
k_2	$6.4 \cdot 10^6$	1	$2.61 \cdot 10^4$
k_3	$4 \cdot 10 \cdot 10^{10}$	$-$	$4.23 \cdot 10^3$
k_4	$1.37 \cdot 10^6$	1	$1.60 \cdot 10^5$
K_{eq}	$2.25 \cdot 10^4$	$-$	$4.96 \cdot 10^5$

in (15) we used the reaction,

which for equilibrium gives

$$[\text{O}] = K_{eq}^{1/2} [\text{O}_2]^{1/2}. \quad (17)$$

Since the NO-formation rate is slow compared to the combustion and the NO concentration is low relative to the concentration of other species in the flame, the NO formation is assumed not to influence combustion. This enables us to compute the NO formation in a post-processor to the combustion code, where the output of the combustion simulations can be used as input for the NO formation computations. A transport equation like (1) (see also table 1) is solved for the NO mass-fraction, in which (15) gives the source-term. A tophat PDF has been used to find the effect of turbulent fluctuations on the NO source term.

2.8 Soot model

The presence of soot in a furnace flame promotes radiation and hence the efficiency of heat transfer from the flame. In order to estimate this effect, the amount of soot and the distribution in the flame have to be known. Despite the highly complex nature of the chemistry of soot formation and oxidation in flames, some general principles begin to be well understood. Four more-or-less separate processes can be recognized:

nucleation: fuel is decomposed and the first soot nuclei appear;

coagulation: the soot particles collide and coalesce;

surface growth: the mechanism by which the bulk of the soot mass is generated;

oxidation: soot is oxidized mainly by O_2 and OH to form gaseous products like CO and CO_2 .

The amount of soot formed depends strongly on the type of fuel. Methane and ethane give relatively low soot concentrations compared to ethylene and acetylene.

The soot formation rates are kinetically limited, especially in the first part of the flame. This means that state relationships, e.g., soot mass concentrations as a function of mixture function f will depend on residence time. Accurate simulation of soot requires solving a transport equation for soot, with source terms for formation and oxidation.

A two-equation model for the evolution of soot volume fraction, f_v , and particle number density, n , is presented by Syed *et al* (1990). Two transport equations like (1) have to be solved for which the following source terms were formulated:

$$\frac{d}{dt} \left(\frac{n}{N_o} \right) = \alpha(f) - \beta(f) \left(\frac{n}{N_o} \right)^2, \quad (18)$$

$$\rho_s \frac{df_v}{dt} = \gamma(f)n + \delta(f), \quad (19)$$

where ρ_s is the density of soot, N_o is Avogadro's number and α , β , γ and δ are functions of the mixture fraction which represent nucleation, coagulation, surface growth and nucleation respectively.

This model does not account for soot oxidation. However the oxidation model described by Magnussen & Hjertager (1976) was used in this study. Coupling of soot concentration to the radiation model is done by using the Planck mean of the absorption coefficient of soot.

3. Description of the simulated furnaces

We simulated two furnaces. One is the semi-technical size experimental furnace of the International Flame Research Foundation (IFRF) in Ijmuiden (The Netherlands). This furnace was used to simulate a glass-melting furnace, by forcing the major part of the heat loss to take place through the bottom of the furnace. In figure 3 a schematic is given of half of the furnace, with the burner port in an underport configuration. The furnace is 3.75 m long, 0.96 m high and 0.88 m wide. The heat input of the furnace is 750 kW, of which 500 kW enters via the natural gas. The temperature of the flue gas is approximately 1700 K. The gas injection velocity typically is 125 m/s, whereas the air inlet velocity is 10 m/s. The air preheat is 1373 K in the standard case.

The other furnace that we modelled is an industrial regenerative side-port fired glass-melting furnace, consisting of six burner compartments, of which three are cyclically fired. Figure 4 gives an overview of one compartment that we have modelled in our simulation studies. The dimensions of the combustion space are length 7.3 m,

Figure 3. View on the IFRF furnace, with underport burner system.

Figure 4. Regenerative side port fired glass furnace. Position of points 1 to 4, for which radiative fluxes have been calculated, are indicated.

height 2.4 m and breadth 3.3 m of one compartment. The secondary air is preheated to 1423 K, the glass bath temperature is 1773 K, air excess is 10%.

4. Numerical method

4.1 Solver

To solve transport equations like (1) we have used a control-volume method combined with finite differences using both the upwind and the hybrid differencing schemes. To solve the hydrodynamical problem we have used the pressure-correction method. While developing our computer program we have paid much attention to flexibility, modularity and clarity of the code. At the moment the program can use several hydrodynamical solvers (like SIMPLE, Patankar 1980, and SIMPLEST, Spalding 1980) and also several solvers for the linear equations involved. These solvers are for most variables plane-TDMA and space-TDMA for pressure correction, mixture fraction f and its fluctuations g . These two solvers are two- and three-dimensional extensions of the well-known Tri-Diagonal-Matrix-Algorithm, see Patankar (1980).

The coupled equations for flow and combustion are solved simultaneously in an iterative manner. The transport equation for NO_x however can be solved separately when a converged flow and temperature field has been obtained. The radiative heat transfer models used (Hottel and DTM) lead to integral equations for the whole furnace space based on the found temperature field. This means that in this case a transport equation cannot be used. However, in the iterative flow solutions one does not need to make a radiation calculation for every iteration. One radiation iteration suffices for every five or ten iterations.

4.2 Non-rectangular geometry

As can be seen from figure 4 the roof of the combustion chamber is curved. Because the finite-differences method as used in our model is only capable of handling rectangular geometries, we had to modify our algorithm. We have chosen a porosity factor method which determines for each cell of the numerical grid the part of the cell-areas and the cell-volume available for the flow, similar to the method described by Moulton *et al* (1979).

Figure 5. Grid and furnace geometry.

4.3 Grid distribution

In all cases 3-D Cartesian nonlinear grids have been used. These grids are finely distributed near the inlet gas mixing zone to obtain a good prediction for the turbulent combustion field. A typical grid for the IFRF furnace with $16 \times 24 \times 20$ points is shown in figure 5. To find grid dependency also $32 \times 48 \times 40$ grids have been used in a few cases, this gave only slightly ($\leq 3\%$) differing results.

For the radiation calculations the volume zones of the Hottel or DTM model do not have to coincide with the finite difference grid. In general we used larger gridsizes for the radiative heat transfer. The radiation source term in the energy transport equations for a finer flow field grid cell uses the contribution from the radiative power and absorption obtained from the coarser grid. We attributed to the distribution of these a weighting factor proportional to the grid volume for the absorption of radiation and to $T_i^4 = (T_i \text{ gridpoint temperature})$ and volume for the emission of radiation. Typically one completely converged solution on the standard grid takes about 6 h of CPU-time on an HP735 computer.

4.4 Validation of the model

Next to the grid refinement study as mentioned under § 4.3, the model has been validated by experiments. For the 3-D flow and mixing of natural gas and air an isothermal experiment has been carried out on a cold (air) furnace model. The flow field and the mixing of a jet of air with an He-tracer and the primary air could well be predicted (Post & Hoogendoorn 1987; Post 1988). This validated the $k-\epsilon$ turbulence modelling for this particular flow configuration of the furnaces studied. The full experimental validation of the complete model will be discussed by comparing with measurements of a semi-technical scale test furnace.

5. Simulations

5.1 Flow and combustion in test-furnace

Some typical calculated fields in the vertical mid-plane through the burner for the IFRF furnace are shown in figures 6 and 7. In figure 6 the velocity vector field has

Figure 6. Velocity vectors in the symmetry plane with 12° underport firing.

been shown. It shows a recirculation zone with low velocities above the main flame jet. Figures 7a, b and c show respectively the isotherms, lines of constant oxygen concentration and constant NO concentrations. The distribution of the radiative heat flux to the load has also been computed and figure 8 shows such a distribution for the 12° underport firing case.

The tests at the IFRF by Van de Kamp *et al* (1991) resulted in two baseline flames that were thoroughly tested during two trial periods. These two flames are both underport fired, at two different gas injection angles (12° and 20°). Plots of the temperature in the symmetry plane for both flames as simulated are shown in figure 9. It is clear from this figure that the mixing pattern is completely different for the two baseline flames. The 20° firing mode results in a much higher mixing rate and thus in faster combustion. As a result the maximum temperature is higher than in the 12° firing model, see also table 3. The predicted NO_x as simulated by FURNACE is also higher: 1074 ppm at 12° against 1470 ppm at 20° (both normalized at 0% O₂). The measured fluegas NO_x concentrations are 1070 ppm and 1170 ppm (0% O₂), at 12° and 20° natural gas injection respectively. Further, the two-step combustion model, extended for combustion to include CO formation and for NO_x formation with a double delta-tophat pdf, has been used.

A comparison can be made with the test at IFRF. In figure 8 the measured heat flux distribution is compared to the simulated one. The agreement is good only near the very end of the furnace, where the measurements show a lower flux, probably due to high radiative heat losses through the outlet and back-wall in the test. Flue gas temperatures (table 3) for two tested firing modes (12° and 20° gas injection angles) differ by 50 and 20 K for the two cases. In view of the measuring accuracy (50 K) of this temperature, good agreement is obtained, meaning that energy efficiency can be well predicted with the "Furnace" code. Taking the accuracy of the NO_x measurements into account (± 150 ppm), the two-step combustion model predicts the NO_x concentrations reasonably well (see also table 3).

To achieve the temperatures normal in glass-melting furnaces, the combustion air is preheated. The preheat temperature normally is approximately 1373 K. The effect of the preheat temperature on the NO_x formation is illustrated in figure 10. At 1573 K air preheat the mean temperature in the furnace is 1800 K, while at 1073 K preheat the mean temperature is 1670 K.

It can be seen from figure 10 that reducing the flame temperature by reducing the air preheat seems a feasible way of reducing NO_x emissions. This is confirmed by the measurements with which the simulations again agree very well. However, the furnace efficiency also decreases significantly when the air preheat temperature is

Figure 7. (a) Temperature, (b) oxygen and (c) NO concentration fields in symmetry plane with 12° underport firing. Temperature in K, O₂ concentrations in % mass fractions, O₂ and NO in ppm. (Horizontal dimension has been scaled down twice as much as vertical dimension.)

Figure 8. Computed and measured heat flux distributions in axial direction.

lowered. This results in a decrease in the heat transfer to the load of 30%, between 1573 K and 1073 K combustion air preheat. At the low preheat temperature the process may no longer be economically feasible. It should also be noted that the process requirements should always be met. Glass melting for high quality glass requires refining and is essentially achieved at high temperatures.

Figure 9. Temperature in the symmetry plane for the baseline flames: (a) 12° firing mode, (b) 20° firing mode.

Table 3. Some characteristics of the baseline 12° and 20° underport flames. Measured data from IFRF. Simulations from FURNACE and complete model.

	Simulated		2-Step combination model		Measured (IFRF)	
	12°	20°	12°	20°	12°	20°
$T_{\max}$ (K)	2395	2450	2330	2390	—	—
T_{flue} (K)	1765	1710	1767	1705	1718	1685
Q'' (kW/m ²)	72.6	73.3	70.7	74.2	68.8	70.1
Flue NO _x (ppm)	1074	1470	930	1020	1070	1170

Glass melting furnaces are normally operated with an excess air level between 5% and 30% (airfactor $\lambda = 1.05$ –1.30). The glass refinement requires that the molten glass is kept in an oxidizing environment, but the furnace efficiency requires an airfactor as low as possible, while still maintaining full burnout of the natural gas. The effect of the airfactor on the NO_x emission is shown in figure 11, in this case also there is good agreement with measurements.

Higher airfactors result in somewhat higher NO_x emissions due to the increasing oxygen concentration. Of course at high airfactors the temperature in the furnace is reduced, due to the mixing of large amounts of relatively cold combustion air. The simulations again predict the measured NO_x emissions quite well. Keeping the airfactor as low as possible is a way both to reduce the NO_x emissions and to increase the furnace efficiency. In general we found that a less intense mixing of natural gas and air results in longer flames with less NO formation.

5.2 Results for industrial furnace

With the full simulation model of the industrial combustion chamber details of the flow, combustion and heat transfer can be obtained (see Post 1987, pp. 884–895, 1988, and Post & Hoogendoorn 1987). Whether the flame is short or long depends

Figure 10. Flue gas NO at several combustion air preheat temperatures.

Figure 11. Flue gas NO at several airfactors.

Figure 12. Flame pictures in the combustion chamber. (a) Surface of constant mixture fraction $f = 0.07$, showing presence of fuel ($f = 0.0612$ stoichiometric); (b) surface at constant temperature ($T = 2000\text{ K}$).

strongly on the inlet conditions. It was found that the initial turbulent length scale is particularly important here. An intense mixing with a large turbulent length scale leads to high μ_t values and consequently to short flames. In this way the flame configuration can be influenced strongly.

Some results for a long flame (small turbulent length scale at inlet port) will now be given. A picture of a long flame can be seen in figure 12a, here the surface of a constant mixture fraction $f = 0.07$, corresponding to an air factor of 0.87, is shown and in figure 12b the 2000 K surface is shown. The prescribed flow profiles at the combustion chamber are for the case of a precombustion of 44% in the burner. From the computations a 97% burnout of the fuel at the outlet is found for the long flame, complete burnout will occur in the passage to the regenerator. For the short flame a 100% burnout has been found. For this hot flame an average heat flow for half of the compartment is found: to glass bath 1.51 MW (99% of this by radiation and only 1% by means of convection), wall losses 0.10 MW and flue gas heat loss 2.20 MW. The efficiency of the furnace, related to total fuel input, is 42% in this case. For a long, relatively cool flame with the same heat input the heat flow to the glass bath is 1.25 MW and the flue gas heat flow is 2.46 MW, where the flue gas still contains unburnt fuel. Combustion chamber efficiency is now 35%.

A short or a long flame also has a large effect on NO-formation. For a short flame the NO-combustion in the outlet is 3481 ppm, whereas for the long flame a value of 4007 has been found. In general these NO-values for the industrial furnace are higher than those for the IFRF-test furnace. The temperatures in the industrial furnace are higher (flue gas temperatures of 1900 K versus 1750 K). For this furnace we could clearly show the large effect of turbulent fluctuations on NO-formation. For the short flame the value of 3481 ppm drops to 1974 ppm (43% lower) if one neglects the turbulent fluctuations (tophat pdf) on the NO-source term.

5.3 Effects of spectral radiation

The main mode of heat transfer to the glass in a high temperature furnace is radiative heat transfer which in general is over 95% of the total heat flux. Previously Post & Hoogendoorn (1987) have shown that for prediction of fuel efficiency a simple single zone or axial flow model is sufficient. To find the effects of the spectral behaviour of gas radiation we included this in a simple model (see Hoogendoorn *et al* 1990). In this model we have the gas multiband radiation spectrum for CO_2 and H_2O at temperatures and partial pressures as occurring in the furnace. For the refractory material a grey surface has been assumed. Most of these materials have a low emissivity at high temperatures. For some specific samples an emissivity of 0.4 at 2000 K has been measured by us. For the glass a grey emissivity of 0.8 has been taken.

Some results for the industrial furnace are given in figure 13. Here the effect of refractory emissivity ϵ_r has been given. Increasing ϵ_r results in a higher total heat flux to the glass Q_{gl} . This is due to the fact that a higher roof emissivity results in a strong increase of the roof radiation because the roof refractory transforms the banded gas radiation to a continuous emitted radiation. However, at low ϵ_r the roof reflects the banded radiation for a large part $(1 - \epsilon_r)$ in the same bands as the gas radiation. In these bands the gases have low transmission and will absorb the reflected radiation to a large extent before it reaches the glass. Figure 13 shows that the direct radiation decreases with higher ϵ_r , due to the somewhat lower gas temperatures, however, the

Figure 13. Heat flux to glass as function of refractory emissivity. Full lines are from spectral calculations, dotted for a grey gas.

Figure 14. Relative enhancement of heat flux to glass as function of refractory emissivity, relative to $\epsilon_r = 0.4$. The mean length $L = 2.8$ m.

net flux (total) still increases. The increase of the roof emissivity ε_r can be obtained by structuring the refractory with cavities and protrusions to make it a "rough" surface or to apply a special coating, see Alexander *et al* (1988) and Fisher (1986). The relative importance of the spectral effects depend on the size of the furnace as expressed by the mean beam length L . Figure 14 gives results of the relative increase of glass load at constant heat input for different values of L . Small furnaces show increases of heat fluxes up to 5%, large furnaces show smaller (3%) benefits of increasing ε_r from 0.4 to 1.

5.4 Turbulence–radiation interaction

In order to estimate effects of turbulence on radiative fluxes in a glass furnace, a number of computations have been done for the industrial furnace. At four locations at the glass melt surface, see figure 4, the calculated spectral incident fluxes will be shown. Three of the points (1–3) lie at the symmetry plane in the centre of the flame. Point 4 is localized at the assumed symmetry plane between two flames. Vertical heights at these points are 1.9, 2.4, 2.0 and 2.4 m for points 1 to 4 respectively. In the vertical direction, the combustion chamber has been divided into 10 volumes. Because of symmetry properties, it is only necessary to consider half a burner compartment of the sideport-fired furnace. In this segment the thermal input of natural gas and preheated secondary air (1423 K) is 3.8 MW. The precombustion of the flame is 44%.

For each point, $\bar{T}$, f , g and mole fractions $\overline{X_{H_2O}}$ and $\overline{X_{CO_2}}$ are shown in figure 15. It is clear that for point 1, near the inflow opening, the path is the least uniform and the mixture fraction fluctuations g are the largest. It may therefore be expected that differences between the three computation methods will be the largest in point 1.

Table 4 gives the total (normal) fluxes from the flame for the four points and for methods 1 to 3, (10)–(13). Results of method 3 (the stochastic method) have a statistical uncertainty, for which the standard deviation is also given. Several things may be noticed from table 4. In the first place, the total flux shows a maximum somewhere halfway in the flame. Towards the end of the flame and away from the flame axis, the flux decreases.

Secondly, the differences between the fluxes calculated according to the three methods are the largest near the inflow. In point 1, the stochastic method predicts

Table 4. Mean total normal radiative fluxes from the combustion gases at points 1 to 4 in the glass furnace, calculated according to methods 1 to 3. For method 3, the standard deviation s in the mean flux is also given.

Point	$q(\text{kW m}^2 \text{sr}^{-1})$			$s(q_3)$ ($\text{kW m}^2 \text{sr}^{-1}$)
	Method 1	Method 2	Method 3	
1	51.49	53.02	65.38	0.34
2	67.05	67.48	70.33	0.26
3	54.89	55.12	56.16	0.19
4	55.39	55.77	57.52	0.18

Figure 15. Mean temperature (T), mixture fraction (f), mixture fraction variation (g), and mole fractions (X) of H_2O and CO_2 vs. distance from the refractory in normal direction above points 1 to 4, (a) to (d).

Table 5. Mean total directional radiative fluxes at point 1 in furnace, for different directions according to methods 1 to 3 as well as one case with a black background at temperature T_b .

$\theta(^{\circ})$	$T_b(\text{K})$	$q(\text{kW m}^2 \text{sr}^{-1})$			$s(q_3)$ ($\text{kW m}^2 \text{sr}^{-1}$)
		Method 1	Method 2	Method 3	
+ 30	0	63.43	64.84	75.47	0.60
+ 60	0	82.05	83.82	96.30	0.60
- 30	0	41.12	42.95	58.25	0.37
- 60	0	18.78	20.40	35.20	0.32
0	1850	210.1	211.7	222.9	0.48

a 27% higher flux than method 1, whereas method 2 only gives a 3.0% higher flux. However, further away from the inflow opening, the effect of turbulence quickly becomes smaller. For point 2, q_3 is only 4.9% higher than q_1 , and in point 3 this difference is only 2.3%. Even method 3 predicts flux increases by turbulence that are lower than are given by Faeth *et al* (1989). This may be a consequence of the fact that they studied vertical diffusion flames where buoyancy can induce strong fluctuations.

Table 5 shows total fluxes in point 1, calculated for different angles with the normal. Positive values of the angle indicate that observation is in the direction of the outflow opening in the symmetry plane of the flame (figure 4). A negative value indicates a beam towards the inflow port. With increasing positive angle, fluxes are found to increase, partly because the path length is increased. Moreover, the influence of turbulence is found to decrease. The latter probably is the result of decreasing values of g towards the end of the flame. The opposite is valid for negative angles.

Also in table 5 fluxes are shown in normal direction in point 1, from the flame with a background flux. The background has been assumed to be a black surface at

Table 6. Influence of soot on model predictions. Soot model of Syed *et al* (1990) has been used. Different values for the constants in the soot model were used for the two different flames to obtain agreement with measurements.

	$T_{\max}$ (K)	T_{flue} (K)	$\text{NO}_{\text{flue}}(0\%)$ (ppm)	Q_{load} (kW/m^2) ($\times 10^7$)	$f_{v,\max}$ ($\times 10^7$)
<i>Underport firing</i>					
no soot	2451	1710	1408	72.25	—
with soot	2451	1701	1314	73.19	1.15
<i>Overport firing</i>					
no soot	2331	1759	1014	71.97	—
with soot	2324	1699	623	76.42	5.39

1850 K. This temperature is approximately the refractory temperature in the furnace. The refractory has been taken as black to avoid severe complication of the program when the calculation of reflected radiation is included. It turns out that with a black background radiation, the effect of turbulence is unchanged in the absolute sense. In relation with the total flux, the relative effect is reduced.

5.5 Effect of soot formation

Based on spectral radiation measurements carried out at the IFRF, Wieringa (1992) has estimated the amount of soot present in the IFRF furnace for two different flames. For the underport flame the maximum f_v is of the order 1.3×10^{-7} ; for the overport flame $f_{v, \max}$ is of the order 5.0×10^{-7} .

The constants of the soot model were adjusted for each of the two flames such that the simulated values of f_v correspond to the experimental values. Table 6 shows the influence of taking soot into account in the simulations. For the underport flame, soot loadings are too low to observe any important effect. The mean temperature decreases slightly and the NO emission level reduces only 7%. However, for the overport flame the temperatures decrease significantly because the flame radiation is stronger. This has the effect that the NO emission level is reduced almost 40%. Figures 16a and b show the [NO] distribution for the overport flame with and without accounting for the effect of soot. Also the flux to the load has increased. Measured NO emission levels are 1214 ppm for the underport flame and 342 ppm for the overport flame.

5.6 Reduction of NO-formation

In the IFRF semi-technical furnace many tests have been done on burner modification to the effect on NO-formation and combustion. Next to underport firing, side-port and overport firing have also been done.

Figure 16. NO concentration (ppm) in overport flame without (a) and with (b) soot. Interval between contourlines – 100 ppm.

Figure 17. Comparison of the simulated and the measured NO emissions of the IFRF tests. (Circles correspond to underport flames, triangles to overport flames, squares to underport/overport flames, diamonds to sideport flames and crossed squares to parallel sideport flames. Also shown are the $\pm 20\%$ deviation lines.)

In general, these tests resulted in lower NO_x concentrations in the flue gases, than for underport firing (see Koster 1992). The injection angle of the natural gas jet into the air flow is important. A large angle enhances mixing of gas and air leading to shorter flames but higher NO_x values. In general, a less intense mixing results in longer flames with less NO-formation. A reduction from 1600 to 400 ppm can be obtained by burner modifications. All tested cases have also been simulated (Koster 1992). Figure 17 shows that within 20% for most tests a good agreement is reached between measurements and simulations, except for a few cases of low NO_x concentrations in the tests. These were the slowly mixing, parallel-fired burner modes. In the simulations we obtained higher NO_x values, probably due to enhanced numerical diffusion in the initial part of the flame for the simulations. However, for practical applications these slowly mixing flames are unacceptable, as they give rise to a low burn-out and very high CO concentration.

Further possibilities to reduce NO-emissions like air- or gas-staging, multiple gas injectors and increased recirculations of the gases can easily be investigated with the simulation model.

6. Conclusions

A complete computational model for turbulent flow, combustion and heat transfer in high temperature furnaces has been developed. It includes radiative heat transfer from combustion gases as well as turbulent flow and flame chemistry. With this model furnace performance can be predicted.

Comparison of computed results with measurements in a semi-technical furnace shows good agreement for heat-flux distribution to load, furnace efficiency and concentration of the pollutant NO in flue gases. With the model many burner configurations could be computed. For the NO-concentration it could be shown that a low-mixing flame can result in a low NO-concentration.

Thermal radiation is the main mode (95%) of heat transfer in these furnaces. Spectral effects of gas radiation are important. Due to this, increasing the refractory emissivity from the usual value of 0.4 to 0.95 can result in 5% increase in furnace efficiency.

Turbulent fluctuations are shown to have a large influence on the radiative heat transfer in the flame zone of the combustion chamber. These fluctuations are also important in the NO-formation. Neglecting them leads to a 43% lower value for the emission of NO in the flue gases. The developed model ("Furnace"-code) can easily be used for the design of new and improved burners or furnaces.

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