THE INFLUENCE OF THE DISCRETIZATION NUMERICAL SCHEME IN HIGH SWIRLING REACTING FLOWS

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Key words: Spray Flame, Swirling Flow, Discretization Scheme.

Abstract. This article describes and evaluates a recent developed discretization numerical methodology for the flow field transport equations. It was used to study the influence of numerical details in the predictions of a high swirling heavy-fuel-oil spray flame. The model is based in the finite volume technique and adopts the exponential model assumptions. Quadratic functions are defined to approximate exponential expressions related to the definition of the coefficients of the discretized algebraic equations and to the definition of the convective coefficients. It was found that the accurate definition of these coefficients, in the interface of the control volumes, is determinant to the accurate prediction of the thermodynamic properties of the flow field. These properties are correlated with the extension of the recirculation zones, which are strongly affected by the methodology adopted to define the convective coefficients. An alternative based in the QUICK scheme was also used to define these coefficients but it was verified that the solution adopted by the QEXP model leads to a greater consistency with the experimental observation.
1 INTRODUCTION

In turbulent reacting flows, the computational models are confronted with many difficulties associated to the high interdependency of the equations that describe physical phenomena.

In many situations of practical concern, the models based in the finite volume approach have demonstrated high versatility and computational robustness. This formulation consists in the discretization of the physical domain in a collection of cells, or control volumes, and in the conversion of the differential equations into algebraic equations, written for each cell.

The conversion of the differential equations into algebraic equations must preserve the correct representation of the physical phenomena and must also ensure numerical stability. Models based in the exponential model proposed in\(^1\) fulfil these two simultaneous restrictions. However, to reduce the computational time, this model is, generally, substituted by an asymptotic approximation, known by hybrid scheme, presented in\(^2\).

Due to its simplicity and computational economy, the hybrid model has been frequently preferred in combustion applications. The results obtained with this approach are often considered satisfactory, when compared with those obtained with higher precision models. Nevertheless, there are situations, like high swirling flows, in which the computational models using this methodology, and others, lead to significant divergences relatively to the experimental observation. The explanations for these discrepancies have been based, mainly, in limitations attributed to the physical models, namely the turbulence model.

The present work provides information that supports the hypothesis that the discretization model has a significant influence in the results. A high swirling spray flame is predicted using two alternative discretization methodologies, which adopt different approaches to evaluate the convective fluxes in the interface of the control volumes.

It has been verified in pervious studies, e.g.\(^3\), that the prediction of thermodynamic properties in high swirling reacting flows are conditioned by the extension of recirculation zones. Using the hybrid scheme to predict a flame with a swirl number of 0.9, it was concluded that the extension of the recirculation zones where inaccurately predicted. However, recently, in\(^4\), it was possible to improve these predictions using a new discretization model, suggested in\(^5\) and identified as QEXP. This approach is based on quadratic approximations of the exponential model; to define both the coefficients of the algebraic equations and the convective coefficients used to evaluate them. Another alternative to the linear interpolation is a quadratic one that can be defined using the methodology suggested in\(^6\) and known by Quick scheme.

Comparatively to pervious studies, in this work, to stress the influence of the numerical models, a flame with a higher swirl number (1.3) is predicted. The results obtained with the QEXP model are compared with those obtained with an approach based in the QUICK scheme, which is more precise than the hybrid approach. It will be concluded that the results obtained with the QEXP model are more consistent with the experimental observation and that those based in the QUICK approach exhibit divergences similar to those verified previously using the hybrid scheme in the lower swirl number flame.
This paper is organised in four sections. This one presents the framing of the problem studied and identifies the main objectives of the work. The next section describes the mathematical and numerical models with emphasis in the discretization scheme. The results are presented and discussed in the third section and the final section highlights the main conclusions of this study.

2 MATHEMATICAL MODEL

The mathematical model that was used and evaluated in this work has been developed to predict the behaviour of spray flames. It is described in detail in\textsuperscript{7,8} and it includes some of the more recent developments that emerged from the continuous effort since 1990 to improve the prediction ability.

Spray flames can be modelled using turbulent diffusion flame procedures but, in general, a two-phase flow approach is required. In this case, a dispersed liquid phase is used to model the vaporisation of the fuel and a continuous gaseous phase is used to describe the mean flow field.

To efficiently account for the several interacting phenomena, the model has been organised in four interacting modules. The main module is used to predict the mean flow field properties according to the information provided by the others that account for the heat transfer by radiation, combustion and vaporisation of the spray.

The mean flow field properties are determined using Eulerian conservation equations for mass, momentum, energy and mass fraction of scalar properties. Turbulent effects are modelled averaging these equations and using the k-ε model, presented in\textsuperscript{9}. A transport equation for the variance of a scalar, \(g\), presented in\textsuperscript{10} and a polynomial probability density function, \(\text{pdf}\), consistent with the experimental observation, presented and evaluated in\textsuperscript{11,12} are used to determine the average values of scalar properties that are directly influenced by the combustion model. The transport differential equations are solved using the finite volume technique, described in the next subsection, implemented in a staggered grid in cylindrical coordinates.

The heat transfer by radiation, which interacts with the energy equation, was quantified using the discrete transfer model presented in\textsuperscript{13} and the Grey-Plus-Clear-Gas model proposed in\textsuperscript{14}. The soot concentration strongly influences the optical properties of the flame and, consequently, the heat transfer by radiation. For this purpose, it was calculated using a transport equation and adopting, for the source terms, the suggestions of\textsuperscript{15} for the formation of soot and the suggestions of\textsuperscript{16} for its oxidation.

The spatial distribution of the vaporised fuel was determined assuming that the spray can be represented by a distribution of droplets. Mathematically, the initial conditions of this distribution are characterised by a mass distribution, a velocity distribution and a size distribution. Lagrangian balance equations of momentum and energy are applied to the droplets, e.g.\textsuperscript{3}, and the turbulent dispersion of the droplets was quantified using a stochastic
approach based in the model presented in\textsuperscript{17}. The interaction between the two phases was quantified using the PSIC technique proposed in\textsuperscript{18}.

The combustion model interacts with the flow field model controlling the transference of latent energy to thermal energy. According to this function, a new combustion model, based in the fast chemistry assumption, has been developed to predict the main intermediate chemical species with significant energy content, such as CO and H\textsubscript{2}. The model used in this work was also used in\textsuperscript{19} and it is described in detail in\textsuperscript{20,21}.

2.1 The discretization of the mean flow field equations

Since the phenomena studied in this work occurs closely to the steady state conditions, the mean flow field equations can be written as:

\[
\frac{1}{A_j} \frac{\partial}{\partial x_j} \left[ A_j \left( \rho u_j \phi - \Gamma_\phi \frac{\partial \phi}{\partial x_j} \right) \right] = S_\phi
\]  

(1)

where $\Gamma_\phi$ is the effective diffusion coefficient of the independent variable $\phi$ and $A_j$ represents the surface area of the infinitesimal control volume, whose normal has the direction of the $x_j$ axis. $S_\phi$ represents a source term, $u_j$ is the velocity component in the $j$ direction and $\rho$ is the density.

The discretized equations are obtained integrating the differential equations in the finite control volumes. A representative node, where the properties of the flow field are calculated, is defined in each volume. Figure 1 shows a typical control volume, and the respective nomenclature, of a bidimensional problem in cartesian co-ordinates.

![Cartesian bidimensional control volume](image)

Figure 1 – Cartesian bidimensional control volume

The central node and its neighbours are usually identified as $P$, $N$, $S$, $E$ and $W$, respectively. The points $n$, $s$, $e$ and $w$ are located in the surfaces of the control volume and in the lines that
link two consecutive nodes. These indexes are also used to identify the components of the surface of the control volume. Integrating equation (1) in the control volume, it follows:

\[
\int \int \int \int \int \int V_r \left( \frac{1}{A_j} \frac{\partial}{\partial x_j} \left[ A_j \left( \rho u_j \phi - \Gamma_\phi \frac{\partial \phi}{\partial x_j} \right) \right] \right) dV = \int \int \int S_\phi dV
\]  

and using the divergence theorem this equation can be written as:

\[
\int \int \left( \rho u_j \phi - \Gamma_\phi \frac{\partial \phi}{\partial x_j} \right) n_j dA = \int \int \int S_\phi dV
\]  

where \( A_p \) is the area of the surface of the control volume \( V_p \) and \( n_j \) is the component, in the \( j \) direction, of the unit vector normal to the surface.

In this equation, the term of the left represents the net total flux (convective and diffusive) through the control surface. For the control volume represented in figure 1 this term can be written as:

\[
\int \int \left( \rho u_j \phi - \Gamma_\phi \frac{\partial \phi}{\partial x_j} \right) n_j dA = J_e - J_w + J_n - J_s
\]  

where, for example, the flux through surface east is defined by:

\[
J_e = \int \int \left( \rho u \phi - \Gamma_\phi \frac{\partial \phi}{\partial x} \right) dA
\]  

If a one-dimension dependence of the variables between consecutive nodes is imposed, equation (5) reduces to:

\[
J_e = \left( \rho u \phi - \Gamma_\phi \frac{\partial \phi}{\partial x} \right) A_e
\]
The integration of the source terms, \( S_\phi \), is obtained, generally, assuming that they are concentrated in the nodes and considering a linear dependence with \( \phi \):

\[
\iiint_V S_\phi \, dV = S_p \phi_p + S_U
\]  

(7)

To conclude the discretization procedure, it is necessary to specify the profile of the physical variables between two consecutive nodes. The density and the diffusion coefficients are, generally, represented by linear functions. However, this type of profile is not appropriated for the transported property \( \phi \), e.g.\(^{22}\). The alternatives used to define the profile of \( \phi \) are based in one-dimensional analytical solutions and in higher order polynomial approximations.

The exponential model\(^1\) is adopted, frequently, as reference but, due to computational inconveniences, it is, generally, substituted by the hybrid scheme\(^2\) which is an asymptotic approximation. A solution based in quadratic polynomials, known by QUICK scheme\(^6\), is also used frequently. Nevertheless, an alternative method\(^5\), identified as QEXP, which is based in quadratic approximations of the exponential model, is privileged in the present study.

Since it is assumed that the source terms are concentrated in the nodes, the evolution of \( \phi \), between two consecutive nodes, can be described by the following equation that balances the convection and diffusion effects:

\[
\rho u \frac{d\phi}{dx} - \Gamma_\phi \frac{d^2 \phi}{dx^2} = 0
\]  

(8)

this equation can be written as:

\[
\phi'' - \frac{P}{L} \phi' = 0
\]  

(9)

where \( L \) represents the distance between the two nodes and \( P \) is the Peclet number:

\[
P = \frac{\rho u L}{\Gamma_\phi}
\]  

(10)

For a constant Peclet number, the solution of equation (8) is:
\[
\phi(x) = \phi_1 + (\phi_2 - \phi_1) \frac{e^{P_0/L} - 1}{e^{P_0} - 1} \quad (11)
\]

where \(\phi_1\) and \(\phi_2\) represent the values of \(\phi\) in the two consecutive nodes.

The introduction of this profile into equation (6) leads to:

\[
J_e = C_e \left[ f_e \phi_p + (1 - f_e)\phi_E \right] \quad (12)
\]

where:

\[
C_e = \rho_e u_e A_e \quad (13)
\]

\[
f_e = \frac{e^{P_e}}{e^{P_e} - 1} \quad (14)
\]

The coefficient \(C_e\) represents the mass flow rate through surface \(east\) and \(P_e\) is the Peclet number in surface \(east\).

Similar expressions can be obtained for the remainder surfaces which, when introduced into equation (3), lead to:

\[
a_p \phi_p = a_E \phi_E + a_W \phi_W + a_N \phi_N + a_S \phi_S + Su \quad (15)
\]

where:

\[
a_E = C_e f_e - C_e \quad (16a)
\]

\[
a_W = C_w f_w \quad (16b)
\]

\[
a_N = C_n f_n - C_n \quad (16c)
\]

\[
a_S = C_s f_s \quad (16d)
\]

\[
a_p = a_E + a_W + a_N + a_S + Sm - Sp \quad (17a)
\]

The term \(Sm\), in the expression of \(a_p\), represents the mass balance to the control volume and it is defined as:

\[
Sm = C_e - C_w + C_n - C_s \quad (17b)
\]

Introducing a diffusion coefficient defined by the expression \(D = \Gamma A/L\), and noting that the Peclet number can be defined as \(P = C/D\), the expressions (16:a,b,c,d) can be written as:
\[ a_E = D_e F_e - C_e \]  
\[ a_w = D_w F_w \]  
\[ a_N = D_n F_n - C_n \]  
\[ a_S = D_s F_s \]  

where the function \( F \) is defined by the expression:

\[ F(P) = P f(P) \]  

Due to the computational time associated to the evaluation of the exponential expression, this function has been substituted by its asymptotic approximation:

\[
F(P) = \begin{cases} 
  P & \leq P \geq 2 \\
  1 + \frac{P}{2} & \leq -2 < P < 2 \\
  0 & \leq P \leq -2 
\end{cases}
\]  

Using this approximation, the coefficient \( a_E \), for example, can be evaluated from:

\[
a_E = \begin{cases} 
  0 & \leq 0.5C_e \geq D_e \\
  D_e - 0.5C_e & \leq 0.5C_e < D_e \\
  -C_e & \leq -0.5C_e \geq D_e 
\end{cases}
\]  

which is usually represented by the following compact expression, e.g.:\n
\[ a_E = \text{Max}\left(0.5C_e, D_e\right) - 0.5C_e \]  

Following the same procedure, similar expressions are obtained for the other coefficients:

\[ a_w = \text{Max}\left(0.5C_w, D_w\right) + 0.5C_w \]  
\[ a_N = \text{Max}\left(0.5C_n, D_n\right) - 0.5C_n \]  
\[ a_S = \text{Max}\left(0.5C_s, D_s\right) + 0.5C_s \]
Although these expressions have been used frequently, they don't provide any computational advantage. The construction of an efficient subprogram to evaluate $F$, using for example the expressions (20), and the evaluation of the coefficients directly from equations (18:a,b,c,d), leads to a significant reduction of the computational time.

Additionally, the function $F$ can be represented by higher order polynomials. For example, a quadratic approximation, defined by the following expressions was suggested in5:

$$F(P) = \begin{cases} 
  P & \iff P \geq 4 \\
  1 + \frac{P}{2} + \frac{P^2}{16} & \iff -4 < P < 4 \\
  0 & \iff P \leq -4 
\end{cases} \quad (23)$$

The degree of approximation of this solution, and of the asymptotic representation, is evaluated graphically in the next figure.

![Figure 2 – Evaluation of $F$ and two approximated solutions.](image)

The precision of the discretization model depends, also, on the evaluation of the total fluxes in the control volume surfaces. From equation (12) it can be concluded that the evaluation of the total fluxes depend on the evaluation of the convective fluxes and on the evaluation of $f$. The asymptotic analysis of this function leads to the conclusion that for high Peclet numbers the coefficients of the algebraic equations represent the inlet convective fluxes (i.e. the inlet mass flow rates). Thus, the definition of $F$ is conditioned to the utilisation of Peclet numbers defined using the velocity components in the control volume surfaces.

The solution of the momentum transport equations is subject to the fulfilment of the continuity equation and to the determination of the pressure field. In this study, these requirements are satisfied using a staggered grid and the Piso algorithm23.
An example of a cartesian bidimensional staggered grid, where a control volume of the velocity component along \( x \) is represented, is shown in the next figure.

![Figure 3 - Example of a staggered grid showing the scalar cells and a \( u \) cell.](image)

This type of grid is characterised by the location of the nodes of the velocity components in the surfaces of the control volumes of the scalar properties, whose nodes are defined by the intersection of lines \( i \) and \( j \). An advantage of this arrangement is that the velocity components become directly available to evaluate the convective fluxes in scalar control volumes but it presents also computational stability benefits, e.g.\(^{22}\).

The evaluation of the convective fluxes in the control volumes of the velocity components is more complicated. The simplest solution corresponds to a linear interpolation, which is adopted in the hybrid scheme. In this study two alternative methodologies are analysed: the solution adopted by the QEXP model, that is based in a quadratic approximation of the exponential solution, and a solution based in the QUICK scheme. These alternatives are illustrated considering the evaluation of the axial velocity in face \( east \), that is represented in figure 3 by \( u_e \).

In the QEXP model, that includes the evaluation of \( F \) using expression (23), the value of \( u_e \) is estimated from equation (11) using a Peclet number based in the average velocity of nodes \( P \) and \( E \). To simplify the evaluation procedure, surface \( east \) is located in the middle of these nodes. In this case, equation (11) leads to the following expression:

\[
\begin{align*}
\frac{u_e}{u} &= \frac{u_p + u_E}{2} + \left( u_E - u_p \right) G(P) \\
&= u_e - u_p + \frac{1}{2} \left( u_E + u_p \right) G(P)
\end{align*}
\]  

(24)

where:
\[ G(P) = \frac{2e^{p/2} - e^p - 1}{2e^p - 2} \quad (25) \]

This equation can be approximated by the following expressions:

\[
G(P) = \begin{cases} 
-\frac{P}{8} + \frac{P|P|}{128} & \iff |P| < 8 \\
-0.5 \frac{P}{|P|} & \iff |P| \geq 8 
\end{cases} \quad (26)
\]

The degree of approximation of this solution, and of an asymptotic representation, is evaluated graphically in the next figure.

\[ \text{Figure 4} \quad \text{Evaluation of } G \text{ and two approximated solutions.} \]

In the alternative solution based in the QUICK scheme \( u_e \) is evaluated using a quadratic function that is defined using nodes \( P \) and \( E \) and a third node that is on the left of \( P \) if the velocity in the three nodes is positive or a node that is on the right of \( E \) if it is negative. If neither of these conditions is verified a linear approximation is used.

Under these conditions, the quadratic profile can be defined by the expression:

\[
u(h) = u_p + \frac{u_E - u_p}{h_{EP}} h + C(h^2 - h_{EP}) \]

(27)
where \( h = x - x_p \) and \( h_{EP} \) is the distance between nodes \( P \) and \( E \). The constant \( C \) is related with the second derivative and it can be evaluated using the following expression:

\[
C = \frac{1}{h_{31}} \left( \frac{u_3 - u_2}{h_{32}} - \frac{u_2 - u_1}{h_{21}} \right) \tag{28}
\]

where the indexes 1, 2 and 3 identify the three consecutive nodes involved in the definition of the profile; \( u_1, u_2 \) and \( u_3 \) represent the velocities in these nodes; and \( h_{21}, h_{32} \) and \( h_{31} \) represent the distances between nodes 1 and 2, between nodes 2 and 3, and between nodes 3 and 1, respectively.

This methodology is subject to the possibility of defining values of the represented variables out of the physical accepted limits which for \( u_e \) are the velocity values in nodes \( P \) and \( E \). This undesired behaviour occurs when the first derivative in these nodes has opposite signs. In this situation, to avoid the possibility of defining unacceptable values, the first derivative in one of these nodes is set to zero, which imposes a maximum absolute value of the second derivative defined by the expression:

\[
|C_{\text{max}}| = \frac{|u_e - u_p|}{h_{EP}^2} \tag{29}
\]

The effect of this condition is illustrated in figure 5 considering a situation of decreasing positive velocity, where nodes 2 and 3 correspond to nodes \( P \) and \( E \), respectively.

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Figure 5 – Examples of quadratic profiles:
- a) Accepted profile;
- b) undesirable profile;
- c) corrected profile.
In this figure, profile \( a \) represents an accepted profile, that will not be modified, while profile \( b \) is undesirable because it leads to inconsistent values between nodes \( P \) and \( E \). Profile \( c \) was obtained from profile \( b \) substituting \( C \) by \( C|_{\max} / C \).

3 RESULTS AND DISCUSSION

The numerical results obtained with the mathematical models described in the previous section are compared with experimental results correspondent to a heavy-fuel-oil spray flame, presented in\(^2\). The flame studied was obtained in a cylindrical furnace with diameter 0.6 m and height 3 m. The main geometry details, relevant for the present work, are related with the burner which is located on the top and is characterised by two coaxial inlets. The centre one is a 35 mm diameter tube with a twin-fluid atomiser characterised by a 6.3 mm exit diameter. A fuel mass flow rate of 12 kg/h, at the temperature of 95 °C, and an atomising air mass flow rate of 15 kg/h, at the temperature of 20 °C, are introduced in the combustion chamber through this inlet. The second inlet is characterised by a tube with an internal diameter, \( D_s \), of 56 mm that is connected to a quarl with a length of 54 mm and an exit diameter of 104 mm. Through this inlet an air mass flow rate of 170.2 kg/h with a temperature of 300 °C and a swirl number of 1.3 is introduced in the combustion chamber.

The fuel is characterised by a carbon and hydrogen mass composition of 86% and 9.8%, respectively, and the combustion model regards the rest of the components as inerts.

The boundary conditions related with the flow field were set assuming uniform axial and angular velocities and standard turbulent properties, in this type of application. In what concerns the radiation model, the wall emissivity was assumed equal to 0.75 and a linear wall temperature distribution was defined assuming that the top and exit temperatures are 1500 K and 600 K, respectively. Assuming that the coalescence of droplets is negligible and that the break-up of the fuel is complete at the atomiser exit, a droplet size distribution obtained experimentally 75 mm downstream, under no reactive conditions, was adopted. This distribution was discretized considering 20 diameter classes. Based in the analysis presented in\(^1\), a uniform inlet mass distribution and a constant initial velocity of the droplets, equal to 75 m/s, are assumed.

The first results presented correspond to predictions obtained using the expressions (23) to evaluate \( F \) and the procedure based in the QUICK approach, described in the previous section, to evaluate the convective fluxes in the interfaces of the velocity's control volumes. Figures 6(a,b,c) show the calculated and experimental radial profiles of the \( O_2 \) and \( CO_2 \) dry volume concentrations and the temperature of the gaseous mixture, respectively, in three axial positions that are defined by \( x / D_s = 1.14 \), \( x / D_s = 2.21 \) and \( x / D_s = 5.07 \). The experimental values of the temperature in the first plan are not available.
Figure 6 – Experimental and calculated radial profiles obtained using the QUICK approach: x1) \( x / Ds = 1.14 \); x2) \( x / Ds = 2.21 \); x3) \( x / Ds = 5.07 \).

These results show that the predictions’ approach to the experimental data is satisfactory in the first plan. However, in the second and third plans there are significant divergences. The location of the peaks in the \( O_2 \) and temperature profiles is not accurately predicted.
The next results correspond to predictions obtained using the QEXP model. Figures 7(a,b,c) show the calculated and experimental radial profiles of $O_2$, $CO_2$ and temperature of the gaseous mixture, respectively, in the three axial positions.

![Graph a) Dry volume concentration of $O_2$](Image)

![Graph b) Dry volume concentration of $CO_2$](Image)

![Graph c) Temperature of the gaseous mixture](Image)

Figure 7 – Experimental and calculated radial profiles obtained using the QEXP approach: x1) $x / Ds = 1.14$; x2) $x / Ds = 2.21$; x3) $x / Ds = 5.07$. 
These results show that, in this case, the predictions approach to the experimental data is, in general, satisfactory. Minor discrepancies can be observed in the location of the inflection points in the \( O_2 \) and \( CO_2 \) profiles, and the temperature profiles are much closer to the experimental observation.

The different behaviour of the thermodynamic properties predicted with the two alternative discretization procedures indicates that they lead to different predictions of the extension of the recirculation zones, that have a strong influence in the results. This conclusion is illustrated in the next figure which presents the predictions of the external recirculation zone. Two streamlines correspondent to 90\% of the total inlet mass flow rate, and lines that define the three planes considered in figures 6 and 7, are shown.

![Figure 8 – Predictions of the external recirculation zone and the location of the plans: \( x/D_s = 1.14 \), \( x/D_s = 2.21 \) and \( x/D_s = 5.07 \):](image)

a) Result obtained with the QUICK approach;
b) Result obtained with the QEXP model.

The correlation between the extension of the external recirculation zone and the profiles of the thermodynamic properties can be explained through the analysis of the behaviour of the \( O_2 \) profiles. The peak of \( O_2 \), in the first and second plans is located near the frontier of the external recirculation zone. However, with the QUICK approach the radial location of this frontier in the second plane is too high which justifies the significant divergences with the experimental results.

A qualitative analysis of the algebraic equations provides some justification for the better performance of the QEXP model, in this application. Close to the quarl the axial velocity decreases but the Peclet number is high. Under these conditions the coefficient \( a_w \) represents the inlet mass flow rate through surface \( w \). The evaluated velocity by the QEXP model in this surface is closer to the velocity in node \( W \) but the evaluated velocity by the QUICK approach is closer to the average of the values in nodes \( W \) and \( P \). Consequently, comparatively to the QEXP model, the QUICK approach underestimates the mass flow rate through surface \( w \). In
this case, the relative weight of the information in node \( W \) is lower which contributes for a faster reduction of the axial velocity and to a less extent external recirculation zone.

The calculations were performed in a carefully specified grid of 122\( \times \)72 scalar nodes. Near the quarl exit the distance in the \( x \) direction, between two consecutive nodes, \( L \), is about 4 mm and the Peclet number is close to 40. As mentioned before, under these conditions the QEXP model assigns a value to \( u_w \) equal to \( u_H \). It should be pointed out that this is consistent with the adopted hypothesis that the source terms are concentrated in the nodes. Since in this situation the diffusion is negligible, the main change of \( u \), between nodes \( W \) and \( P \), is due to the source term in \( P \) and should be concentrated near this node. By contrast, the QUICK approach will assign a value to \( u_w \) that will not be so far from the average of the values \( u_H \) and \( u_P \), which under the exponential model assumptions, corresponds to a high diffusion effect.

Since the evolution of the external recirculation zone is strongly influenced by the equilibrium of forces near the quarl exit, e.g.\(^{25} \), it is unlikely that with the present level of grid refinement different results are obtained with a different turbulence model. Turbulence Reynolds stresses have a diffusive effect and, under the QEXP model, close to quarl exit, they would have to lead to an effective diffusion coefficient two orders of magnitude higher to lead to a different value of \( u_w \).

On the other hand, it is interesting to notice that not all properties are so influenced by the details of the mean flow field that have been discussed. For example, the next figure shows the experimental values and the predictions of the incident radiation flux in the lateral wall, obtained with the two methodologies considered.

![Figure 9](image)

**Figure 9** – Experimental values and predictions of the incident radiation flux:

a) Results obtained using the QEXP model;

b) Results obtained using the QUICK approach.

It is evident from these figure that the two profiles correspondent to the QEXP model and to the QUICK approach are almost coincident and agree very well with the experimental results. Since this variable highly influences the evaluation of the efficiency of the furnace, it may be concluded that for many practical purposes the two methodologies are acceptable.
4 CONCLUSIONS

The present study was dedicated to the evaluation of the influence of numerical details related with the mathematical modelling of high swirling flows with combustion. A model that has been developed to predict the behaviour of spray flames in industrial furnaces was described. Special attention was dedicated to the discretization numerical methodologies of the transport differential equations that are used to describe the behaviour of the mean flow field.

The finite volume formulation was adopted to convert the differential equations into algebraic equations and two alternative discretization schemes were analysed in detail. Both of these alternatives adopt the exponential model as reference, which preserves the correct representation of the physical phenomena and ensures numerical stability. The main differences are related with the evaluation of velocity components in the interface of the respective control volumes, which are used to evaluate the convective fluxes in the interfaces of the velocity control volumes. The model identified as QEXP, was built defining quadratic functions to approximate exponential expressions related with the definition of the coefficients of the algebraic equations and with the definition of convective coefficients. The other solution was defined using some assumptions of the exponential model but using the QUICK approach to define the convective coefficients.

It was found that the results correspondent to the thermodynamic properties of the mean flow field, in the near burner region, are very sensitive to the alternative discretization methodologies. Furthermore, it was concluded that the predictions obtained with the QEXP model are more consistent with the experimental observation.

The differences of the two alternatives were explained identifying the correlation of the profiles' shape of the thermodynamic properties with the extension of the recirculation zones. In particular, it was seen that the solution based in the QUICK approach lead to an underestimation of the extension of the external recirculation zone. This behaviour was justified by the underestimation of the upstream convective fluxes in the near burner region, which contributes to a faster reduction of the axial velocity.

Finally, it was found that not all properties have the same sensitivity to the extension of the recirculation zones and, consequently, to the discretization numerical scheme. For example, the predictions of the incident radiation flux in the lateral wall of the furnace, obtained with the two alternatives, are almost coincident.

REFERENCES


