TURBULENT FLOW MODELLING IN SPAIN. OVERVIEW AND DEVELOPMENTS.
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ABSTRACT
A brief overview of ongoing flow modelling activities in Spain in the fields of turbulent boundary layers, two-phase flows and turbulent reactive flows is presented. Turbulent shear flows laden with small solid particles and the turbulent isothermal mixing of two chemical species undergoing a second order irreversible chemical reaction are discussed in more detail. An eulerian approach is followed in the former, employing a phase indicator function conditioning technique for the continuous phase and a Boltzmann type velocity distribution function for the dispersed phase. The latter is treated via a probability density function (pdf) formalism where the joint statistics of concentrations and concentration-gradients is investigated. Predictions are compared with available experimental results in both cases.

Some concluding remarks on the specific needs on modelling or turbulent two-phase and reacting flows are listed.

1. INTRODUCTION
As in most fields of scientific research, the ultimate goal in the investigation of turbulent flows is to develop a quantitative tractable predictive theory. This objective is hampered by the existence of a wide spectrum of length and time scales, ranging from the characteristic sizes and frequencies of the large turbulent structures to the Kolmogorov length and time microscales. This prevents direct numerical simulation (DNS) of turbulent flows in most cases of practical interest. DNS\textsuperscript{13, 16, 31, 36} of some idealized and limit cases can provide useful information on the asymptotic behavior of turbulent fields.

Existing computers set a limit on the length and time scales that can be numerically resolved. Large eddy simulation (LES) methodology\textsuperscript{21} filters the contribution to a fluctuating variable coming from large structures averaging the effects of small scales below a given threshold. The latter introduce unknown terms in the resulting equations. Models or closure hypothesis must be proposed in order to proceed further to the numerical simulation. In some instances, dumping the small scale contributions into a collective pool may yield good results. This can be the case of the turbulence modelling where most energy production and energy transfer processes are dominated by large/intermediate size eddies, while the overall small-scale action upon the flow can be simulated and quantified as a diffusive-like irreversible mechanism. However, if a process is tied to the small fluctuating scales the closure difficulties might render LES strategies useless. This is the case of chemically reacting turbulent flows.

Reynolds averaging techniques consider the contribution to a fluctuating variable coming from the whole spectrum of length and/or time scales\textsuperscript{22}. The closure problem can be more severe and difficult to solve than the equivalent one in LES for the velocity field or of the same order to complexity for a reactive scalar in a turbulent flow. Moment and probability density function (pdf) equations have been obtained after Reynolds-averaging the corresponding local-instantaneous conservation equations. Most modelling activity has revolved around moment-equations\textsuperscript{18, 19}. Pdf transport equations condense the information equivalent to an infinite hierarchy of moment equations\textsuperscript{9, 10, 25}. It has been shown that the pdf formalism is the natural one for turbulent reactive flows\textsuperscript{10} and that pdf models can be proposed based on second order closure models\textsuperscript{29}.

An overview of ongoing activities on turbulent flow modelling in Spain is presented in Section 2. Modelling work on turbulent boundary layers, two-phase flows and turbulent reactive flows is briefly described. More details on the specific needs on closure models are provided in Section 3 for two selected cases: Turbulent shear flows laden with small solid particles and turbulent isothermal mixing of an acid and a base undergoing a second order irreversible chemical reaction; these cases exemplify two areas in which significant modelling efforts are required. In the former even the basic equations and methodologies to be used as a starting point are being questioned. The latter is adequate to illustrate the difference between what seems to be the natural pdf approach and what most moment modellers in the field are doing. Section 4 contains some concluding remarks on the two selected cases.

2. OVERVIEW
The following ongoing turbulent flow modelling activities in Spain have been brought to the attention of the authors:

2.1 Turbulent Boundary Layers
2.1.1 Asymptotic Expansion Techniques\textsuperscript{7, 26}
Turbulence modelling is being conducted via the asymptotic techniques originated within the framework of "periodic homogeneization theory". The flow variables are asymptotically expanded and the model can, thus, be formally justified. The averaged partial differential equations have a structure analogous to that of the compressible Navier-Stokes equations.

The starting point is the so called MPP turbulence models\textsuperscript{20}, valid for incompressible flows of ideal or weakly viscous fluids. These models have been generalised in a first attempt\textsuperscript{7} to inviscid compressible
isentropic flows. No closure hypothesis are required at this level. The Reynolds stress tensor is obtained from the solution of a non-linear differential equation. The gradient of the inverse lagrangian coordinate associated to the mean velocity field, the average turbulent kinetic energy and the average helicity appear as parameters in that equation. The unclosed terms can then be tabulated and it is to be expected that the corresponding table has a universal character. These models do not take into account the flow behavior near solid walls. On the other hand, mechanisms for turbulence generation are not considered and models are typically non-stationary.

As a first step, a reformulation of asymptotic models for moderately high Reynolds number and moderate Mach number compressible isentropic flows has been achieved. Non-standard boundary conditions adding new non-linearities to the problem and based on the well known logarithmic law of the wall have been introduced to take into account the existence of boundary layers. The methodology followed to numerically solve the problem is described in detail in Reference 26 where a large number of numerical results are presented.

In a second step, new models describing the turbulent motion of the fluid over the whole domain, including the regions near solid walls, have been formulated. The flow domain is decomposed into a turbulent boundary layer and an inviscid outer zone. Small parameters are introduced and asymptotic expansions for the flow variables are hypothesized for the different zones. Formal manipulation of the equations, identifying the coefficients of the various powers of the small parameters, lead to averaged variable equations for the inner and outer zones. The original initial and boundary conditions are supplemented with those obtained from "matching" the inner and outer variables. The use of these models allows, among other things, to rigorously justify, from the asymptotic point of view, the laws of the wall.

The numerical solution rest upon semi-implicit time discretization schemes and finite element type approximation for the space variables. A least square type formulation is utilized followed by an algorithm of the Buckley-Le Nir conjugate gradient. Finally, the numerical problem is reduced to the solution of a "cascade" of linear problems, some of them analogous in nature to the Stokes problem, which can be solved using, for example, the Glowinski-Pironneau method, and others of the Poisson type.

These techniques are being developed within the framework of the HERMES Project of the European Space Agency (ESA) in order to predict the thermal behavior of this space aircraft during its reentry into the earth's atmosphere.

2.1.2 Algebraic Model of Turbulence

The two-dimensional (2D) compressible laminar Navier-Stokes equations are considered in a non-dimensional form,

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = 0 \quad (1)$$

where the flux vectors $F$ and $G$ can be expressed as $F = F^I + F^V$, $G = G^I + G^V$. The superscripts $I$ and $V$ denote inviscid and viscous contributions, respectively, and

$$U = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho e \\ \rho \mu \\ \rho \nu \\ \rho \psi \\ \rho \phi \end{bmatrix}, \quad F^I = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho u v \\ \rho u h \\ \rho v u \\ \rho \mu^2 + p \\ \rho \nu u \\ \rho \phi u \end{bmatrix}, \quad G^I = \begin{bmatrix} \rho v \\ \rho v u \\ \rho v^2 + p \\ \rho \mu v \\ \rho \nu v \\ \rho \phi v \end{bmatrix}$$

Here $Re$ and $Pr$ denote the Reynolds and Prandtl numbers respectively, $\rho$ and $\nu$ the two components of the velocity vector and $\rho$, $e$, $p$, $h$ and $T$ are the dimensionless density, specific total energy, pressure, specific total enthalpy and temperature of the fluid. The Sutherland relation is used to take into account the dependence of the molecular viscosity coefficient, $\mu$, on temperature and Mach number. The non-dimensional components of the stress tensor, $\tau_{11}$, $\tau_{12}$ and $\tau_{22}$ are assumed to follow the Navier-Poisson relation for laminar flows. The equation of state complete the problem specification.

For turbulent flows $\mu$ is replaced by $\mu + \mu_t$. $\mu$ is the laminar viscosity. For the "eddy viscosity coefficient", $\mu_t$, the Baldwin-Lomax algebraic model is used. The variables in Equ. (2) stand then for average values. Cebeci's modifications avoid the calculation of the boundary layer edge.

In this two-layer model the turbulent viscosity is given by,

$$\mu_t = \begin{cases} \mu \text{ for } y \leq y_c \text{ for } y \leq y_c \\ \mu_t \text{ for } y > y_c \end{cases}$$

where $\mu_t$ and $\mu_0$ stand for inner and outer values of $\mu$, $y$ is the normal distance to the wall and $y_c$ is the crossover value, the minimum $y$ for which the inner and outer values of $\mu_t$ are equal.

Van-Driest formulation is followed for $\mu_t$,

$$\mu_t = C_l \rho L^2 w$$

where $C_l$ is a constant, and

$$l = k \left( \left[ 1 - \exp \left( - \frac{y}{y_c} \right) \right] \right)$$

$w$ is the mean vorticity module given by,
and \( y^+ = y u_*/n \), with \( u_* \) being the friction velocity and \( v \) the kinematic viscosity.

Clauser formulation is used to express \( \mu_0 \).

\[
\mu_0 = K \ C_{cp} \ F_w \ F_k(y)
\]  

(7)

\( K \) is Clauser constant, \( C_{cp} \) is an additional constant and

\[
F_w = \min (y_{\text{max}}, \ F_{\text{max}}, \ C_{wk} \ y_{\text{max}}, \ u_{\text{diff}}^2 / F_{\text{max}})
\]  

(8)

\( F_{\text{max}} \) is the maximum value of

\[
F(y) = y \left[ 1 - \exp (- y^+ / A^+) \right]
\]  

(9)

and \( y_{\text{max}} \) is the value of \( y \) at which \( F(y) = F_{\text{max}} \). \( F_k(y) \) is the Klebanoff intermittency factor,

\[
F_k(y) = [1 - 5.5 (C_k y/y_{\text{max}})]
\]  

(10)

\( u_{\text{diff}} \) is the difference between the maximum and minimum values of the velocity for a profile. The standard values are assigned to the constants.

The solution is obtained by advancing the unsteady non-dimensional form of the equations to steady state by means of a hybrid timestepping scheme. The convergence is accelerated by the use of local timestepping and the incorporation of implicit residual averaging. Spatial discretization is accomplished by means of a Galerkin finite element method assuming a general unstructured grid of linear three-noded triangular elements. In the code, this is achieved by the equivalent process of computing the element contributions from a loop over all the element sides in the mesh. To ensure complete vectorisation of this procedure, the element sides are automatically coloured by the mesh generator. The resulting scheme is stabilised by the application of an artificial dissipation operator which is formed as a blended combination of second and fourth differences.

2.2 Two-Phase Flows

2.2.1 Dispersed Phase as a Continuum

A monodispersed cloud of rigid spheres suspended in an incompressible isothermal viscous gas is considered. No mass transfer between the phases is included. The dynamic behavior of the particles is characterized by continuous velocity, pressure and concentration fields. For a distribution of particle sizes, as many velocity, pressure and concentration fields are required as the number of size families to be treated.

The particle/particle and particle/fluid interactions are simulated by the introduction of a "pressure" and a "viscosity" of the particle cloud and an inter-phase force taking into account the momentum transfer between the phases.

Should the particle cloud viscosity be ignored no macroscopic mechanism exists to set a limit to strong gradients. A discrete system of particles has been analysed in order to find a strong-gradients limiting mechanism for the continuum model. The inviscid flow around an ensemble of spherical particles has been investigated. None of the microscopic terms can prevent the development of strong gradients in the particle concentration. The consideration of the cloud viscosity seems thus to be necessary in order to describe small wavelengths.

On the other hand, the functional dependence of the particle cloud pressure is important and has significant macroscopic consequences upon the flow development.

The specification of the particle cloud viscosity and pressure are therefore open topics. The viscosity data measured by Schürgel for glass spherical particles of various diameters have been analysed. The viscosity increases considerably when the fluidised bed concentration approaches the maximum packing concentration; on the other hand, it has been observed that a dimensionless viscosity can be obtained by scaling the experimental data with the particle density, the fluidization velocity and a characteristic length which is a function of the particle diameter and Reynolds number. A universal curve of the dimensionless viscosity as a function of the volume concentration can then be plotted. More experiments are however necessary in order to ascertain the suspension rheological behavior. At moderately high loads the particles interact mainly with the surrounding fluid and the stresses of the cloud are mostly due to particle/fluid interactions. On the other hand, for high cloud concentrations the frequency of collisions between particles increases and the pressure of the particle cloud should substantially grow, preventing the cloud from attaining concentrations above that of maximum packing. Neither experimental data nor theoretical developments exist to model the cloud pressure at high concentration. However, the correct modelling of the pressure is essential, as this is an important mechanism limiting the maximum value of particle concentration.

2.2.2 Eulerian Formulation of Average Equations

In the theoretical derivation of two-phase flow equations, extensive use is made of conditioned averaging techniques. Spatial, temporal, or ensemble average and double/mixed average operators are frequently found in the literature. Two consecutive averages are also encountered in turbulent two-phase flow modeling. Nevertheless the existing formalisms are not quite satisfactory, specially in dealing with turbulent flows. Volume or time averaging produce filtering of small-scale turbulent structures or large fluctuating frequencies. To avoid that filtering effect, dispersed elements must be much smaller than Kolmogorov scales and the number of elements inside the probe volume large enough to get stable values. Those situations rarely occur in practice and are impossible to satisfy in dilute flows. Ensemble averages
avoid these problems but the interaction terms have no straightforward meaning and must be interpreted by comparison with other averages. Applying two consecutive averages lead to equations with a large number of terms with no direct physical meaning and include high order fluctuation correlations, creating some serious closure problems.

Following the usual conditioning technique based on a phase-indicator function and properly defining a joint probability density function to describe the dispersed phase dynamics, some of the ideas pointed out by Herczynski and Pienkowski are generalized. Theorems and associated properties are given allowing a general, rigorous and systematic treatment of the continuous phase of a dispersed two-phase flow system. The conditioned mean value of any variable derivative can be expressed as the derivative of the variable conditioned mean value, plus an extra interface source term, which will introduce in the equations information about the action of the second phase. The formalism employed, shares some features in common with those previously developed. The difficulties mentioned above are however overcome. Using those results conditioned average continuity, momentum turbulent kinetic energy and turbulence dissipation rate equations for the continuous phase can be obtained. The main characteristics of these equations are:

- General applicability. In principle no restrictions are placed on the sizes of dispersed elements or their concentrations.
- Continuous phase variables appear statistically averaged. Therefore no spatial or temporal filtering is performed.
- Continuous phase equations are obtained in a single-step averaging operation.
- Continuous phase equations are formally identical to those in classical turbulent single-phase flows, with similar terms and the same order of fluctuation correlations.
- A few additional interaction terms, with direct physical interpretation and mathematical properties which help in modeling them, enter the continuous phase equations.

General eulerian equations for the moments of the particle velocity are next obtained. This is done from a "Boltzmann type" probability density function transport equation which is assumed to correctly represent the particle cloud dynamics. Dispersed phase average continuity, momentum and fluctuating kinetic energy equations are then generated. Neither a particle cloud pressure nor viscosity appear in the average equations. Particle fluctuating velocity correlations and phase interaction terms are unknowns.

A k-ε turbulence model is used for the continuous phase. The dispersed phase is modelled via a gradient transport approximation where the particle turbulent diffusivity is rephrased in terms of a root mean square particle fluctuating velocity and, in the case of a dilute dispersed phase, a particle relaxation length. Closure hypothesis are also proposed for the phase interaction terms.

An axisymmetric turbulent jet configuration has been chosen to validate the model for both single phase and two-phase flows. A classical finite volume four-node formula space-marching fully-implicit scheme has been used. Validation has been conducted by comparing the model predictions with available experimental data. Preliminary predictions indicate a reasonably good agreement.

2.3 Turbulent Reacting Flows

The mixing of dynamically passive inert and reactive scalars convected by a field of nearly homogeneous turbulence is being investigated. The transport equation for the joint probability density function (pdf) of scalars and their gradients is used. Exact treatment is possible of the processes of the straining by mean velocity gradients, the chemical reaction and the dissipation of scalar fluctuations. Closure approximations are required for the non-closed terms describing the straining of scalar gradients by fluctuating velocity gradients and the dissipation of scalar/scalar-gradient and of scalar-gradient correlations by molecular diffusion.

A cumulant expansion technique is used to treat the turbulent straining term. The limit of large Kubo or Reynolds number ("strong perturbation limit") is identified. Furthermore, the "small time limit" allows to truncate the cumulant function operator series expansion at the second-order level. This small time pdf behavior is all that is required in order to derive a scalar-gradient increment random equation. For isotropic turbulent velocity gradients the straining is inversely proportional to the square of the Kolmogorov time micro-scale. The scalar gradients display a tendency to grow and to become isotropic.

A binomial sampling model is used to close the molecular dissipation terms. This model has features in common with the LMSE closure approximation and with Langevin models. This closure model leads to a qualitatively reasonable relaxation process and produces correct asymptotic results. A stochastic scalar-gradient straining model is proposed in terms of products of two random vectors. This simulation also implies a model for the turbulent velocity gradient and, therefore, for the turbulent strain rate tensor and for the fluctuating vorticity. Only the consequences of this model on scalar gradients have been explored until now.

A Monte Carlo simulation of the molecular dissipation processes is performed considering non-interacting particles. During a time step, all the particles are affected by a LMSE process, while only a fraction acquire new values via a binomial or gaussian sampling technique. Scalar mixing frequencies can be calculated as a part of this joint pdf formulation. The ratio of scalar-gradient to scalar characteristic mixing frequencies is assumed to be a constant greater than one.

The previous formulation is then applied to study the evolution of an inert scalar in grid generated turbulence. In particular, the prediction of the concentration...
variance and the characteristic mixing frequency displays an excellent agreement with the experimental data for the evolution of dilute CINa injected at the grid into a main water flow. The flatness factor of the concentration gradient grows to values significantly greater than 3. The latter can be taken as an indication of the internal intermittency of the scalar field.

The reaction between sodium hydroxide diluted in the main flow and methyl formiate injected as a dilute solution at the grid generating the turbulence has been investigated in detail by Bennani et al.5 Predicted means and variances agree very well with experimental data. The experimentally determined segregation coefficient of skewness of the injected species is positive while that of the species diluted in the main flow are negative, both increasing downstream. Large values of the flatness factors of both species clearly suggest the spatial segregation of reactants. The computation of characteristic mixing frequencies for both species shows how moderately fast chemical reaction (Damköhler number of order unity) can significantly modify the time and length scales of the scalar fields. This is a call of attention on some extended practices in turbulent combustion modeling which overlook this fact. The number of order unity) can significantly modify the time and length scales of the scalar fields. This is a call of attention on some extended practices in turbulent combustion modeling which overlook this fact.

Information on the statistics of length scales defined as the ratio of concentration and concentration gradients could be obtained from the formulation. The sensitivity of the strain-rate/scalar-dissipation correlation coefficient to changes in the Schmidt or Prandtl numbers could also be evaluated. The same formalism could probably be extended to investigate the fluctuating vorticity dynamics in nearly homogeneous shear flows with constant mean velocity gradients.

3. PRESENTATION OF TWO SELECTED CASES

The following two cases have been selected for a more detail description:

3.1 Eulerian Formulation of Two-Phase Flow Average Equations

3.1.1 Fluid Phase Conditioning Technique

A phase indicator function, I, is defined such that8,11,

\[ I (x,t) = \begin{cases} 
1 & \text{if } (x,t) \text{ is inside the continuous phase} \\
0 & \text{otherwise} 
\end{cases} \]

In the process of averaging the Navier-Stokes equations conditioned upon the presence of the fluid phase the indicator function appears as a factor of time and space derivatives. The following relation holds11,

\[ \langle I \phi, \lambda \rangle = \langle I \phi \rangle, \lambda - \langle I \phi, \lambda \rangle \]

(11)

\( \phi \) stands for any continuous phase variable and, \( \lambda \) for the derivative with respect to \( \lambda \) (time or space). \( \langle \cdot \rangle \) is meant for statistical average. The last term in equ. (11) represents the phase interaction. Should the characteristic length of the dispersed elements be much smaller that the mean overall flow characteristic length, this interaction term can be expressed as3

\[ \langle I \phi, \lambda \rangle = \frac{\alpha^d}{v^d} \int_S \frac{\phi}{S_p} n \, dS + \varepsilon \phi \lambda \]

(12)

where \( \alpha^d \) is the "particle concentration", the overbar followed by a star denotes statistical average conditioned to the center of the dispersed elements being positioned at point \( x \) at time \( t \), \( \bar{v}^d \) is the dispersed element average volume, the surface integral extends over the interface, \( S_p, \varepsilon \phi \lambda \) is a residue usually much smaller than the first term on the right side of equ. (12) and

\[ n^\lambda = \begin{cases} -v^k & \text{if } \lambda = t \\
0 & \text{if } \lambda = x_k \end{cases} \]

(13)

\( v^k \) and \( n \) are the interface velocity and the unit vector perpendicular to the interface element located at \( x_k \), pointing towards the continuous phase, respectively. The subscript \( k \) designates the \( k \) component of the corresponding vector.

3.1.2 Continuous Phase Conditioned Equations and Modeling

The instantaneous conservation equations multiplied by \( I \) and averaged, after making use of Equ. (12) yield the continuity, momentum, turbulent kinetic energy and dissipation rate averaged equations.

A k-\( \varepsilon \) model is used to represent the turbulence. The following expressions are used for the unclosed terms,

\[ -\alpha \left( \mathbf{u}' \cdot \mathbf{u}' \right) = -\alpha \frac{2}{3} \kappa \delta_{ij} + \nu_T \left[ \left( \alpha \mathbf{U} \right)_j + \left( \alpha \mathbf{U} \right)_i \right] \]

(14)

\[ -\alpha \left( \mathbf{u}' \cdot \mathbf{k}' + \frac{1}{P} \mathbf{u}' \cdot \mathbf{p}' \right) = \frac{\nu_T}{\sigma_k} \left( \alpha \mathbf{k} \right)_i \]

(15)

where \( \alpha \) is the void fraction, \( \mathbf{U} \) and \( \mathbf{u}' \) are the mean and fluctuating velocity, respectively, \( k \) and \( k' \) are the average and the instantaneous-fluctuating turbulent kinetic energy, respectively, \( \delta_{ij} \) is the Kronecker delta, \( \mathbf{p}' \) is the fluctuating pressure, \( \sigma_k \) is set equal to one and \( \nu_T = C_D (P, \varepsilon) k^2 / \varepsilon \) is the turbulent viscosity. \( P \) and \( \varepsilon \) stand for the turbulent kinetic energy production and dissipation rates, respectively.
The weakest point in the model is the $\varepsilon$-transport equation, which is replaced by

$$ (\alpha \varepsilon)_t + (\alpha U_j \varepsilon)_j = \left[ \left( v + \frac{V_T}{\sigma_\varepsilon} \right) (\alpha \varepsilon)_j \right] + $$

$$ + \alpha_k \left( C_{e_2} P - C_{e_1} \varepsilon \right) + I_\varepsilon $$

where the constants $\sigma_\varepsilon$, $C_{e_1}$ and $C_{e_2}$ are assigned the values corresponding to single-phase flows and the phase interaction term is designated by $I_\varepsilon$. Based on dimensional considerations and order of magnitude estimates the following model is proposed,

$$ I_\varepsilon = \frac{\rho_d}{\rho} a \frac{\varepsilon}{k} \left\{ - C_{e_3} (k - k_d) + C_{e_4} K \left( U_i - V_i \right)^2 + k (1 - \theta) \right\} $$

where $\rho_d$ and $k_d$ are the dispersed phase density and fluctuating kinetic energy, respectively, $a$ is the inverse of the particle relaxation time, $K = (R/n) + a \tau_L$, with $R$ and $n$ being the particle radius and Kolmogorov length microscale respectively and $\tau_\varepsilon = 0.5$ (k/\varepsilon), $V$ is the mean dispersed phase velocity and $\theta = \tau_\varepsilon / (\tau_L + 1/a)$.

$C_{e_3}$ and $C_{e_4}$ are both tentatively taken equal to one.

The phase interaction terms in the momentum and turbulent kinetic energy equations are modelled as,

$$ I_{U_i} = - \frac{\rho_d}{\rho} a \left( U_i - V_i \right) $$

$$ I_k = \frac{\rho_d}{\rho} a (1 - \theta) - \frac{\rho_d}{\rho} a \left( k - k_d \right) $$

Should mass transfer at the interface be negligible and for solid particles the $I_{U_j}$, $I_k$ and $I_\varepsilon$ include all the significant phenomena taking place at the solid/fluid interface.

A rigorous presentation of the equations and closure assumptions is contained in Reference 3.

### 3.1.3 Dispersed Phase Average Equations and Closures

A Boltzmann type equation is assumed to accurately describe the particle cloud dynamics. The generalised transport equation for the particle velocity distribution function can be multiplied by any function of the velocity field and integrated over the phase-space in order to generate moment equations. For clouds of solid non-diffusive particles undergoing elastic collisions and allowing neither disaggregation nor agglomeration, average continuity, momentum and fluctuating kinetic equations are easily obtained.

The unknown terms are then modelled as,

$$ - \alpha_d v'_i \cdot v'_j * = - \alpha_d \frac{2}{3} k_d \delta_{ij} + $$

$$ + v^d \left[ \left( \alpha_d V_i \right)_j + \left( \alpha_d V_j \right)_i \right] $$

(20)

$$ - \alpha_d k \cdot v'_j * = \frac{v^d}{\sigma_k^d} \left( \alpha_d k_d \right)_j $$

(21)

where $v^d$ is the dispersed phase fluctuating velocity and $v^d$ is the particle turbulent diffusivity, which for a dilute dispersed phase is given by, $v^d = C_p k_d / a$. $\sigma_k^d$ has been set equal to one.

The phase interaction terms to be modelled in the dispersed phase equations are identical to those entering the fluid phase equations and closure assumptions have already been proposed.

A detailed derivation of the equations and a justification of the models are presented in References 2 and 3.

### 3.1.4 Numerical Results

An axisymmetric turbulent jet configuration has been chosen to validate this model for both single phase and two-phase flows. The pressure is assumed constant throughout the flow field.

A classical finite volume, four node formula, space marching, fully implicit scheme has been used. Due to this particular methodology applied to a parabolic shear flow, the radial momentum equation is not solved. An additional closure assumption is required for $W_r = U_r - V_r$ (the radial relative velocity) namely

$$ W_r = C_\alpha \frac{v^d}{\sigma_k^d} \frac{\partial \sigma_k^d}{\partial r} $$

(22)

with $C_\alpha = 0.5$. Justification for this hypothesis is provided in Reference 3.

The standard values for the single-phase $k - \varepsilon$ model coefficients are used:

$$ C_D = 0.09 \left( 1 - 0.44 G \right), C_{e_1} = 1.44 $$

$$ C_{e_2} = 1.92 \left( 1 - 0.035 G \right), \sigma_k = 1.0, \sigma_\varepsilon = 1.3 $$

$G$ is the deceleration parameter, modifying the traditional $C_D$ and $C_{e_2}$ values, introduced by Rodi in order to get the proper single phase jet spreading rate.

Based on a few initial runs, the preliminary values for the additional two-phase model coefficients are:

$$ C_p = 0.1, \sigma_k^d = 1.0, C_{e_3} = 1.0, C_{e_4} = 1.0 $$

The standard values for the single-phase $k - \varepsilon$ model coefficients are used:
3.1.5 Model Predictions

Available experimental data for turbulent jets of air, laden with solid particles or liquid droplets in highly dilute concentrations, were scrutinized. Restrictions setting the range of applicability for the model, are not fully satisfied by most of the published works. Furthermore, only a few publications supply direct measurement of each individual phase, and on measured turbulent parameters and boundary conditions required for proper model calibration. Nevertheless, the experimental data from References 12 and 24 have been selected to test the model predictions. Three basic cases have been documented:

<table>
<thead>
<tr>
<th>Case</th>
<th>(2R(\mu m))</th>
<th>(\phi_0)</th>
<th>(R/t)</th>
<th>(R \cdot W_0/V)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>50</td>
<td>0.32</td>
<td>0(1)</td>
<td>0(10)</td>
</tr>
<tr>
<td>2</td>
<td>50</td>
<td>0.85</td>
<td>0(1)</td>
<td>0(10)</td>
</tr>
<tr>
<td>3</td>
<td>200</td>
<td>0.80</td>
<td>0(1)</td>
<td>0(100)</td>
</tr>
</tbody>
</table>

where \(\phi_0\) stands for the initial particle mass loading ratio.

Comparison between model predictions and experiments are shown in Figures 1 to 6. Comments are self-explanatory. \(r\) and \(x\) represent the radial and axial coordinates, respectively. \(x = 0\) is located at the nozzle exit. The nozzle diameter is \(D\). In order to make clear the dispersed phase influence upon the flow, single phase jet measurements and predictions are included in each figure. Single phase jet data were taken from References 24 and 35.

Figures 1 to 3 relate to case 1, the best documented one. Predicted and measured mean velocity, turbulence intensity and turbulent shear stress profiles are presented for both phases. The agreement is reasonable.

Figures 4 and 5 refer to case 2. The values of the variables at the centerline are slightly underpredicted. The turbulent axial velocity is accurately estimated. Centerline velocity values have been shown to be very sensitive to the value of \(C_p\).

Figure 6 belongs to case 3. Centerline particle and fluid velocity are correctly predicted. However, the computed profile for the dispersed phase seems to be sharper than what the few experimental points available suggests.

3.2 Turbulent Mixing and Chemical Reactions

It seems now clear that neither large-eddy simulation (LES) nor direct numerical simulation (DNS) can be successfully applied at present to solve general turbulent reacting flow problems. Some investigators advocate the presumed pdf method in order to evaluate the average chemical source terms entering the moment equations. However, the use of a pdf transport equation is by far the most rigorous methodology to cope with the non-linear chemical rate terms. These terms are close in the pdf formulation. Should a transport equation for the joint pdf of velocity, kinetic energy dissipation rate, concentration and scalar dissipation rate be used, the closure problem associated with the turbulent transport can also be avoided. Here some preliminary ideas on the use of the joint pdf of scalar fields and their gradients are presented.

3.2.1 Basic Equations

The isothermal turbulent mixing of two scalar fields undergoing a second order chemical reaction obeys the local instantaneous equation,

\[
L_c \alpha = S_\alpha (C) \tag{23}
\]

where

\[
L = \frac{\partial}{\partial t} + v_j \frac{\partial}{\partial x_j} - D \nabla^2 \nabla^{2}
\]

is the convection/diffusion operator. \(v_j (x,t)\) is the local instantaneous velocity field at point \(x\) and time \(t\), which can be decomposed into a mean field, \(U_j (x,t)\), and fluctuation, \(u_j (x,t)\). \(D\) is the molecular diffusivity assumed identical for the two species. \(C = (C_\alpha)\), for \(\alpha=1,2\), stands for the concentrations of the two chemical species. \(C_\alpha (x,t)\) can also be decomposed into a mean, \(<C_\alpha (x,t)>\), and a fluctuating field, \(c_\alpha (x,t)\). For a second order irreversible chemical reaction the chemical source term is expressed as

\[
S_\alpha (C) = - K_c C_1 C_2, \text{ for } \alpha=1,2, \text{ where } K_c \text{ is the chemical rate constant.}
\]

Let the gradient \(C_\alpha\) be defined as \(C_\alpha,i = \partial C_\alpha / \partial x_i\). Its evolution follows the equation,

\[
L C_\alpha, i = - \frac{\partial v_j}{\partial x_i} C_\alpha, j + \frac{\partial S_\alpha}{\partial C_\beta} C_\beta, i \tag{25}
\]

Summation over repeated latin and greek indexes is implied. A transport equation for the joint pdf of the scalar and scalar-gradient fields can readily be derived,

\[
\frac{\partial P}{\partial t} + \frac{\partial}{\partial x \alpha} \left[ S_\alpha (\Gamma) P \right] + \frac{\partial}{\partial x \alpha} \left[ \frac{\partial S_\alpha (\Gamma)}{\partial x \beta} \chi_{\beta i} P \right] +
\]

\[
D \frac{\partial^2}{\partial x \alpha \partial x \beta} \left( \chi_{\alpha i} \chi_{\beta i} P \right) = \frac{\partial}{\partial x \alpha} \left( \frac{\partial u_j}{\partial x_j} | \Gamma, \chi \right) \chi_{\alpha j} P \]

\[
- 2D \frac{\partial^2}{\partial x \alpha \partial x \beta} \left( \chi_{\alpha j} \chi_{\beta j} P \right) \]

\[
- D \frac{\partial^2}{\partial x \alpha \partial x \beta} \left( \chi_{\alpha j} \chi_{\beta k} P \right) \tag{26}
\]

where \(P \Gamma d x = P (\Gamma, x, t) d \Gamma d x\) is the probability of the joint event \(\Gamma_\alpha \leq C_\alpha (x,t) < \Gamma_\alpha + d \Gamma_\alpha\) and
\[ \chi_{ai} \leq C_{ai} (x,t) < \chi_{ai} + d \chi_{ai} \]  
Equation (26) has been restricted to the case of statistically homogeneous turbulence and scalar fields. \( \langle V | \Gamma \chi \rangle \) stands for the expectation of the variable V conditional upon \( C(x,t) = \Gamma \) and \( \nabla C(x,t) = \chi \).

All the terms on the left hand side (LHS) of Equation (26) are closed and physically represent the accumulation of probability, the probability transport in concentration and concentration-gradient spaces due to chemical reaction and due to molecular mixing of concentrations, respectively. The terms on the right hand side (RHS) of Equation (26) are not closed. The phenomenon of turbulence straining of scalar-gradients (similar to the vortex stretching mechanism of turbulence\(^{25}\)) is ascribed to the first term on the RHS. The last two terms represent the cross-dissipation of scalars/scalar-gradients and the dissipation of scalar-gradient/scalar-gradient correlations due to molecular mixing, respectively. In order to use Equation (26) the three terms on its RHS must be approximated.

3.2.2 Turbulence Straining of Scalar-Gradients

Since a sequential Monte Carlo (MC) simulation\(^{27}\) of Equation (26) will be conducted hereafter, the effect on P of the terms on the RHS can be separately treated. In the limit of large turbulent Reynolds number and of small time, Kubo technique\(^{17}\) leads to the following representation of the first term on the RHS of Equation (26).

\[
\frac{dP}{dt}_1 = \langle \frac{dQ}{dx_i} \, \frac{dQ}{dx_k} \rangle \frac{\partial}{\partial x_{ai}} \left[ \chi_{ai} \frac{\partial}{\partial x_{bi}} \left( \chi_{bi} P \right) \right]
\]  
(27)

The subscript 1 on the LHS of Equation (27) indicates that the P variation is due only to the first term on the RHS of Equation (26). It is pertinent to remark that Equation (27) implies only mathematical approximations but no closure hypothesis in the classical sense.

For statistically homogeneous and isotropic fluctuating velocity-gradient fields and incompressible flows Equation (27) finally becomes,

\[
\frac{dP}{dt}_1 = \frac{1}{3} \frac{e}{v} \left( 4 \chi_{ai} \chi_{bj} \delta_{ij} - \chi_{ai} \chi_{bj} - \chi_{ai} \chi_{bi} \right)
\]  
(28)

where \( \langle e \rangle \) is the average turbulent kinetic energy dissipation rate\(^{25}\) and \( v \) is the kinematic viscosity.

3.2.3 Monte Carlo Simulation

Due to the high dimensionality of P, Equation (26) is simulated via a sequential MC technique\(^{27}\). Every physical process represented by the various terms in Equation (26) is then considered to act separately and sequentially upon N stochastic particles which approximate P(\( \Gamma, \chi; t \)). A stochastic particle n is defined by its concentration and concentration-gradient values, \( \{ C^{(n)}, (\nabla C)^{(n)} \} \).

3.2.3.1 Turbulence Straining

Equation (28) can be formally transformed into a finite-increment equation by using the definition of the P derivative and a Taylor series expansion. After a few algebraic manipulations, the following stochastic model (equivalent to a closure assumption) is proposed\(^{34}\),

\[
\Delta \delta t \chi_{ai,1}^{(n)}(t) = \left( \frac{1}{600v} \right)^{1/2} \delta t \left( x \eta_i^{(n)} \xi_j^{(n)} + y \eta_j^{(n)} \xi_i^{(n)} + z \eta_k^{(n)} \xi_k^{(n)} \right) + \xi_{ij}^{(n)} C_{ai,1}^{(n)}(t)
\]  
(29)

The LHS is the change experienced during a time step, \( \delta t \), by the \( i \)th component of the gradient of the scalar \( \alpha \) for the stochastic particle \( n \) at time \( t \). \( x, y \) and \( z \) are constants with analytically determined values, \( x = 0.35634, y = 2.8059, z = 0.8165 \) \( \eta \) and \( \xi \) are statistically independent random vectors with zero mean and unity correlation matrix.

3.2.3.2 Molecular Mixing

A recently developed binomial sampling model\(^{33,34}\) is used to close the last two terms on the RHS of Equation (26). Although the last term on the LHS of Equation (26) is closed, it is also treated in this manner. It has been shown that this model produces a qualitatively reasonable evolution and the correct asymptotically gaussian relaxation for large times.

3.2.3.3 Chemical Reaction

The change of scalar and scalar-gradient in a time step, \( \delta t \), due to chemical reaction are exactly given by,

\[
\Delta \delta t C_{\alpha}^{(n)}(t) = (\delta t) S_{\alpha} \left[ C_{\alpha}^{(n)}(t) \right] \]  
(30)

\[
\Delta \delta t C_{\alpha,1}^{(n)}(t) = (\delta t) \frac{\partial S_{\alpha}}{\partial C_{\beta}^{(n)}} \left[ C_{\alpha}^{(n)}(t) \right] C_{\beta,1}^{(n)}(t) \]  
(31)

3.2.4 Numerical Results

The mixing and chemical reaction of an acid and an alkali diluted in water in a field of grid generated turbulence have been investigated by Bennani et al.\(^{5}\). The acid is injected at the grid and the base is convected by the main flow. These experiment has been predicted using the previously explained pdf methodology. The evolution of concentration means and variances is presented in Figure 7 showing a good agreement with the experimental data. The segregation coefficient in Figure 8 also shows a reasonable agreement with the measured constant experimental value of -0.7. The skewness and flatness factors for the concentration and concentration-gradients are presented in Figures 9 and
10; no experimental data are available. The large values of the flatness factors of the concentrations are a clear indication of the spatial segregation of the reactants, while those of the concentration-gradients might also reflect the internal intermittency of the scalar fields. The evolution of the characteristic turbulent frequencies for both reactants is plotted in Figure 11. Due probably to the difference in the initial condition of the acid and the base the frequencies for both reactants evolve in a different way. This is not taken into account in present combustion models.

4. CONCLUDING REMARKS

An overview of turbulent flow modelling activities in Spain have been presented. Two selected examples have been described in detail: turbulent two-phase flows and turbulent reactive flows. While there seems to be a consensus that a moderately significant progress in the last two decades has been achieved in the field of turbulence models using moment equations, there are not reasons to be so optimistic in the two cases described. The following comments seem then pertinent:

4.1 Turbulent Two-Phase Flows

- No agreement has been reached on the local instantaneous basic equations to be used as a starting point, in particular for the dispersed phase. While some investigators treat the dispersed phase as a continuum, defining a particle cloud pressure and viscosity, others prefer to describe the particle cloud dynamics in terms of moments of a Boltzmann type equation.

- The type of average employed to generate moment equations also leads to significantly different transport equation structure.

- Classical k - e or Reynolds stress models can be used for the fluid phase. However, the unknown terms in the dispersed phase equations and the phase interaction terms deserve special and careful consideration.

- LES or vortex dynamics techniques can help to gain significant knowledge on peculiar phenomena influencing the particle dynamics.

- DNS of some simplified two-phase flow systems can provide rational basis to the asymptotic behavior of the proposed models.

- Reliable experimental data for simple flow configurations to validate model predictions are scarce.

4.2 Turbulent Reactive Flows

- The non-linearities in the chemical source terms introduce important difficulties in moment formulations. Even for some idealized situations (diffusion controlled limit, premixed systems, etc.) existing models are not as accurate as desirable.

- The pdf formalism overcomes the closure problem associated with the chemical source terms. The closure of the molecular diffusion effects has proved however to be a very difficult one.

- The conceptually different framework of the pdf methodology makes it appear somehow unnecessarily cumbersome to some investigators.

- Moreover the inclusion of the velocity and/or dissipation rates or gradients into the formulation leads to a pdf with a large number of independent variables. Non-standard Monte Carlo simulations must be used to obtain numerical solutions.

- Since reaction takes place at the molecular level, LES or vortex dynamics techniques are also confronted with closure problems identical to those present in moment formulations.

- DNS of simplified chemical kinetics in simple flows can be of some help as a guidance for the asymptotic behavior of models.

- Most available experimental data pertain to the field of turbulent combustion. Experiments on irreversible bimolecular chemical reactions in incompressible grid-generated turbulence where the interactions among turbulent straining, molecular mixing and chemical reaction can best be evaluated are badly needed in order to validate model predictions.

In summary, in the foreseeable future significant effort will be required to model turbulent two-phase and reactive flows. A judicious combination of physical insight, theoretical developments, analysis via LES and/or DNS of simplified flows and examination of reliable experimental data is the best support for successful modelling endeavors.

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Figure 5. Turbulence intensity profiles at x/D = 20

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Figure 6. Mean velocity profiles at x/D=20

Data of Elghobashi et al. (12) Case 3

Figure 7. Evolution of means and variances of two reactive scalars. Comparison with Benanni et al.'s experimental data (Kc = 47.5 l/mol s).

Figure 8. Evolution of the segregation coefficient. The approximate experimental value is 0.7. (Kc = 47.5 l/mol s).
Figure 9. Evolution of the skewness coefficients and flatness factor of two reactive scalars ($Kc = 47.5$ l/mol s).

Figure 10. Evolution of the skewness coefficients and flatness factor of two reactive scalar gradients (downstream direction derivative) ($Kc = 47.5$ l/mol s).

Figure 11. Evolution of the characteristic turbulent frequencies of two reactive scalars ($Kc = 47.5$ l/mol s).