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CFD Experience on Industrial Combustors

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ABSTRACT

This paper summarises the authors' perspective of the current status of computational fluid mechanics (CFD) with regard to engineering application, especially those relating to combustion processes. Particular emphasis is placed on the physical modelling of the turbulence, combustion and thermal radiation. The summary is supported by several example applications, again drawn from the authors' own experience.

It is concluded that CFD is now an established design tool when expertly used. However, its accuracy and applicability remain tethered by several difficult problem areas in need of continuing research and development. These comprise the need for: an improved simulation of the turbulence for affordable computational cost; an economic simulation of the turbulence/chemistry interaction; usable reduced chemistry modelling of the combustion, of the 'engineering hydrocarbon fuel', including the role of soot; simulations of the very many pollutants that are increasingly a matter of public concern; better simulation of the char burnout of solid fuel combustion; and enhanced routines which enable the unskilled user to generate effective grids for complex geometries for acceptable effort. The total research effort implied by these tasks is very considerable. The incentive is, however, powerful: every advance will lead, through the increased applicability and usefulness of CFD, to improved equipment for minimised development cost.

HISTORICAL SETTING

Terminology

This paper concerns 'CFD', or computational fluid dynamics, sometimes called 'mathematical modelling' (MM). The latter term, although currently less fashionable, is probably the more appropriate since it admits heat transfer and combustion processes. It is particularly appropriate here since this paper deals specifically with the application of mathematical modelling to engineering combustion. The MM terminology is still imprecise since it properly embraces all analytical models of complex problems. However, both CFD and MM have come to designate the numerical solution of the partial differential equations which describe the behaviour of fluids, reacting or non-reacting. In spite of the imprecision, the terminology is now widely understood and seems destined to become yet another example of the curious blend of flexibility and vagueness which characterises the English language.

Beginnings

The advent of the modern digital computer gave birth to the subject of MM as we know it today. Computer-based technology enabled the generalised numerical solution of the complex Navier Stokes equations such that, for the first time, real industry flow problems could be tackled without the need for excessive simplification. Spalding and his co-workers were perhaps the first to take advantage of the new technology. For example, he and his then student Patankar devised the landmark GENMIX program (1) for the calculation of flows of the boundary layer type. Many of the concepts of this landmark code endure today. Spalding was able to combine mathematical flare which a copious amount of physical intuition which led to a scientific methodology which was universally appreciated by the engineer at the 'sharp end' of real industry problems. His seminal volume (2) on turbulence modelling, with Launder, another of his renowned students, is testimony to his ability to find usable and fundamentally based descriptions to immensely complicated physical phenomena. Spalding was also the driving force behind a second landmark computer method which could be applied to recirculating or elliptic flows (3). The method was formulated around the solution of the vorticity and stream function variables and was therefore restricted to two-dimensional flows. Initial enthusiasm within the engineering community soon faded since virtually all of their problems were three-dimensional. As a result, methods based on the so-called primitive variables, the velocity components and pressure, quickly evolved, again largely due to Spalding and co-workers (4). The classic volume by Patankar (5) appeared during this period and remains much cited. Commercial CFD software developers are not always noted for their generosity of acknowledgement so there is merit in remarking that virtually all of the commercial codes being marketed today owe much to Sthe pioneering work of Spalding and co-workers.

The literature which has evolved in the wake of these initial computational methods is far beyond the scope of this paper. In the main it has concentrated on improved numerical techniques to ensure more reliable convergence and improved precision, and on meshing techniques capable of accommodating the intricate geometry's of engineering equipment (6,7). It should however be noted that, in spite of the vast development and applications of the finite element methods for solving systems of partial differential equations, the solution schemes deployed in fluid/combustion dynamics have remained firmly based on the finite volume concept, primarily because it ensures that the principals of conservation, fundamental to the analysis of fluid flows, are not violated.

Combustor Calculations

Prior to the deployment of modern mathematical modelling, furnace/combustor design was almost entirely a 'black art'. In the main combustors evolved slowly on the back of expensive and time-consuming experimentation. The analytical treatments which did exist were almost entirely due to Hoyt Hottel who offered what as for its day was remarkable physical understanding combined with simple zero and one dimensional analytical treatments (8,9). The first modern furnace prediction procedure, the so-called 'zone method' for the calculation of the radiation heat transfer in combustors, must also be attributed to him and his co-worker Sarofim (10,11). This was a fully-fledged numerical method for the solution of the three-dimensional integro partial differential equation which governs radiative transfer. The combination of this method, plus the above-mentioned finite volume methods which were soon to be developed for the fluid mechanics, set a foundation for the realisation of fundamental predictive methods for furnaces, provided that suitable treatments for the combustion processes could be found.

Fortunately, for the bulk of engineering combustion systems the mixing process proceeds much more slowly than the chemistry and as a result the mixing rate almost always determines the rate of combustion. Therefore, for the predominant industry case of 'diffusion' or unpremixed combustion for example, it normally suffices to solve a conservation equation for a mixing variable called the 'mixture fraction' in order to determine the temperature and concentrations of major species. Researchers trumpeted the potential of the new computer-based technology to an engineering combustion community which quickly became ecstatic with the prospect of designing improved furnaces. Commercial software packages emerged which developed user-friendly versions of these new mathematical models. However, engineering users soon found that the technology was inevitably sophisticated demanding considerable user expertise and, more importantly, that the predictions were often flawed. The errors arose primarily because almost all engineering flows are turbulent. Now the time scales of the smallest vortices of the turbulent spectrum are very small indeed, too small to be resolved by existing or foreseeable computers. So Reynolds (or Favre) averaged variables are solved for, with the effects of the turbulence on the mean flow motion being accounted for by a turbulence model (2). Turbulence modelling has proved to be an extraordinarily complex area. The development of usable models of turbulence has progressed little over the past 20 years, and while combustors embrace many complex phenomena which require to be modelled, the turbulence model remains a major uncertainty in combustor predictions.

Value of CFD

Given that the predictions are frequently erroneous, why then do the commercial software enjoy continuing success? There are three primary reasons: (a) apart from very expensive experimental programmes or excessively simple engineering models, design engineers have no other options; (b) trends are almost always correctly predicted; and (c), the predictions very often reveal important physical features which were previously unrecognised. The word 'erroneous' needs further comment. When conditions are right the experienced user of mathematical modelling might anticipate an accuracy as good as plus or minus 10%. However, the predictions may be much worse, especially locally, but such a user will normally know the level of accuracy he can expect. Given that the trends and major physical features of the flow are likely to be correctly predicted by the skilled user, and assuming that the user is also skilled in the application of such knowledge, the scope for design improvement is very considerable.

Environmental Pollution

In the early years of the application of MM to combustors, essentially in the decade of the 1970's, the heat release and its transfer to the process were the primary concerns. Since combustion could most often be considered to be mixing controlled, combustion was considered to proceed to completion yielding 'harmless' carbon dioxide and water vapour, with the 'inert' nitrogen content of the air transgressing the combustor unaffected Concern about the greenhouse effect of CO_2 arose only later. Also subsequent to the early days, it became increasingly recognised that many compounds were emitted, which although only present in trace quantities, were harmful to the environment. The most notable of these where the oxides of nitrogen which give rise to photochemical smog and acid rain, the effects of which first traumatised the inhabitants of the Los Angeles basin. Generally, the trace concentration pollutants are emitted because some facet of their governing chemistry is slow. Chemistry can then no longer be ignored and combustion engineers, who traditionally needed only rudimentary knowledge of chemistry, have been forced to recognise this. The combination of increasing public concern about health and increasing world prosperity, and so combustion, has caused the list of combustion generated pollutants to lengthen continually. Examples include: particulate matter such as soot and fly ash; toxic metals such as cadmium, lead and mercury; the oxides of nitrogen and sulphur; and volatile organic/chlorinated compounds such as formaldehyde.

Range of Application

The application of CFD software has been hugely diverse, particularly with the introduction of faster computers, encompassing everything from inert flow calculations inside single rooms of simple geometry's, to intricate flows inside entire building complexes, and from mixing controlled reacting flows to hazardous chemistry driven explosions (12-14). CFD has been widely used to assist designers in formulating low emission burners (15). The use of CFD has also shown promising results in the design of advanced higher efficiency and lower emission power systems (16). Computational fluid dynamics

simulations are frequently used to visualise the aerodynamics, combustion environment and emission performance of a combustor at the design stage, to assist permit acquisition from regulatory bodies, to verify operational performance at the commissioning stage. In respect of regulatory compliance for example, statutory waste incineration requirements of minimum temperatures and residence times and of flue gas condition for a novel type of waste and/or incineration technology can be demonstrated using CFD predictions.

Present Paper

In a single paper, it is not possible to present a balanced and fair review of the very many significant contributions by researchers across the very broad area of computational fluid dynamics. As a result, we must apologise for confining the material primarily to that of our own experience, a fact which we accept may have already with justification irritated some readers.

GRID GENERATION

Industrial combustors are characterised by a multitude of shapes. Moreover, they often exhibit regions of elaborate geometric detail. In particular, the geometry of the typical combustor exhibits two features which impede its solution by conventional methods: the discrepancy of scale between the burners and of the much larger volume of the combustion chamber, and the discrepancy between the typically three dimensional cylindrical geometry of the burners and the largely Cartesian geometry formed by the confining walls of the combustion chamber. Also modern combustion chambers, e.g., gas turbine combustors have complex topological features in their geometry which prevents the use of simple orthogonal meshing techniques. These difficulties would be surmounted by the existence of a numerical treatment based on a flexible unstructured grid capable of being locally refined.

This end has been partially achieved through previous work on, for example, grid embedding or zoning methods (17,18) and multigrid methods (19,20). These involve subdividing the solution domain into fine-grid regions near the burners and patching them to more coarsely gridded regions elsewhere. These regions can be solved as a single spanned domain, or as multiple domains with periodic information transfer. The principal disadvantage of the methodology is that the transfer of information across the frontiers between regions can lead to severe convergence rate problems. This difficulty is circumvented by the local grid refinement (LGR) method of (21) where the solution for all zones is effected simultaneously. However, the extension of this method beyond application to Cartesian forms is fraught with computational uncertainty. Some authors (e.g. (22)) have recently argued that this is of little consequence since even quite awkward shapes can be perfectly well fitted in a castellated manner using locally refined cartesian grids.

The use of boundary fitted co-ordinate (BFC) methods have served marvellously for the specialised geometry's with complex topology such as gas turbine combustors (7) and in principal the BFC methodology is applicable to the geometry's typical of industy furnaces. However, the above-mentioned geometric particularities of the typical furnace may give rise to highly skewed control volumes which seriously impede convergence, in the situations where BFC method are deployed in a structured framework. This problem can be circumvented by the advanced meshing practices of *unstructured* domain-discretisation methods. As the name implies these methods may involve multiple cell-type definitions and, in general, may also vary the cell topological characteristics (e.g. the number of cells sharing a host cell). In this category the use of triangular/tetrahedral as well as quadrilatral/hexahedral has become popular in the finite volume based methods, while some researches (23,24) have also attempted the use general polyhedral cells.

The use of hexahedral cells in an unstructured domain is, however, particularly attractive for finite volume methods because: (a) of the ease of maintaining grid line alignment with stream lines so minimising numerical diffusion, and (b) the meshes may be conveniently defined and generated as multi-block general-coordinate-frame orientated tensor product meshes with different embedded structures. The use of polyhedral mesh types (eg. octa-hedral, do-decahedral) for CFD should not, in principle, pose difficulties in formulating the numerics, their practicality appears to be limited since the mesh generation for such cells in geometry's of arbitrary complexity can be particularly cumbersome.

TURBULENCE MODELLING

An established method to describe turbulence supposes that the flow is composed of a mean motion superimposed by turbulent fluctuations (25). The spectrum of the length and the time scales of these fluctuations usually ranges from the smallest Kolmogorov scales to the large integral scales of energy containing eddies. An accepted view on high Reynolds number flows is that, the mean motion generates the large scale turbulence fluctuations and the large scale fluctuations interact with neighbouring fluctuations and generate smaller scales. The fluctuations smaller than the Kolmogorov scale are considered to be dissipated by molecular viscous action, thereby transferring energy from the mean motion to the turbulence. Due to the small magnitudes of the Kolmogorov scales that are important in tracing the energy transfer, the solution of transport equations by direct numerical simulation (DNS) requires extremely fine time-space resolution, which in turn requires extensive computational resources in terms of storage and execution time. Thus, direct numerical simulations, although successfully performed for simple flows, see (26,27) for example, are totally impractical for engineering usage. A more practical approach to solve turbulent flows is the large eddy simulation (LES) method (see for example (28 and 29) which is based on direct numerical simulation of the large scale motion of turbulence by parameterising the small scales on a subgrid with an eddy viscosity type model. The renormalised method (e.g., renormalising group theory (30); renormalising perturbation(31)) can also be regarded as large eddy simulation methods, where the small scales of turbulence are successively eliminated from the Navier-Stokes equations leading to a description of large scale motion. These methods assume that the small scale motion is statistically equivalent to the modelled Navier-Stokes equation perturbed with a random noise source, and in a frequency domain solution. LES methods are perhaps the ones with the most promise for improving engineering calculations in the future, but because they under developed and remain computationally expensive they have received little applied exploitation.

A much more computationally economical and a widely used method to simulate turbulent flows is the statistical method involving the decomposition of the flow variables to their mean and fluctuating components, where the solution of the mean motion is sought by appropriate modelling of lower order correlations of turbulent fluctuations. The bulk of such methods rely on characterising the turbulence with just two variables solved for in their own differential equations. The most common, known by name to all engineers who have applied CFD as the 'k-ε model', has the turbulence kinetic energy, k, and its dissipation rate, ε, as the two variables. Other two-variable models have been proposed (2), with none displaying marked superiority. Clearly only so much can be achieved in any attempt to describe a phenomenon as complex as turbulence with just two variables.

A more elaborate description of the turbulence clearly involves the specification of further parameters. Much work has been performed on models where modelled equations having the six turbulence stress correlations as their dependent variables. Such models have the additional advantage over two-equation ones through negating the need to model the complex turbulence transport as a gradient diffusion process. We have explored these so-called 'Reynolds stress turbulence models' in respect of two types of pulverised coal combustion: a non-swirling flame typical of cement kilns and a swirling flame typical of power stations (32). Various options appear in the literature for some of the modelled terms and it is not clear which are to be preferred, we have experimented with two versions. Moreover, serious convergence difficulties were encountered not simply because of the extra equations which require to be solved, but primarily because of the transfer of the effects of turbulence out of inherently stabilising diffusion terms and into source terms. Rather surprisingly, when converged results were eventually procured the Reynolds stress model did not demonstrate any consistent advantage over the simple k-ε model, at least within the constraints of the limited two phase velocity data. The evidence suggested that the second-moment closure should be extended to the scalar equations if improved predictions are to be secured. However, for pulverised solid fuel combustion modelling this requires the solution of at least a further three transport equations which for engineering purposes is impractical. In sum, we have concluded that although it is fashionable to blame the much used k-ε turbulence model for all weaknesses of engineering calculations, it is our experience that the worst predictive discrepancies are all too often due to numerical inaccuracies and that the use of a finer grid and/or higher order difference schemes are the remedies. Nonetheless, there can be no denying the need for improved and usable turbulence models and, as indicated above, it is our suspicion at this time, and that is all that it is, that those of the LES variety have the most promise.

COMBUSTION MODELLING

Analysis is in general considerably complicated by the inclusion of chemical reactions. There are two principal reasons. Firstly, the combustion of the typical engineering hydrocarbon fuel involves literally hundreds of elementary reactions. Secondly, there are significant interactions between the turbulence and the chemistry, particularly because of the typically non-linear dependence of the reaction rate on the fluctuating temperature. Fortunately, the first difficulty may most often be circumvented in practical applications because, as mentioned above, the speed of the overall reaction is much faster than the physical processes such as mixing. When this is not the case, for example for flames near extinction, or in the case of slow reactions involving important pollutants in trace concentrations, reduced chemistry schemes (33) with the controlling reaction paths appropriately modelled would be preferred over detailed schemes, except in the limited applications of simple flames that are typical of fundamental combustion studies. The typical reduced scheme might identify just some 5 to7 key reactons.

When the assumption of fast overall chemistry is valid the concentrations of the major species can be linked to conserved scalars usually denoted as mixture fractions, and the chemical state of the flow may then be determined by scalar state relations. Fig 8 applies to a system of two fuels plus an oxidant, normally air. By way of a currently important practical example one may consider the 'reburn' technology applied to reduce the emission of nitric oxide from combustors, especially power stations and especially those which are coal fired. In this a fraction of the total energy input is introduced downstream of the main burners which are fired with the normal quantity of excess air. This secondary fuel, which is normally gaseous, creates a fuel rich region, and has the effect of reducing the NO formed upstream to molecualar nitrogen. (34). Still further downstream, the requisite quantity of additional air is introduced to ensure good burnout of the fuel. The reburn process may be modelled by a set of three mixture fractions according to the following;

For fuel rich conditions, ; $\dfrac{f_1}{f_1^{st}} + \dfrac{f_2}{f_2^{st}} \le 1 - \dfrac{f_3}{f_3^{st}}$

$$[m]_{ox} = \left\{ \left(1 - \frac{f_3}{f_3^{st}} \right) - \left(\frac{f_1}{f_1^{st}} + \frac{f_2}{f_2^{st}} \right) \right\} [m]_{ox}^{*}$$

$$[m]_{fu} = 0$$

For fuel lean conditions, ; $\dfrac{f_1}{f_1^{st}} + \dfrac{f_2}{f_2^{st}} \le 1 - \dfrac{f_3}{f_3^{st}}$

$$[m]_{ox} = 0$$

$$[m]_{fu_i} = \frac{\left\{ \left(\dfrac{f_1}{f_1^{st}} + \dfrac{f_2}{f_2^{st}} \right) - \left(1 - \dfrac{f_3}{f_3^{st}} \right) \right\}}{\left\{ \left(\dfrac{f_1}{f_1^{st}} + \dfrac{f_2}{f_2^{st}} \right) - (f_1 + f_2) \right\}} f_i \, [m]_{fu_i}^{*} \qquad i = 1, 2$$

where, f_1 and f_2 are considered as the mixture fractions of the re-burn fuel and volatiles from coal, while f_3 is considered as that of for the char carbon fraction released by the hetrogenous combustion of the solid phase. The temperature and the density field are then defined by the state relation for the total enthalpy and the equation of state; it should be noted that, in a radiating medium, the enthalpy field is determined by a

transport equation for the total enthalpy. The thermo-chemical properties obtained as such represent in general the instantaneous values of the variables, and the averaged properties are usually determined by the first moments of those relations with presumed shape pdf's, in which the second moments of the pdf's are obtained by modelled transport equations.

When the chemical rates are not fast with respect to the physical ones the turbulence/chemistry interaction cannot be ignored. This represents one of the most challenging aspects of current day combustion research. The scope of the subject cannot even in summary fashion be adequately dealt with for the purposes of this review. It suffices to comment that a number of methods are being explored including, by way of example, laminar flamelet models (35), transport pdf procedures (36) that may be of eularian or lagrangian based methods (37), or perhaps other schemes, such as conditional momement closers (38), or the flame wrinkling combustion model of Weller et.al. (39).

CALCULATION OF THERMAL RADIATION

Energy transport by thermal radiation becomes significant for 'luminous' particle laden flames, such as those produced by oil or coal fuels, when the characteristic dimension of the combustor is, generally, of the order of a metre. For the 'non-luminous' flames of gaseous fuels the radiation influence is somewhat less. Nevertheless, thermal radiation transport is significant for almost all atmospheric-industry combustors, and for large coal-fired utility boilers it accounts for well over of 90% of the heat transfer to the walls of the combustor, the remainder being by convection. The 'optical thickness' of the combustor fluid is pressure dependent so that radiation effects in combustors operating at elevated pressures, such as gas turbines and internal combustion engines, may be significant for quite small sizes.

The equation of radiation transport may be simply expressed by:

$$\frac{dI}{ds} + \kappa I = \frac{\kappa E}{\pi}$$

where, I is the radiation intensity, k is the absorption coefficient, $E=\sigma T^4$ is the black body emissive power and s is a distance measure along the path of a ray.

Clearly, the form of this equation differs from the Navier-Stokes type fluid equations, where a directional derivative $d/ds \equiv \Omega_o\nabla$ replaces the Eulerian form spatial derivatives $\nabla_o(\underline{u} - \mu\nabla)$ of the latter. For this reason, fluid flow researchers are often reluctant to address the thermal radiation problem. When the transport equation is written for all directions, a complex integro three-dimensional partial differential equation results which has been the subject of many highly mathematical and voluminous specialist textbooks. Fortunately, numerical solution methods have been devised which are applicable to engineering combustors. One of the first was the so-called 'zone method' due to Hottel (10), a numerical procedure which was a forerunner for the whole subject of numerical analysis when later applied to equations of the Navier-Stokes form. A drawback of the zone method is its geometric inflexibility and because of this related methods based on Monte Carlo techniques developed (40). However, both the zone and Monte Carlo methods are computationally expensive, a major consideration in view of the totality of computations required for combustor simulation, so that 'flux model' approximations (41), centred on the solution of simple ordinary differential equations of the diffusion kind, were popular for a time. Nowadays, commercially available codes almost universally use the 'Discrete Transfer' procedure (42) which offers geometric flexibility for acceptable computational economy. This method is distinguished by the direct integration of the transport equation (42) to yield a simple recurrence relation:

$$I_{n+1} = \frac{E}{p}\left(1 - e^{-? \delta s}\right) + I_n e^{-? \delta s}$$

where, the indices n and n+1 denote two adjacent locations along a mean radiation ray, separated by a spatial distance of δs.

This relation is integrated starting at a location on the combustor wall and within the discretised solid angle elements of the hemisphere open to the combustor domain, until an opposing wall is intercepted. The starting locations are often the mid-points of the fluid flow control volume surfaces coincident with the wall.

The physical difficulties of the thermal radiation problem concern the specification of the absorption, emissive and scattering, or optical, properties of the transport medium in the combustor. Strictly, the evaluation of these properties is extremely difficult for numerous reasons. For instance: the radiative behaviour of gas flames is highly non-grey, it is not possible to predict the concentrations of soot in oil and coal flames, and the radiative properties of the soot are flame dependent and equally difficult to specify. Fortunately, experimentally-based correlations have been derived to approximate the radiative properties of gaseous combustion (43), while sooty flames are so optically dense that for flames of industry dimensions good prediction of the radiation transfer to the combustor walls does require an accurate specification of the optical properties of the soot.

It is not here possible to pursue further the challenging problem of the calculation of the radiative transport in combustors. In summary it suffices to reiterate that the transport equation is now amenable to efficient numerical solution and a methodology exists for dealing with the optical properties of flames which is sufficient for the bulk of engineering purposes.

MODELLING OF A PULVERISED SOLID FUEL

We here primarily concerned with coal. However, because of the growing concern about the 'greenhouse effect', biomass fuels which do not 'short circuit' the carbon cycle, such as forestery and agriculture wastes, are being increasingly advocated. Solid fuels are frequently pulverised to maximise their specific surface area prior to burning.

Turbulence Dispersion of the Particulate Phase

Fluid turbulence bedevils all aspects of combustion. The interaction between the turbulence and the particulate phase serves to perturb the particles velocities and so disperse their spatial locations and this has implications for flame stability and the deposition of ash on heat transfer surfaces. The vast majority of the reported mathematical models treat the particulate phase in Lagrangian fashion by tracking the flights of particles belonging to representative uniform diameter size groups released from representative entry locations, throughout the computational domain. The overall modelling procedure is then a hybrid one, where the influences of the particles are made known to the Eulerian solution of the gas phase equations through source terms appended to these equations (44). It is common practice to handle the dispersion of the particle flights stochastically by tracking successive releases of a particle in a given class and subjecting these to the random influences of the turbulence. (45). However, in order to ensure statistical reliability a sample size of 1000 to 10000 is least required for each representative class. The computer demands are impossible with the result that such treatments are never implemented correctly and the solutions are little more than indicative.

In order to circumvent this problem we have developed a method which predicts the evolution of the probability density function of the particles velocities starting from the known distribution at entry (46). The method is fundamentally based with the starting point in its derivation being the momentum conservation equation for a particle. An analysis based on probability theory leads to the following equation for the rate of change of the velocity probability, $P(v_p,t)$, of a particle

where

Here, C_D is the drag coefficient, SIGN is the sign of the relative velocity $(u_f - u_p)$, σ's are the rms velocities, and ρ_{fp} is the gas-particle fluctuating velocity correlation coefficient.

In the solution method the initial pdf is discretised into a sufficient number of 'bins' and the governing equation is solved by the method of characteristics. The procedure has proved orders of magnitude faster than conventional stochastic treatments (47).

Volatiles Release

The rate of release of the gaseous (volatile) content of coal when has important consequences for flame stability and pollutant emissions. Since the volatile matter is chemically bound in the solid fuel, the evolution of the volatilic substances is controlled by chemical kinetic parameters and temperature. For coal, as well as biomass, the mechanisms by which this occurs is clearly very complicated. Although simplified schemes have been proposed to model the thermal decomposition it is, given the extreme variability of coal and biomass, the authors' opinion that, where possible, the release rates should be obtained for each fuel in characterisation experiments for which the heating rates are high enough to be representative of combustor conditions. In general, empirical relations are required for the mass release as a function of the heat transfer to the particle. For other than fairly small particles, less than 20 microns say, other physical influences, such as the conduction heat from the surface to the interior of the partile, may also be important. These are not normally modelled in practice but they would be accounted for in characterisation experiments if these could be effected for the representative range of particle sizes.

Volatiles Combustion

In the very early stages of the heating of a solid fuel a small quantity of light species is released. The particle very quickly softens and tar vapours are evolved, entraining and ejecting molten material as they do so. Ease of ignition requires that these heavy hydrocarbons should crack and an additional time scale is implied. However this time scale is expected to be short in the vicinity of the flame front due to the high temperatures thereof and can probably be ignored. It has been customary to presume partial premixing of the volatiles with the combustion air prior to ignition, and therefore is reasonably accounted for by the eddy-bread-up model of Magnussen and Hjertager (47). While some premixing may occur, the assumption of diffusion combustion is probably not too far from reality as confirmed by some recent calculations (48). In any case, a suitable combustion modelling method as discussed earlier may be deployed for the volatile combustion in the continuous phase, away from the particles boundary layers. In view of solid fuel combustion, where particle mass release also occurs due to heterogeneous combustion, the above-described two-mixture mixture fraction approach for a single pf fuel, or a general n-mixture fraction approach for the

case of co-combustion with several combustible streams, may be used to formulate the homogenous combustion.

Char Combustion

Good burnout of the char, that is the solid carbonaceous material remaining after volatile release, is essential, none the least to ensure that the carbon in the exit ash is low enough to ensure that ash is a viable commercial product in, for example, the building industry. It is not usually difficult to achieve good burnout of the majority of the char, but there will always be a 'least likely to burn fraction' characterised primarily by large particles or ash rich particles compounded by the inevitable heterogeneity of the fuel, particularly where coal is concerned. The 'standard' mathematical model allows for external diffusion near the particle surface, probably with adequate accuracy, and simulates the chemical reactivity of the solid fuel by presuming a first order reaction having a single pre-exponential factor and a unique activation energy entirely confined to the surface of an equivalent spherical particle. Fuel variability remains the primary problem and again it is preferable to attempt to determine the kinetic behaviour, as characterised by the just-mentioned two kinetics parameters, of each fuel in suitable characterisation experiments. This is not easy since there is now evidence that the char undergoes thermal deactivation in the high temperatures of the combustor (49). This could reduce the pre-exponential factor by as much as two orders of magnitude, although the activation energy might not vary much. Modelling studies tend to confirm this since the use of char kinetic parameters established in conventional characterisation experiments, which are unable simulate the full range of combustor conditions, almost always lead to a serious over prediction of the char burnout.

EXAMPLE APPLICATIONS

The following examples are intended to illustrate the scope of application of CFD to engineering equipment. Each example in its entirety is rather complex and only an outline description is possible. The interested reader requiring full information is kindly requested to contact the corresponding author.

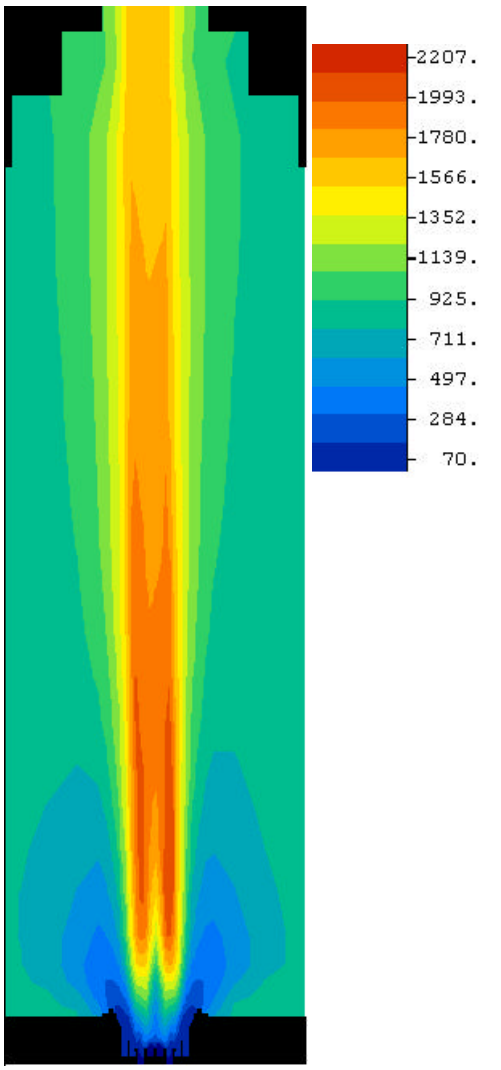
Simulation of a Reheating Furnace

A steel reheating furnace has been simulated using a Cartesian mesh of 69x69x46 (Fig 1). Such furnaces are employed to ensure uniformity of temperature within steel billets prior to further forming, rolling into strip material for example, which might be used to fabricate motor cars. Successive hot steel billets(~1200 K) enter the soak zone from the left of the figure, and are pushed towards the exit to be discharged down a chute and through a flap door fitted at the bottom of the furnace. The action of the discharge door allows an air flow into the furnace. The furnace has an array of gas fired burners arranged across its width (into the page). In the interests of computational economy, a furnace 'slice' containing a single burner is computed, bounded by symmetry planes situated midway between this burner and its neighbours.

The operation of this furnace was plagued by an excessive ingress of air through the exit flap which corrupted the temperature uniformity of the billets prior to their falling down the exit chute. The computational challenge was to determine furnace aerodynamics through appropriate adjustment of the burner firing conditions, which eliminated the ingress. The simulation shows that firing conditions, which are proprietary, have been found that prevent contact of cold air with the billet about to descend the chute.

A Single Burner Test Facility

An industrial-scale single burner (40 MW) fired with coal fitted to a refractory lined, box-shaped test furnace, is predicted using a mesh of 67x67x49. Figure 2 shows the temperature and oxygen profiles across the furnace. A common measure of the numerical quality of the predictions in such cases is the degree of symmetry achieved. The slight asymmetry observed in the predictions is a statistical error



resulting from the random specification of the turbulence intensity used in the particulate phase calculations. The level of agreement achieved here is typical to that which may be currently expected for the computation of engineering equipment.

Simulation of a Full-Scale Power Station Combustor

The combustor, which is typical of that of an electric power station boiler, consists of 48 wall-fired burners arranged in four rows (12 burners/row). In this example (see,Figs 3 a and b), all the burners in the two central rows are in operation and the six central burners in each of the top and bottom rows out-of-service in an effort to reduce the emissions of nitric oxide. The fuel is pulverised coal which is widely used throughout the world for the generation of electric power. The configuration implies the existence of a symmetry plane in the flow configuration, and therefore, only a half of boiler geometry is modelled in the numerical simulation. A mesh of 79x86x22 nodes is used for the simulations. The burner design implemented in the boiler, which is typical of modern low nitric oxide emission burners, describes four concentric inlets: a core air stream, surrounded by so-termed primary, secondary and tertiary streams. The

pulverised coal fuel is suspended in the primary stream. All the streams are swirled (i.e. given a circumferental component of velocity) which except for the primary stream assists in promoting flame stability. The primary stream swirl is subsequently eliminated near its discharge location by the inclusion of four circumferencially distributed radial plates which serve to concentrate the pulverised coal causing it to enter the combustion zone in 'fingers', which helps to reduce NO formation.

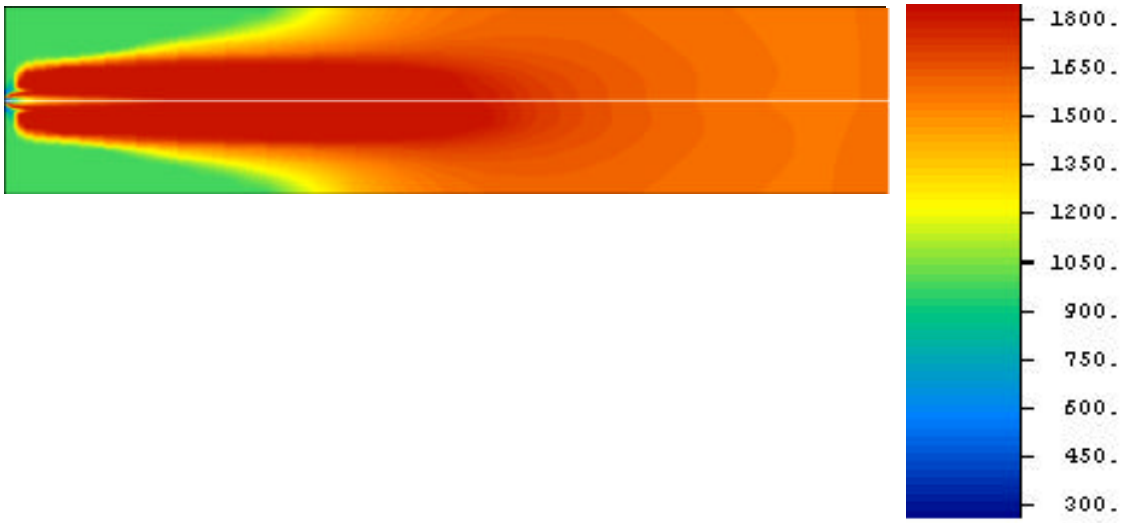
There is some flame impingement from the upper burners on the back wall, with the lower burner flame being deflected into the hopper region. The outlet temperature to the superheater pendants is, however, relatively uniform. It is observed that most of the NOx generation is confined to the near burner regions and along the particle trajectories where the temperature is high.

Fig.3 a - Temperature Contours of a Full scale power station boiler

Fig.3 b - Temperature Contours of a Full scale power station boiler

Cement Kiln Predictions

In the above examples, the interlinkage between the combustion and the process it is powering is mainly in the direction of flame to process. However, there are many examples where there is a complex two-way interaction. Such is the case of the cement kiln. The cement kiln consists of a large, slightly inclined and



rotating combustion chamber fired from its lower end with the charge of limestone and clay introduced from its upper end. The rotation of the kiln causes the charge to tumble down the kiln to exit as cement clinker at its lower end. The present rotary kiln performance prediction method is based on a technique where the flame calculation, and thus the heat transfer from the flame, is dynamically linked with a procedure which computes the cement chemistry and which provides the thermal boundary conditions of the former. The cement clinker formation routine is based on the reactions between the species: H_2O, $CaCO_3$, SiO_2, Al_2O_3, Fe_2O_3, CaO, C_2S, C_3S, C_3A, C_4AF

The prediction procedure incorporates the above-described multi-stream mixing formulation to accommodate further fuel streams. In cement kilns the modern tendency is to supplement the main coal or petroleum coke fuel with a waste fuel. The high temperatures within cement kilns permit the safe destruction of waste-derived fuels such as car tyres, solvents, sewage sludge, plastics etc., reducing the quantity of expensive fossil fuels required per unit of cement production. The task is quite simply to find burner conditions which enable the quantity of waste fuel to be maximised, and the fossil fuel requirement to be correspondingly reduced, with no loss of cement quality. The figures show the predicted temperature contours of a cement furnace and the resultant species concentration profiles along the kiln length.

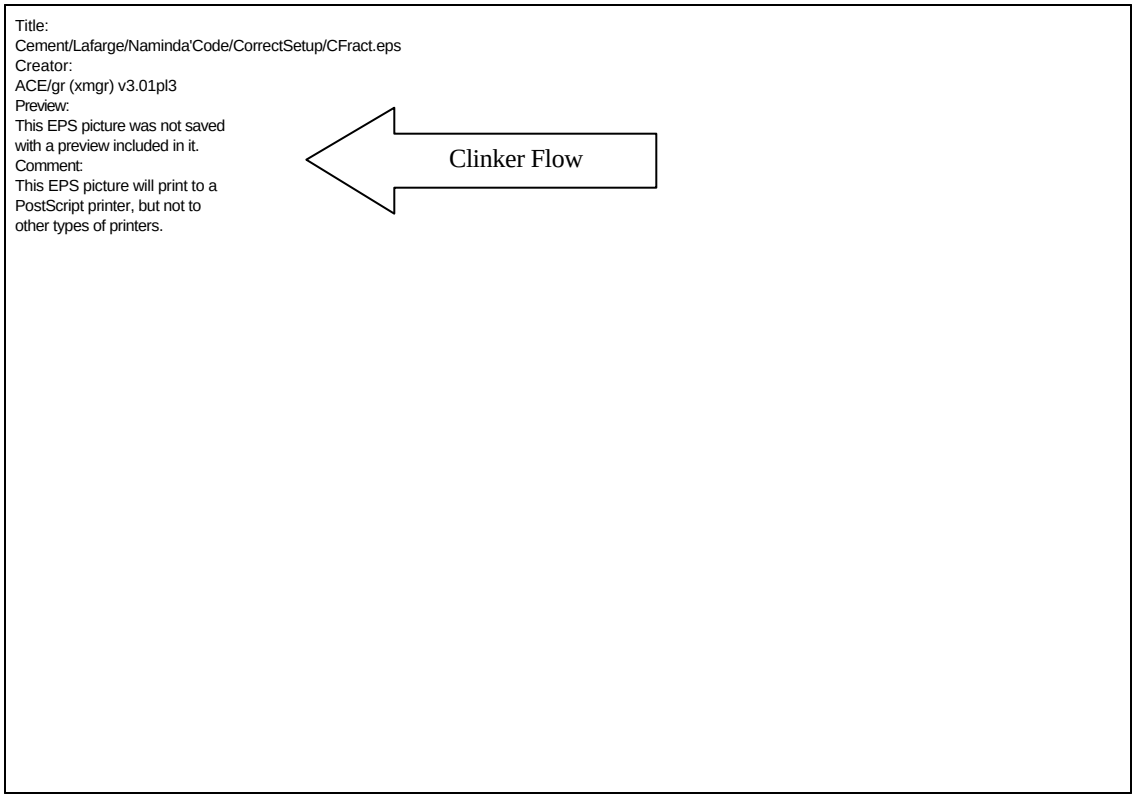
Fig. 4 a – Temperature contours of a Cement Kiln Flame

Fig 4 b – Mass fractions of clinker species and products

Gas Turbine Combustor

The gas turbine has traditionally been best suited to large scale applications such as air transport and power generation. Attempts to scale down to smaller applications have been thwarted by efficiency losses. The design constraints, blade tip losses for example, impeding scale reduction are being overcome. As a result small scale gas turbine combustors require to be designed, which in view of the many land-based applications envisaged, transport for example, require to be fuel tolerant.

The computations shown below are for a 325 kW annular gas turbine combustor, for example for power generation on the scale of an apartment building, fired with natural gas is presented below. The combustor consists of nine injectors firing a premixed air-fuel stream in the tangential direction, with a single intermediate air port per symmetry section and two sets of dilution rows of holes in the inner and outer surface of the flame tube. The design also includes an additional cooling air stage on the outer periphery of the flame tube in the exhaust section, to control the exhaust gas pattern factor. The geometric complexity of the combustor is self-evident, and computations are performed for a one ninth symmetry sector of the combustor using an unstructured computational mesh conforming precisely with the combustor geometry



(Fig. 5 a). The predictions reveal that this combustor design, which is the result of several trials, exhibits good performance characteristics. The combustion efficiency is high within the primary zone, the exhaust gas pattern factor of 6% is excellent, and the NO emission is acceptable and is observed to be mainly due to the thermal NO pathway, with the majority of the NO formation occurring at the high-temperature high-oxygen intersection cross-section upstream to the dilution zone.

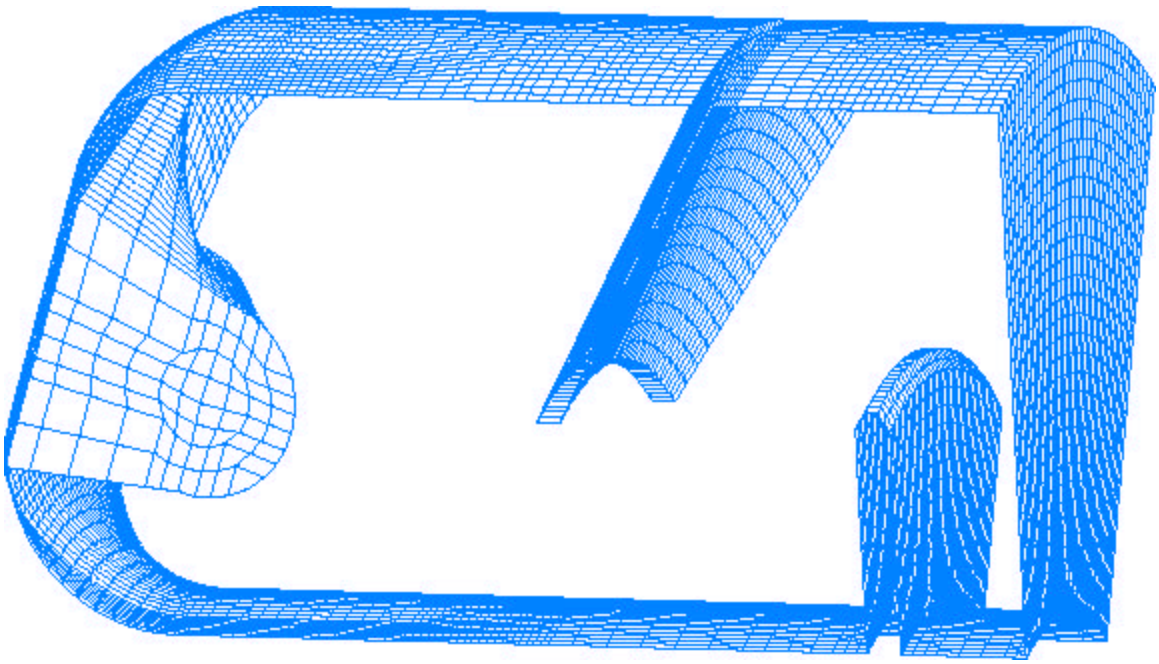


Fig. 5 a - Computational mesh

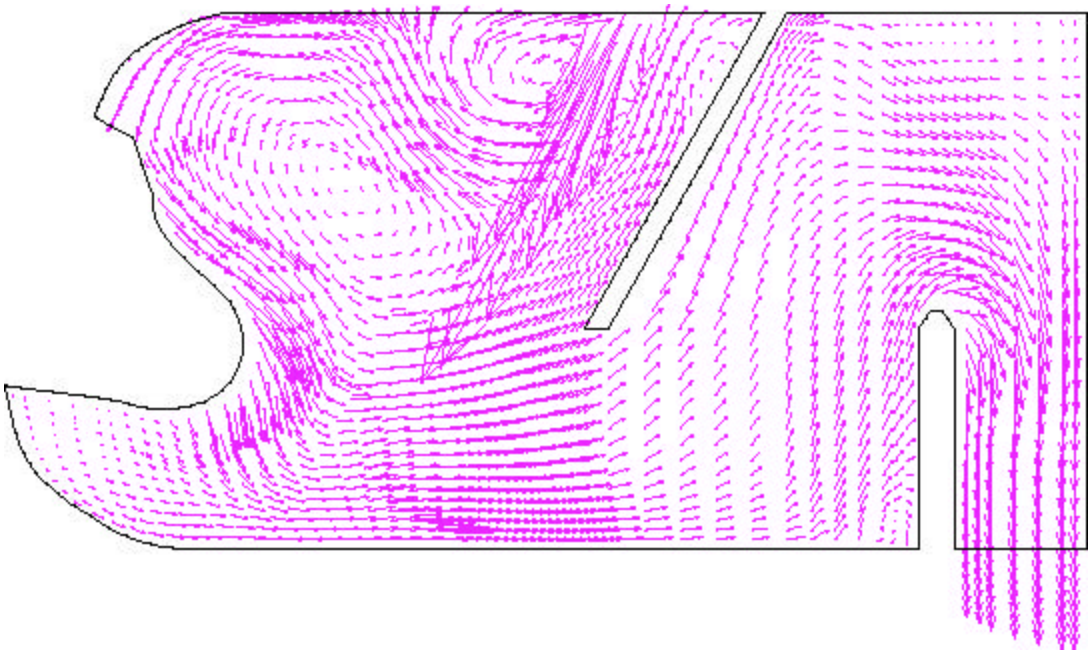


Fig. 5 b - Flow pattern on the centre plane of the computational sector

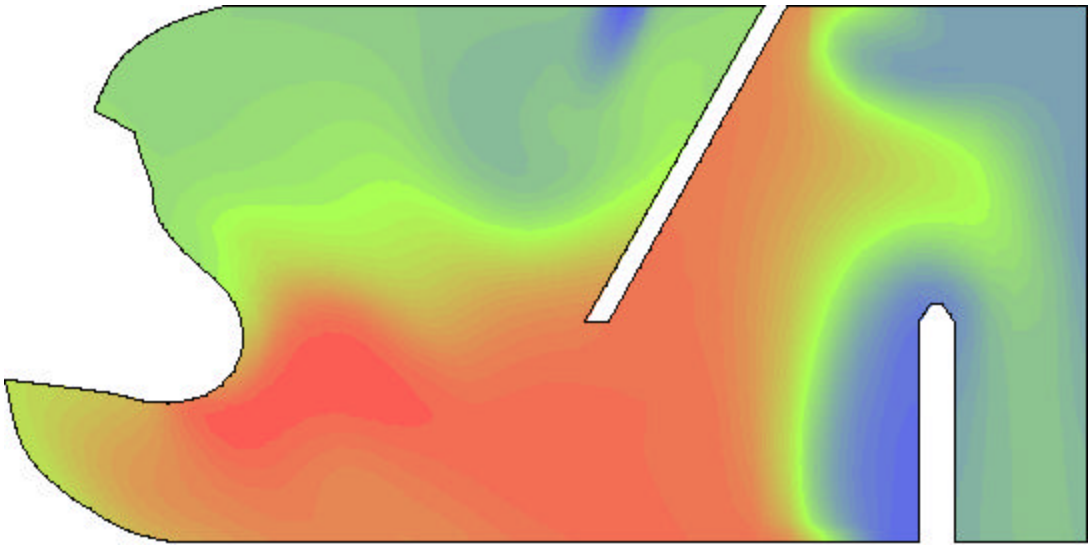


Fig. 5 d - Temperature contours on the centre plane of the computational sector

(T_{max} = 2500 K, T_{min} = 835K)

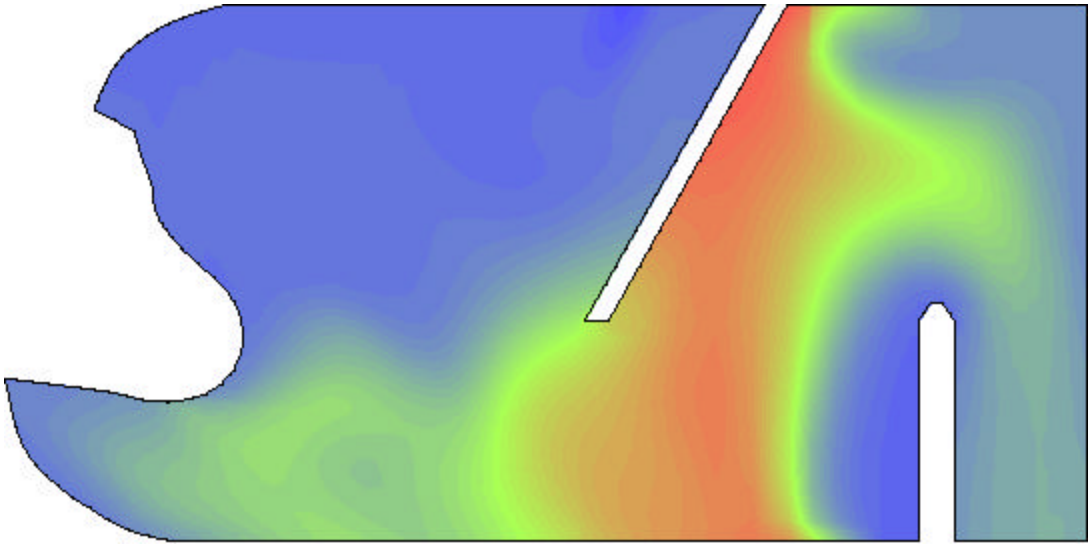


Fig. 5 e - NO concentration on the centre plane of the computational sector

(NO_{max} =432 ppmv, NO_{min}=3 ppmv)

CONCLUDING REMARKS

The modern subject of CFD is complex and extensive. The material which can be presented in a single review is therefore very limited. Faced with this restriction we have chosen to give especial attention to our own work and experience and we apologise to the many other and excellent workers in the CFD field. As engineers we have also strongly biased the need for applicability while recognising that there is much instructive and erudite physical modelling that we have ignored simply because it is not yet usable in practical calculations. We hope that we have demonstrated that CFD enables the deign of much engineering equipment to be refined in spite physical the current modelling limitations. In particular it is our experience that even if the absolute accuracy of the predictions is in some cases wanting, engineers almost always gain through the application of CFD the considerable benefit of fresh physical insight.

It is important to stress that the successful application of CFD is largely dependent on the experience and skill of the user. In our opinion the areas on which further development should be concentrated are: an improved simulation of the turbulence for affordable computational cost; an economic simulation of the turbulence/chemistry interaction; usable reduced chemistry modelling of the combustion of the 'engineering hydrocarbon fuel' including the role of soot; simulations of the very many pollutants that are increasingly a matter of public concern; better simulation of the char burnout of solid fuel combustion; and enhanced routines which enable the less than highly skilled user to generate effective grids for complex geometries for acceptable effort.

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