MODELLING FREE AND IMPACTING UNDEREXPANDED JET FIRES

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A numerical model for predicting jet fires resulting from high pressure, sonic releases of natural gas is described. The model embodies mathematical descriptions of all the important processes occurring in such fires, and is capable of accurately resolving the near field shock structure which occurs in these flows as well as including a realistic sub-model for flame lift-off height and a novel implementation of the discrete transfer method for calculating thermal radiation fields. The accuracy of the complete model is assessed by simulating a number of free jet fires, and a horizontal jet fire impinging a pressure vessel. Predicted flow and heat transfer fields are compared with available field scale measurements, with good agreement with the data being obtained.

Keywords: Sonic releases, jet fires, mathematical modelling

INTRODUCTION

This paper describes a numerical model for simulating jet fires which result from underexpanded releases of natural gas. An ability to predict the consequences associated with such fires is a necessary prerequisite to performing safety and risk assessments of operational and accidental releases of flammable gas from high pressure pipework and gas handling plant.

A number of mathematical models of jet fires have been reported in the literature. These vary in their level of sophistication and generality, and range from empirical approaches (e.g. Cook et al. (1)) and integral-based methods (e.g. Caulfield et al. (2)), through to numerical models based on computational fluid dynamics techniques. Despite their relatively long computer run times, numerical models provide the capability to predict all fire properties of interest to the safety engineer, including the interaction of fires with complex plant. The level of detailed information such models provide, and their potential accuracy, also encourages further development of these predictive methods.

Several authors have derived numerical models, based on solutions of the fluid dynamic equations, for wind blown jet fires that result from subsonic releases. The various models generally allow the prediction of fire structure and external radiation fields, with the major difference between them being in terms of the formulation used to describe the turbulent non-premixed combustion process. Botros and Brzustowski (3) implemented a flame sheet combustion model, whereas Galant et al. (4) used an approach based on Magnussen's (5) version of the eddy break-up method. Fairweather et al. (6, 7) described turbulent combustion using a conserved scalar/prescribed probability density function approach coupled to a laminar flamelet model. Models of fires from sonic releases are fewer in number, although Gore et al. (8)

predicted field scale fires studied experimentally by Pfenning (9) using a pseudo-source to account for the near field shock containing region. Barker et al. (10) also described a novel modelling study of free, horizontal jet fires, and demonstrated good agreement between predicted levels of thermal radiation external to such fires and data obtained from a large scale release.

DESCRIPTION OF UNDEREXPANDED JET FIRES

Underexpanded free jet fires are characterised by a non-reacting near field region upstream of the combusting portion of the jet, with the distance downstream of the release point separating these two regions being known as the lift-off height of the flame. For high pressure jets the near field region resembles a free underexpanded non-reacting jet, with a system of shocks being located immediately downstream of the release point. The qualitative behaviour of this region is dictated by the ratio of the pressure at the release point to the ambient value. For values of this pressure ratio just above the critical value at which the source flow is at sonic velocities, a moderately underexpanded jet is formed which is characterised by a system of oblique shocks. At larger pressure ratios a Mach disc, or barrel shock, is formed normal to the flow downstream of the release point, with such jets being referred to as highly underexpanded. The pressure ratio separating these two flow regimes is dependent on the gas being discharged. Figure 1 shows predicted Mach number fields for two underexpanded jets, with pressure ratios of 1.8 and 3.6, derived from a non-reacting version of the numerical model described below. The qualitatively different shock patterns occurring in moderately and highly underexpanded jets is clearly apparent from these results.

Beyond the lift-off height, combustion occurs within subsonic regions of the flow and thermal radiation is emitted from high temperature, gaseous combustion products. In large scale fires from subsonic releases, residence times are sufficient for significant levels of soot to be formed which in turn enhance radiative heat transfer both within the flame and to the surroundings (7). In sonic releases, however, residence times are much shorter, and for low hydrocarbon fuels such as natural gas, significant levels of soot may not be formed. This finding has been verified experimentally (1) for large scale natural gas fires, where the radiative heat loss from the flame is found to decrease significantly with increasing jet exit velocity. Lastly, for items of plant engulfed by such a fire, convective heat transfer to the impacted object enhances the thermal loading due to radiation.

MATHEMATICAL MODEL

The model was based on solutions of a system of partial differential equations which describe the conservation of mass, momentum, energy and conserved scalar variables. These equations were written in their density-weighted (Favre averaged) and high Reynolds number forms for solution. The equation set was closed, and turbulence quantities described, through use of the standard k-ε turbulence model, modified to account for compressibility effects through the recommendations of Sarker et al. (11).

The turbulent non-premixed combustion process was modelled by assuming fast gas-phase chemical reaction and a shape for the probability density function (pdf) of a conserved scalar, the latter being taken to be mixture fraction. A two-parameter, β-pdf was used, with the form of this pdf specified in terms of the mean and variance of mixture fraction obtained from solution of modelled transport equations for these variables. The density weighted pdf constructed in this way was then used to evaluate both density weighted and unweighted values of any scalar quantity that could be uniquely related to mixture fraction. The laminar flamelet concept was used to provide a library of relationships between the instantaneous thermochemical state of the burnt mixture and mixture fraction, with mean properties such as density, temperature and species mass fractions being obtained by integration over the pdf. The flamelet library was derived from a full chemical kinetic scheme for methane-air combustion, with laminar flame calculations performed for a strain rate of 115 s^{-1} and a radiative heat loss of 5%. Fairweather et al. (7) have shown that mean flow fields are relatively insensitive to the strain rate used, with the level of radiative heat loss introduced being consistent with measurements from field scale jet fires (1). Turbulent flow calculations were also performed using the soot formation and oxidation model described in (7), although in the results given later the levels of soot formed were found to be sufficiently small to not contribute significantly to radiative heat transfer within the fires.

The mean lift-off height of the flame was calculated using the approach of Sanders and Lamers (12) which assumes that combustion does not occur within the lift-off region due to flame quenching by the turbulent flow field. Mean thermochemical fields are then determined by taking a weighted average of mean values calculated from the laminar flamelet library and those derived by assuming isothermal mixing. The weighting function used has two components - the probability of burning, based on a model for the mean strain rate of large turbulent eddies, and a prescribed triangular pdf for the instantaneous lift-off height. This model can therefore be viewed as a multi-flamelet model comprising a burning and a non-reacting flamelet. More details of this approach can be found in (12).

Thermal radiation received at any point of interest was calculated using the discrete transfer method developed by Lockwood and Shah (13), as extended by Cumber (14). In this approach the field of view of a receiver is partitioned into a number of elements, with the incident radiative intensity being assumed constant over each element and taking the value determined at its centroid. The incident intensity at each centroid is calculated by tracing rays through the computational domain, with a ray's orientation defined by the centroid location on the unit hemisphere. For each ray the temperature and participating species concentrations in each finite-volume cell traversed are noted and input to a statistical narrow band radiation model (see Grosshandler (15)) to calculate the incident intensity. The incident flux integral is then evaluated by summing the incident intensity distribution in a numerical quadrature. In the present work, the computational cost of evaluating incident fluxes was reduced significantly by improving the efficiency of the ray quadrature using an adaptive algorithm in which rays were directed at a fire in an automatic fashion. The adaption criteria was based on an estimation of the local numerical error calculated by Richardson extrapolation - see Gerald and Wheatley (16). This allowed a numerically accurate prediction of incident flux to be obtained using, typically, 100 rays, compared to the 700 rays that are generally needed when using a more conventional ray distribution. Lastly, convective heat transfer rates to impinged obstacles were determined from the predicted temperature gradient normal to the vessel multiplied by the turbulent thermal conductivity, with the latter value calculated from predicted turbulent viscosity and prescribed Prandtl number values adjacent to the vessel.

NUMERICAL SOLUTION METHOD AND BOUNDARY CONDITIONS

Numerical solution of systems of transport equations for subsonic flows is typically achieved using some variant of the pressure correction, or SIMPLE, algorithm originally proposed by

Patankar and Spalding (17). This method has been extended to compressible flows, and applied successfully to the simulation of moderately underexpanded non-reacting jets by Page and McGuirk (18). However, the compressible pressure correction method is computationally expensive compared to numerical solution methods originally developed for high speed gas dynamics such as Godunov's method (see, for example, Hirsch (19)). A further complication in adopting a numerical solution strategy for flows that contain both sonic and subsonic regions is that compressible solvers are very inefficient at low Mach numbers where the mass and energy conservation equations become decoupled.

The approach adopted in the present work was to treat the non-reacting, near field region as an axisymmetric, underexpanded jet, and at the predicted lift-off height calculated profiles were used as a source specification for a fully three-dimensional simulation of the subsonic, reacting portion of the flow. The main advantage of this solution strategy is that the most appropriate numerical methods can be applied within the two different flow regimes. A further benefit is that the combusting portion of the fire can be treated as an incompressible flow with the density field prescribed by the laminar flamelet library, which in turn makes solution of an energy equation unnecessary. Decoupling the combusting region from the near field, non-reacting region at this stage of development is considered an acceptable approximation as the flow upstream of the lift-off height is influenced to a negligible extent by the downstream conditions (12).

For the underexpanded, non-reacting jet simulations the system of transport equations were discretised over a finite-volume mesh superimposed on the domain of interest, with inviscid fluxes approximated using a second-order variant of Godunov's method. The system of algebraic equations derived in this way was then converged by time marching to a steady state. This convergence strategy is efficient for high Mach number flows, and allows grid independent resolution of the shock structures downstream of the release point at a modest computational cost. To further enhance the efficiency of the model, hierarchical adaptive grids were also used, with local grid refinement taking place in regions of steep gradients. A detailed discussion of the numerical solution method employed can be found in Falle and Giddings (20). In the simulations the release pipe was represented as a thin walled tube, with the hyperbolic nature of the sonic flow at the exit plane of the pipe requiring pressure, velocity and density to be fixed. Turbulent kinetic energy and its dissipation rate were set to values typical of fully developed turbulent pipe flow (see Hinze (21)), with the source boundary condition being completed by setting the mixture fraction to one and its variance to zero. The computational domain used for the underexpanded jets was sufficiently large in both the radial and downstream directions to ensure that the fixed pressure and free flow boundary conditions imposed, respectively, in each of these co-ordinate directions had no influence on the predicted jet structure.

In the three-dimensional simulations of the combusting portion of the jet fires an adaptive, Cartesian mesh was superimposed on the domain of interest. Over each control volume defined by the mesh, the system of transport equations was approximated using a finite-volume scheme. In this scheme diffusion terms were represented by a second-order accurate central difference scheme, with advection terms represented using a total variation diminishing version of the QUICK scheme. The composite finite-volume scheme is nominally second-order accurate and reproduces the physically correct monotonic behaviour in the vicinity of steep gradients. Fixed pressure boundary conditions were imposed over the majority of the calculation domain boundaries, with the exception of the jet source and inlet plane boundaries over which mean velocity and turbulence quantities consistent with an atmospheric boundary layer were imposed.

At solid boundaries, such as the ground or a pressure vessel engulfed by a horizontal jet fire, turbulent law-of-the-wall profiles and non-slip conditions were employed. The boundary conditions and finite-volume scheme approximation to the system of transport equations form a non-linear algebraic system which was converged using the pressure correction algorithm. In all the computations performed, a sufficiently large number of grid nodes was used to ensure that the results presented below were effectively free of numerical error.

RESULTS AND DISCUSSION

In applying any mathematical model the user must have confidence that the predicted flow and heat transfer fields are reliable. Some assessment of a model's accuracy and range of applicability must therefore be made. To this end, a number of comparisons between predictions of the model described and appropriate and reliable experimental data are presented below. Space limitations do, however, necessitate that discussion is restricted to a representative subset of the comparisons with experimental data which have been used to validate the model.

As the mathematical model consists of a number of sub-models, each accounting for some physico-chemical aspect of high pressure jet fires, it is beneficial, as far as the scarcity of experimental data allows, to validate each component of the model in turn. This ultimately gives an appreciation of the capabilities of the composite model, but moreover helps identify any weaknesses in the sub-models so that effort can be focused on critical aspects to improve performance.

Considering the shock containing, non-reacting region immediately downstream of the release point, an extensive validation of the model for both moderately and highly underexpanded jets exists in the open literature - see Cumber et al. (22, 23). In brief, the mathematical model has been demonstrated to give reliable predictions for all jets for which measurements are available. In particular, mean and turbulence velocities, mean concentrations and the number, strength and orientation of the shocks formed have been found to be well predicted for a range of drive pressures up to 70 bar. As an example, Figure 2 shows comparisons between model predictions and data for velocity decay (non-dimensionalised with respect to a reference velocity taken as the square root of the ratio of ambient pressure to density) along the centre-line (non-dimensionalised by a pipe diameter of 2.7 mm) of two highly underexpanded jets studied experimentally by Birch et al. (24). One aspect of compressible releases not encountered in subsonic jets is the observed reduced mixing rate caused by additional turbulence dissipation mechanisms which occur in shock containing flows. The results of Figure 2 demonstrate that compressibility effects can significantly affect the rate of velocity decay within such jets, as exemplified by model results derived with and without a compressibility correction (11), and that incorporation of such effects within the model does lead to accurate predictions.

The second aspect of the model requiring evaluation is the method for determining the flame lift-off height. Predictions of the mean temperature field in a subsonic lifted jet fire are shown in Figure 3. Two predictions are given: the first based on initiating combustion when a turbulence time scale (k/ε) on the jet axis has increased to 5×10^{-3} s, as advocated by Chakravarty et al. (25) and applied previously to jets in a cross-wind by Fairweather et al. (6, 7), and the second determined using the multi-flamelet model described earlier. Comparing the two predictions, the main point of note is that although the calculated lift-off heights are similar the transition from the non-reacting region to the combusting zone, and hence the way combustion is initiated, is quite different. Predictions of the multi-flamelet combustion model are in fact physically realistic, whereas the threshold model creates an unrealistic step change in the temperature field at the lift-off height. In the predictions given later, however, heat flux results were not found to be affected significantly by the flame lift-off height model employed. The accuracy of the multi-flamelet model is assessed in Figure 4 which compares predictions of the asymptotic (with respect to pressure) lift-off heights observed in sonic jet releases by Birch and Hargrave (26), plotted as a function of the square root of release pipe diameter (d), for natural gas jets with a static exit pressure of 30 bar. As is evident from these results, the more elaborate lift-off height model is capable of yielding reliable predictions of the distance from the sonic source at which combustion is initiated.

Turning to predictions for complete sonic jet fires, Figure 5 compares results for radial mean temperatures, at three downstream locations, within an essentially vertical, natural gas fire studied by Pfenning (9). The initial jet source and atmospheric conditions for this fire are given in Table 1. Predictions of temperature are seen to be in reasonable agreement with observations in the far field of the fire, with the spreading rate of the jet being accurately predicted. Temperatures at the first downstream station do tend to be overpredicted, although this measurement location is just beyond the lift-off height of the flame where comparisons are prone to error due to the fluctuating nature of the lift-off zone. Further downstream, where the bulk of the high temperature gases which are responsible for radiative heat loading are located, agreement with observation is more satisfactory. Measured and predicted radiative fluxes received at a number of locations and orientations about the fire are given in Table 2. Overall, agreement between theoretical results and observations is encouraging.

Predictions of the model were also compared with a natural gas jet fire which was studied (1) at the British Gas Spadeadam test facility in Cumbria as part of a series of field trials on flares. The jet source and atmospheric conditions for this release are again given in Table 1. The particular fire considered is significantly larger than that examined by Pfenning (9), with a much greater mass flow rate, and was exposed to higher wind speeds. Figure 6 compares the observed flame envelope and radiative fluxes received by a line of radiometers located downwind of the release with the predicted centre-line flame trajectory and flux levels. Again, agreement between theory and experiment is satisfactory, with reliable predictions of radiative fluxes received about the fire being obtained.

The final comparison is for a horizontal, sonic natural gas jet fire which impacted a cylindrical pressure vessel. This release was again studied (27) at the Spadeadam test site, with the jet source and atmospheric conditions being given in Table 1. The fire considered was stabilised on a release from a pipe whose centre-line was 1.7 m above ground level, and impinged on a pressure vessel which was orientated normal to the wind direction and the release pipe, and which was located 21.5 m from the source and 3 m above the ground. The pressure vessel itself was 2.2 m in diameter and 8.8 m long. A clearer understanding of the location of the vessel relative to the fire can be obtained from Figure 7 which shows reasonable agreement between predicted (corresponding to a mean temperature of 1400 K) and observed flame envelopes.

Radiative heat fluxes received external to this fire were measured using a line of radiometers positioned in a cross-wind direction, orthogonal to the centre-line of the fire, and located 15 m downstream of the release. In addition, the pressure vessel itself was also instrumented with total (convective and radiative) heat transfer gauges. Figures 8 and 9 show, respectively, radiative fluxes external to the fire and total fluxes on the stagnation line along the front surface of the vessel. Agreement between theory and experiment is again good, and in particular predictions of the high thermal loading to the vessel are both qualitatively and quantitatively correct.

CONCLUSIONS

A numerical model capable of predicting the structure of, and heat transfer from, jet fires resulting from high pressure, sonic releases of natural gas has been described. The accuracy of the model has been assessed by comparing its predictions with experimental velocity data obtained in the near field, shock containing regions of such releases, and with observed flame lift-off heights. Comparisons have also been made with measurements of flame temperature, trajectory and the radiative flux received about large scale free jet fires, as well as with internal and external heat fluxes measured in a fire which impacted a cylindrical pressure vessel. In all cases, good agreement was found between predictions of the model and available data.

Further work remains to be performed in order to more fully validate individual components of the model, and to assess the ability of the complete model to predict the full, three-dimensional distribution of heat loading on impacted vessels. From the comparisons described, however, it is clear that computational fluid dynamic techniques offer the potential to be very useful in promoting the safe design and operation of industrial plant. In particular, they can be applied, with only minor modification, to a wide range of complex release scenarios which, due to the dimensionality of the flow fields created, are difficult to address using simpler modelling approaches. They can be used in the detailed analysis of critical release scenarios, and their firm basis in physical understanding also means that they can be employed in the design of simpler phenomenological models which can be used routinely due to their short computer run times.

In the past the safety engineering community has been reluctant to take up computational fluid dynamics techniques, primarily because the advantages of using this technology must be weighed against the relatively long computer run times and additional technical knowledge required to realise the full benefits. Improvements in the price performance of computer technology and the use of parallel computer architectures are, however, set to reduce turn-round times to more acceptable levels and to thereby mitigate the long run-time issue. The more serious difficulty of understanding and mastering a new technology is also currently being addressed by simplifying problem specification using graphical user interfaces, and results interpretation is being revolutionised by the application of animation techniques and virtual reality. All in all, therefore, computational fluid dynamics is a technology that is reaching maturity and will, in the coming years, find its place in the safety engineers' "tool chest".

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Table 1. Jet source and atmospheric conditions.

Reference	Configuration	Stack Height /m	Stack Diameter /mm	Pressure Ratio	Mass Flow Rate /kg s^{-1}	Wind Speed /m s^{-1}
Pfenning (9)	Free Jet	1.5	102	1.64	3.7	0.4
Cook et al. (1)	Free Jet	16.2	385	1.68	65.1	6.4
Bennett et al. (27)	Horizontal Jet	-	75	12.00	8.2	5.5

Table 2. Measured and predicted radiative fluxes about the fire studied by Pfenning (9).

Radiometer Location * /m			Radiometer Orientation ** /Degrees		Radiative Heat Flux kW m^{-2}	
x	y	z	φ_{twist}	θ_{tilt}	Measured	Predicted
-1.7	7.4	20.4	283	90	8.3	6.9
-2.1	8.9	-1.5	283	32	5.0	5.1
-1.7	7.4	1.8	283	34	5.8	8.5
-0.3	1.5	-1.5	0	0	7.1	6.9

* Origin taken on the axis of the vent stack at the stack exit plane, x - direction parallel to wind direction, y - direction normal to wind direction, and z - vertical direction.

** φ_{twist} - angle of rotation in the x-y plane of the radiometer orientation, θ_{tilt} - angle of inclination between the radiometer and the z axis.

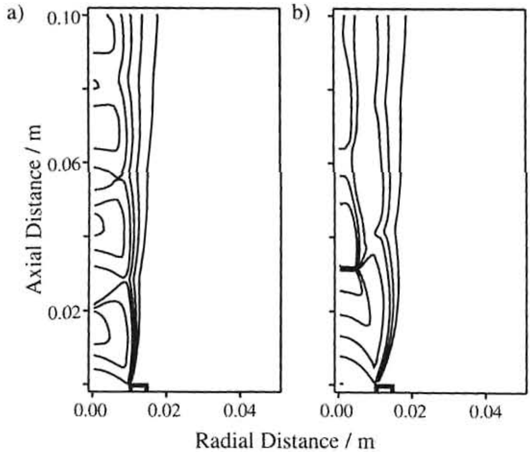


Figure 1. Predicted Mach number fields in a) moderately and b) highly underexpanded jets

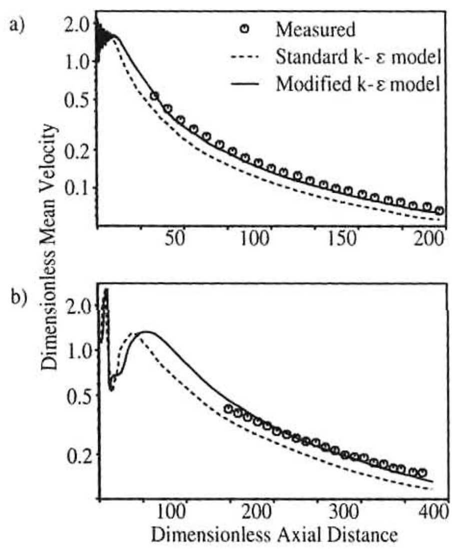
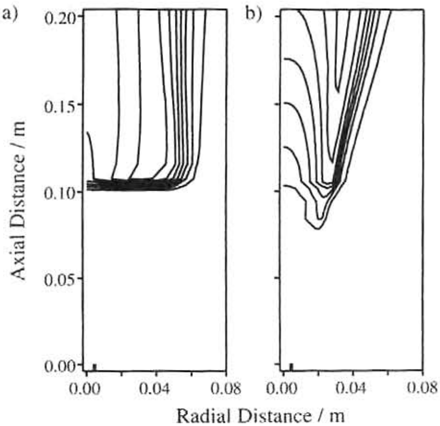


Figure 2. Decay of mean velocity in underexpanded jets with pressure ratios a) 3.1 and b) 36.9



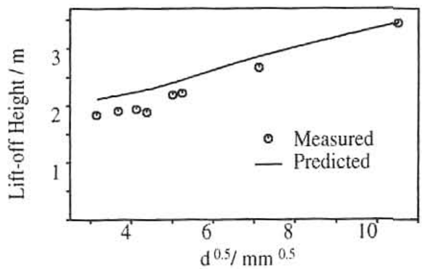


Figure 3. Mean temperatures in a subsonic fire using a) threshold and b) multi-flamelet models (upstream contour 500 K, decreasing in 200 K steps downstream)

Figure 4. Asymptotic lift-off heights in sonic, natural gas fires

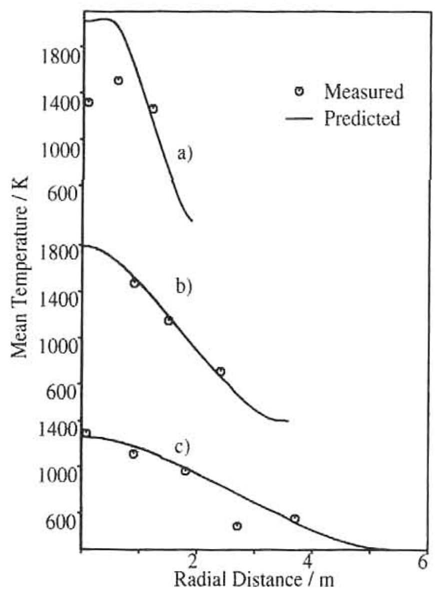


Figure 5. Radial mean temperatures in a sonic fire at a) 7.6, b) 13.1 and c) 20.4 m downstream

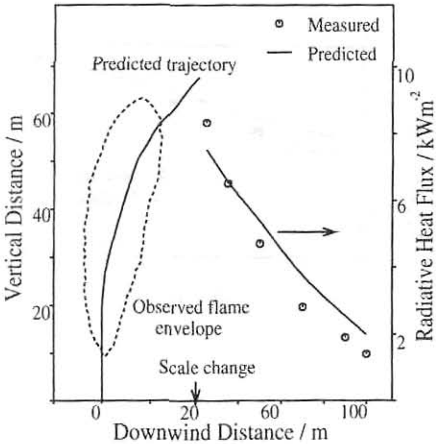


Figure 6. Flame trajectory and radiative fluxes received external to a sonic fire

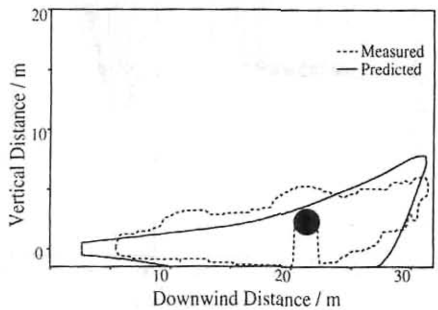


Figure 7. Flame envelopes for a sonic fire impacting a cylindrical vessel

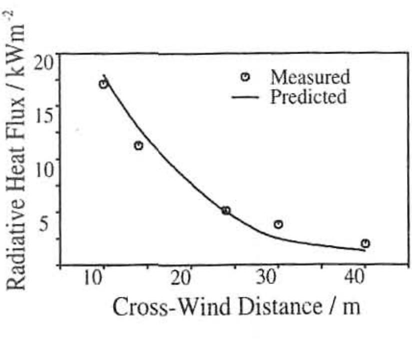


Figure 8. Radiative fluxes received external to a sonic fire

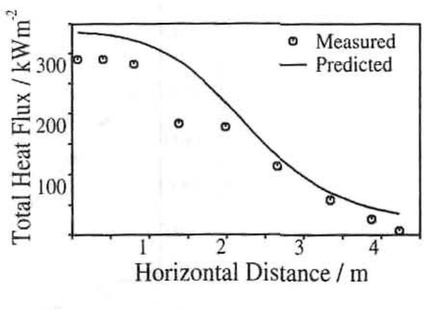


Figure 9. Total fluxes received along the stagnation line of the impacted vessel