LARGE-SCALE FREE AND IMPINGING TURBULENT JET FLAMES - NUMERICAL MODELLING AND EXPERIMENTS

A.D. Johnson, A. Ebbinghaus, T. Imanari, S.P. Lennon and N. Marie
Shell Research and Technology Centre, Thornton, P.O. Box 1, Chester CH1 3SH

This paper summarises progress in the development and validation of a suite of computational fluid dynamics sub-models for the calculation of open air and impinging turbulent gas jet flames. The sub-models are implemented in the commercial flow and radiative heat transfer solvers CFX-FLOW3D and CFX-RADIATION. Demonstration calculations are reported for an open air sonic 0.3 kg/s propane flame, and a 2.5 kg/s subsonic natural gas flame in the open air and impinging on a 2m diameter cylindrical target. Improvements for the calculation of under-expanded jet shock structures, flame lift-off, and combustion in the main bulk of the flame are reported. A practical model for predicting convective heat transfer is identified. Results of preliminary calculations of flame impingement heat transfer are presented.

keywords: CFD, Jet Flame Impingement, Heat transfer

1. INTRODUCTION

The Piper Alpha disaster in 1988 highlighted the risks of hydrocarbon jet fires on offshore installations and graphically demonstrated the potential for escalation of hazards when jet fires impinge on structures. Jet fires may also present a hazard in onshore petrochemical plants, the main difference being that in the confines of a remote offshore platform the consequences are more likely to result in the loss of life. Lord Cullen's report on the Piper Alpha disaster[1] emphasised the need for accurate determination of the potential hazards on offshore installations in Safety Cases and where necessary the measures to mitigate them.

For more than ten years Shell Research has been studying the hazards posed by impinging jet fires using large-scale experiments. The experimental measurements have provided unique information about the extent of flame engulfment and the heat loading to structures. However, the measurements are limited in their application to the prediction of hazard consequences for jet fire and impingement target scenarios that are similar to the experiments. In this paper we describe a CFD model that is being developed for the determination of radiative and convective heat loading for a wide range of gaseous jet flames and obstacle geometries.

The CFD model consists of a suite of modular sub-models, based around the commercial computer codes CFX-FLOW3D and CFX-RADIATION from AEA technology[2]. These codes are used to generate numerical grids and to solve turbulent transport and radiative heat transfer equations. New physical sub-models have been added for turbulent combustion, soot formation and radiative heat transfer[3]. This paper summarises progress on the following extensions of the model.

1. Application of new algorithms for calculating the structure of under-expanded gas jets.

2. Improvements in the model for calculating flame lift-off.

3. Extension of the model to propane gas flames.

4. Improvements in the combustion model for the main bulk of the flame.

5. Preliminary results of the application of the model to predict flame impingement and impingement heat transfer for natural gas flames.

2. CALCULATION METHODOLGY

Figure 1 illustrates the method we have adopted for splitting the problem of calculating the structure of a turbulent jet flame arising from the ignition of a high pressure release of gas into manageable parts.

2.1 Jet shock structure

If the stagnation pressure of the gas in the system is above about 2 bara, the emerging jet will be sonic and the pressure in the jet at the exit plane will be above ambient. As the jet expands to atmospheric pressure it forms a series of complex shock structures. The turbulent straining and shearing of the flow at the edge of the jet, where the mixture is flammable, is much too high in this expansion region for a flame to exist, whilst the fuel/air mixture in the centre of the jet is too rich to support combustion. Only after the jet has expanded down to atmospheric pressure and the strain rate in the flammable region at the edge of the jet has reduced can the first turbulent burning be established - at the flame lift-off point. The under-expanded jet is unaffected by the downstream combustion, therefore, the flowfield and shock structure can be determined using an axisymmetric fully compressible CFD calculation without combustion. High Mach number modifications to the pressure correction algorithm derived by AEA technology and an additional modification to the turbulence model originally proposed by Sarker[4], which reduces the turbulent viscosity in regions where the mach number is high, are used to calculate the flowfield. The turbulent viscosity constant C_μ in the k-ε model is also reduced from 0.09 to 0.06, according to the recommendations of Sanders[5], to give better representation of scalar mixing in round jets. This value is used for all the jet flame calculations. Higher-order upwind differencing schemes are also used for the convective terms to give better resolution of sharp gradients in variables. Radial profiles of jet properties are taken at an axial position where the local pressure is close to ambient, but far enough upstream for the local turbulent strain rate to be too high to support combustion. These profiles are then used as inlet conditions for the flame lift-off calculation. Figure 2 shows a comparison between measurements[6] and predictions of dynamic pressure along the axis of the jet.

2.2 Flame Lift-off

The amount of mixing in the initial jet expansion and the fact that the local mean turbulent strain rate is much higher than the extinction strain rate of laminar diffusion flames suggests strongly that the combustion process at the flame lift-off point in high-pressure gas jet flames is pre-mixed. Therefore the flame lift-off is calculated using an assumed probability density function (PDF), premixed laminar flamelet model, first used by Gu[7] for modelling the lift-off of subsonic natural gas jet flames. The model is an extension of work by Bradley et al.[8] on the calculation of premixed turbulent burning velocities. The model is based on the specification of a mean turbulent volumetric heat release rate, $\bar{q}_t$ which is a source term in the transport equation for thermal enthalpy

$$\bar{q}_t = \int_{f_{min}}^{f_{max}} P_b(f) \int_0^1 q_l(\theta, f) p(\theta, f) d\theta df \qquad (1)$$

$q(\theta, f)$ is the laminar unstretched heat release rate (W/m^3), determined from calculations using the PREMIX code from Sandia[9] and a full chemical kinetic scheme for 31 species and 97 reactions, $p(\theta, f)$ is a joint PDF, which can be expressed as the product of conditional single variate beta-function PDF's $p(\theta / f)$ and $p(f)$ whose form is given respectively by the mean and variance of a reaction progress variable θ and by the mean and variance of the mixture fraction f. $P_b(f) = P_b(K_t(f)Le)$ is the turbulent probability of burning, which is a function of the fuel Lewis number *Le* (the ratio of thermal diffusivity to the molecular diffusivity) and the turbulent Karlovitz number (the ratio of the chemical timescale to the Taylor timescale) $K_t = \left(\frac{\varepsilon \nu}{15}\right)^{1/2} \frac{1}{u_l^2(f)}$, where $u_l(f)$ is the laminar unstretched burning velocity for mixtures between the flammable limits f_{min} and f_{max}, ε is the rate of dissipation of turbulent kinetic energy and ν is the kinematic viscosity. The turbulence model used is the standard k-ε model[2], with added terms to take into account mean density and pressure gradients created due to the heat released by the combustion process[10]. CCCT differencing is used for the convective terms to give good resolution of sharp gradients in variables. Figure 3 shows measured[6] and predicted dynamic pressures taken radially at a distance of 1 m from the nozzle of a 0.3 kg/s sonic propane release.

The flame lift-off position is defined as the axial position at which the mean turbulent heat release rate achieves a threshold value. Figure 4 shows a comparison of measured[6,11] and predicted flame lift-off positions for propane jet flames. The lift-off position is defined as the point at which the mean turbulent heat release rate is 10 MW/m^3. The x-axis for this figure is the jet velocity after it has expanded isentropically to atmospheric pressure as described by Chamberlain[12]. Also shown are the predictions from a correlation proposed by Kalghatgi[13].

2.3 3-Dimensional flame structure

Once the flame lift-off position has been determined, the CFX-FLOW3D is run with combustion switched on downstream of the lift-off point to calculate the 3-Dimensional flame structure. At present the flame structure is calculated using an assumed PDF and strained laminar diffusion flamelet combustion model similar to that described in reference 3. This is because the premixed combustion model used in the flame lift-off calculation does not as yet include the calculation of soot formation or radiative heat loss. In reference 3 the effect of radiative heat loss was defined a-priori using a formula for the reduction in the laminar diffusion flamelet temperature originally defined by Crauford et al[14].

$$T(f) = T_{ad}(f)[1 - \chi(T_{ad}(f) / T_{ad}^{max})^4] \qquad (2)$$

where χ is a constant throughout the flame. Radiative heat transfer can thus be calculated as a post-process. The 3-D flame structure and flame centreline temperatures shown in the lower half of figure 1, for a horizontal 0.3 kg/s propane jet flame, are derived from calculations based on a 280 s^{-1} laminar diffusion flamelet with $\chi = 0.21$, as recommended by Fairweather et al[15] for calculating subsonic nonpremixed propane jet flames. The flame centreline trajectory is well predicted. However, the centreline temperatures are overpredicted considerably in the first two metres of flame, because the laminar diffusion flamelet model overpredicts combustion in the fuel-rich core at the start of the jet. The centreline temperatures are well predicted in the bulk of the flame however, beyond 2m from the release point.

3. MODIFICATIONS TO THE 3-D FLAME COMBUSTION MODEL

Two modifications to the combustion model have been made recently in an attempt to improve the accuracy of the predictions of gas temperatures and radiative heat transfer. Firstly, a transport equation is solved for the thermal enthalpy loss due to radiative heat transfer, $\tilde{h}_{loss}$. The reduced Favre temperature due to radiative loss $\tilde{T}$ is approximated by

$$\tilde{h}_{loss} = \overline{Cp_{ad}}\ (\tilde{T}_{ad} - \tilde{T}) \qquad (3)$$

If it is assumed that the reduced temperature profile follows the form of equation (2), taking the Favre average and equating to the above provides a local χ value,

$$\chi = \frac{\tilde{h}_{loss}}{\overline{Cp_{ad}}\ (\widetilde{T_{ad}^{5}} / T_{ad}^{max^4})} \qquad (4)$$

Thus, a local χ value can be calculated for each numerical cell from the local enthalpy loss and adiabatic flame properties. The second modification is to select a laminar diffusion flamelet according to the local turbulent mean eulerian strain rate $\bar{s} = \frac{u'}{\lambda} = \left(\frac{\varepsilon}{15\nu}\right)^{0.5}$ where λ is the Taylor microscale and u' is the rms turbulence velocity. If $\bar{s}$ at points downstream of the flame lift-off point is greater than the counterflow laminar diffusion flame extinction strain rate, the extinction strain rate flamelet is used. Thus the effect of strain on reducing turbulent combustion rates is incorporated in a crude manner.

This model has been applied to the calculation of a series of large-scale horizontally released natural gas flames[16]. As an example of results, figure 5 shows results of the application of the new combustion model for a 2.5 kg/s natural gas jet flame released horizontally from a 152 mm pipe[16]. Figure 6 shows temperature profiles taken horizontally across the flame at various distances downstream of the release point at heights of 0.5m and 0.8 m above the release point. The predictions are in good agreement with the measurements, with the exception of the profile taken 12.8 m from the release point, which is almost on the edge of the jet flame.

Table 1 shows measured and predicted radiative heat fluxes located to the side of the flame. By setting the radiative absorption coefficient of the ambient air to zero it is possible to estimate the fraction of the combustion energy that is released as thermal radiation. For this flame the radiated energy fraction is 0.21, which is the same as that obtained by direct calculation from the radiometer measurements and as predicted by a physically based model[18].

4. FLAME IMPINGEMENT

In the previous sections, the suite of CFD models developed by Shell Research has been shown to give reasonable predictions of flame shape, temperatures, and external radiation heat fluxes for open-air jet flames. In this section we describe preliminary results of our work to validate application of the models to the calculation of impinging jet flames.

The initial validation required is the ability to predict convective heat transfer. There is a lack of suitable published measurements from impinging jet diffusion flames to validate convective heat transfer models. Therefore validation was performed against heat transfer measurements for isothermal jets impinging on heated flat plates[19]. Figure 7 shows a comparison of measured and predicted Nusselt numbers as a function of non-dimensional radial distance from the jet centreline for a round jet impinging on a plate positioned 2 diameters from the jet nozzle. The predictions were derived using the standard High Reynolds number (HRN) k-ε turbulence model, the Low Reynolds number (LRN) k-ε model available within CFX-FLOW3D Version 3.3 and a modification of the LRN model due to Yap[20]. The LRN+YAP model produces the most accurate predictions. However, the Yap correction suffers from the inconvenience that the normal distance to the nearest wall has to be calculated for every numerical cell. Given that the region of inaccuracy is quite small and that there is a significantly higher numerical effort required to use the LRN+Yap model, the first calculations of impingement heat transfer for combusting flows were performed using the HRN model.

As an initial test of the CFD combustion model, comparison was made between prediction of a 2.5 kg/s subsonic natural gas jet flame impinging on a 2m diameter tank placed 9 m downstream of the release point[20]. The combustion model used was the simple model described in reference 3, with the flame temperatures given by equation (2), $\chi = 0.15$ and $T_{ad}(f)$ taken from counterflow laminar flamelets with a strain rates of $60 s^{-1}$ and $500 s^{-1}$. These strain rates effectively span the range of possible strain rates that are used in the modified combustion model described in section 3. Figure 8 shows that the modification of the flame shape due to the obstacle is reasonably well predicted, the overall flame shape is similar for both strain rates. Comparison with temperature measurements taken in front of the tank show that using a strain rate of $60 s^{-1}$ overpredicts the temperatures. The effect of the overpredicted temperature is also reflected in the heat flux prediction which are significantly higher than measured. The results using a strain rate of $500 s^{-1}$ are much closer to the measurements, both temperature and heat fluxes. See Figure 9 for a comparison between measured and predicted heat fluxes for the 40 calorimeters used. The heat fluxes are plotted on a development of the tank surface where the tank has been opened out so that the centre of the development is the front of the target and the top and bottom of the development is the back of the target. An explanation for the better performance of the higher strain rate can be found when considering the calculated strain rates presented for the same jet release conditions in Figure 5. For the main part of the flame, especially in the region where the target would be located, the strain rates are predicted to be in excess of $500 s^{-1}$. If a coupled calculation is performed, using the modifications to the combustion model as described in section 3, it is expected that the predicted convective heat fluxes will not change significantly, whereas the radiative heat fluxes should be improved.

5. CONCLUSIONS AND RECOMMENDATIONS FOR FURTHER WORK

1. Shell Research has developed a suite of sub-models within the commercial codes CFX-FLOW3D and CFX-Radiation that are designed to model turbulent high pressure gas jet flames.

2. Reliable predictions have been obtained for under-expanded sonic jet structure, jet flame trajectory, flame lift-off position, flame temperatures, soot formation and external thermal radiation.

3. Prediction of heat fluxes to objects inside the flame show correct trends.

Further work is required to validate turbulence sub-models to enable accurate prediction of convective heat transfer for flames impinging on curved surfaces and for recirculation regions behind obstacles. Application of the new modifications to the 3-D combustion model is required to give better predictions of radiative heat transfer to engulfed objects. A unification of the premixed and diffusion flame sub-models would also prevent the overprediction of temperatures in the fuel-rich core of the early part of the flame.

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7. REFERENCES

1. The Hon. Lord Cullen, The Public Inquiry into the Piper Alpha Disaster, DEn (HMSO), November 1990.
2. FLOW3D Release 3.3: User Manual, CFD Department AEA Industrial Technology, June, 1994, C. Hesketh and P.W. Guilbert, "RAD3D user manual Version 1.2", AERE-R 13710, HCCP/R32/1989, 1989.
3. P W H Barker, A D Johnson and N Goto, CFD Calculation of the Combustion and Radiation Properties of Large-scale Natural Gas Jet Flames, Major Hazards Onshore and Offshore II, I.ChemE Series No.139, Manchester, October 1995.
4. S. Sarker, G. Erlebacher, M.Y. Hussaini and H.O. Kreiss, "The analysis and modelling of dilational terms in compressible turbulence", J. Fluid Mech. 227, pp 473-493, 1991.
5. J.P. Sanders, "Scalar transport and flamelet modelling in turbulent jet diffusion flames", PhD thesis, ISBN.90 386 01433.
6. Measurements taken from a 0.3 kg/s sonic propane jet flame, performed by Southwest Research Institute, San Antonio Texas, Private communication.
7. X.J. Gu, PhD Thesis, Leeds University, 1994.
8. D. Bradley, A.K. Lau and M. Lawes, "Flame stretch rate as a determinant of turbulent burning velocity", Phil. Trans. R. Soc. Lond. A 338, pp 359-387, 1992.
9. R.J. Kee, J.F. Grcar, M.D. Smooke and J.A. Miller, "A Fortran Program for modelling steady one-dimensional premixed flames", SAND85-8240. UC-401, 1991.

10. D. Bradley, L.K. Kwa, A.K. Law and M. Missaghi, "Laminar Flamelet Modelling of Recirculating Premixed Methane and Propane-Air Combustion", Comb. & Flame, 71, pp 109-122, 1988.
11. N.A. Rokke, J.E. Hustad and O.K. Sonju, "A study of partially premixed unconfined propane flames", Comb. & Flame, 97, pp 88-106, 1994.
12. G.A. Chamberlain, "Developments in design methods for predicting thermal radiation from flares", Chem. Eng. Res. Des. 65, pp 299-310, July, 1987.
13. G.T. Kalghatgi, "Lift-off heights and visible flame lengths of vertical turbulent jet diffusion flames in still air", Comb. Sci. & Tech. , 41, Nos 1-2, pp 17-29, 1984.
14. N. L. Crauford, S. K. Liew and J. B. Moss, Combust. Flame 61: 63-77, 1985.
15. M. Fairweather, W.P. Jones, H.S. Ledin and R.P. Lindstedt, "Predictions of soot formation in turbulent non-premixed propane jet flames", 24th Int. Symp. Comb., pp 1067-1074, 1992.
16. J. N. Davenport, J.F. Bennett, L.T. Cowley and J.J. Rowson, "Large-scale natural gas and LPG jet fires. Final report to the CEC", TNER.91.022, publ. Shell Research Ltd, 1991.
17. J. N. Davenport, J.F. Bennett, L.T. Cowley and J.J. Rowson, "Large-scale natural gas and LPG jet fires. Data report for test 1072", TNER.91.081, publ. Shell Research Ltd, 1991.
18. Johnson A.D.; Brightwell H.M.; Carsley A.J. "A model for predicting the thermal radiation hazards from large- scale horizontally released natural gas jet fires", Trans I. Chem. E., Vol 72, Part B, August 1994.
19. J.W. Baughn and S. Shimizu, "Heat transfer measurements from surface with uniform heat flux and impinging jet", Int. J. Heat Mass Transfer, 111, pp. 1096-1098, 1989.
20. C.R. Yap, "Turbulent heat and momentum transfer in recirculating and impinging flows", PhD Thesis, Faculty of Technology, University of Manchester, 1987.
21. J. N. Davenport, J.F. Bennett, L.T. Cowley and J.J. Rowson, "Large-scale natural gas and LPG jet fires. Data report for test 1061", TNER.91.031, publ. Shell Research Ltd, 1991.

Downstream distance, m	Cross stream distance, m	Height above ground, m	Radiation heat flux kW/m^2	
			Measured	Predicted
9	10	1	10.4	10.7
9	14	1	7.1	6.9
9	18	1	4.6	4.8
9	22	1	3.2	3.5

Table 1. Comparison of measured and predicted radiative heat fluxes outside a 2.5 kg/s subsonic natural gas jet flame.

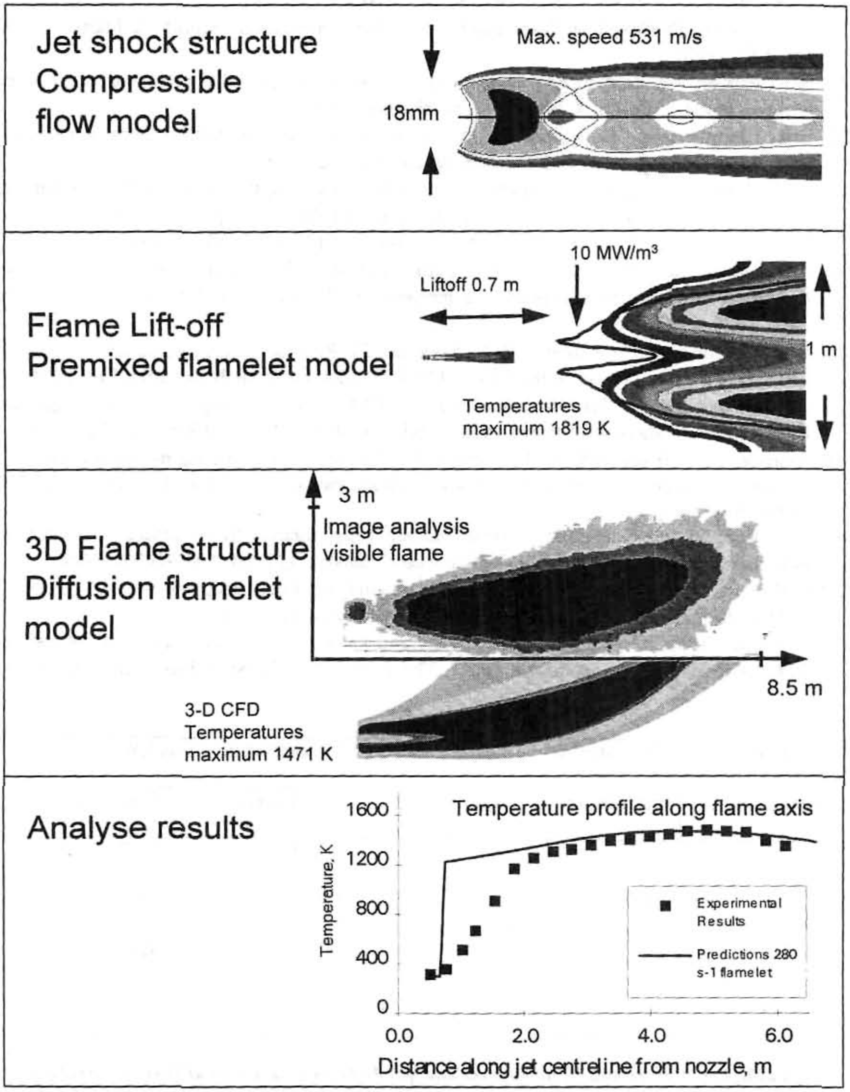


Figure 1. Calculation Methodology

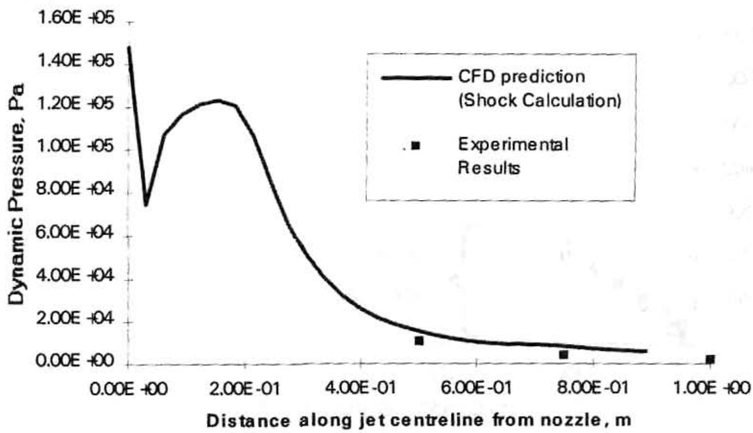


Figure 2. Measured[6] and predicted dynamic pressure along the centreline of a 0.3 kg/s sonic propane release.

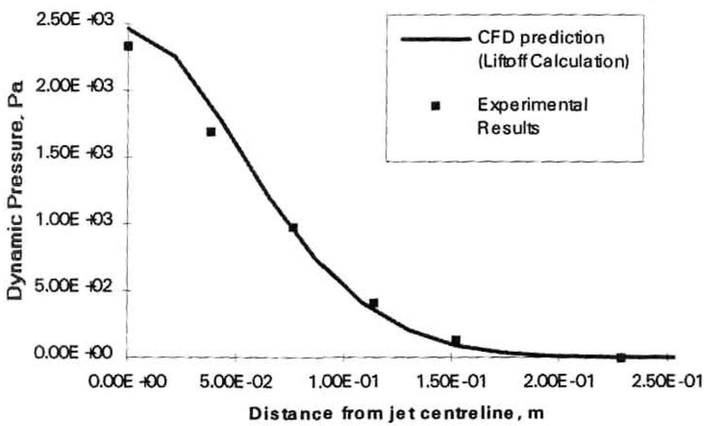


Figure 3. Radial plot of measured[6] and predicted dynamic pressure 1 m from the nozzle of a 0.3 kg/s sonic propane release.

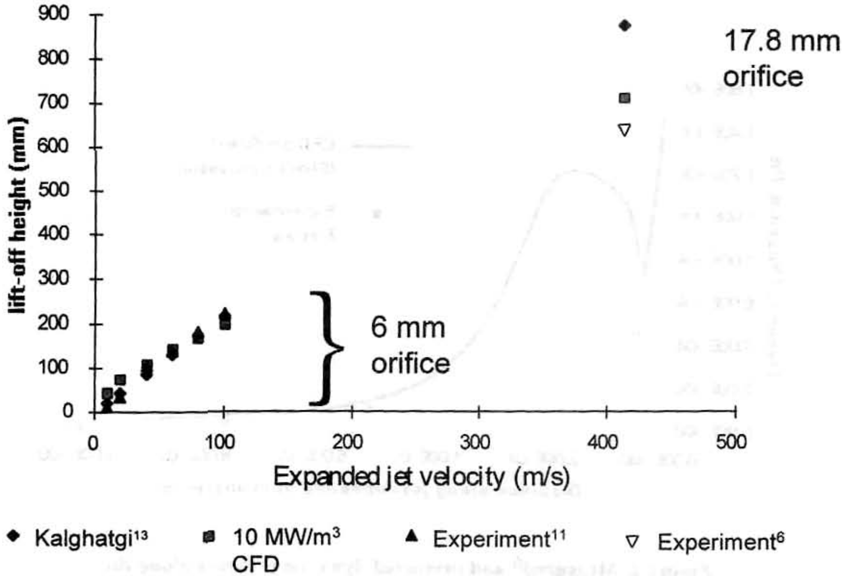


Figure 4. Comparison of measured and predicted flame lift-offs for propane jet flames

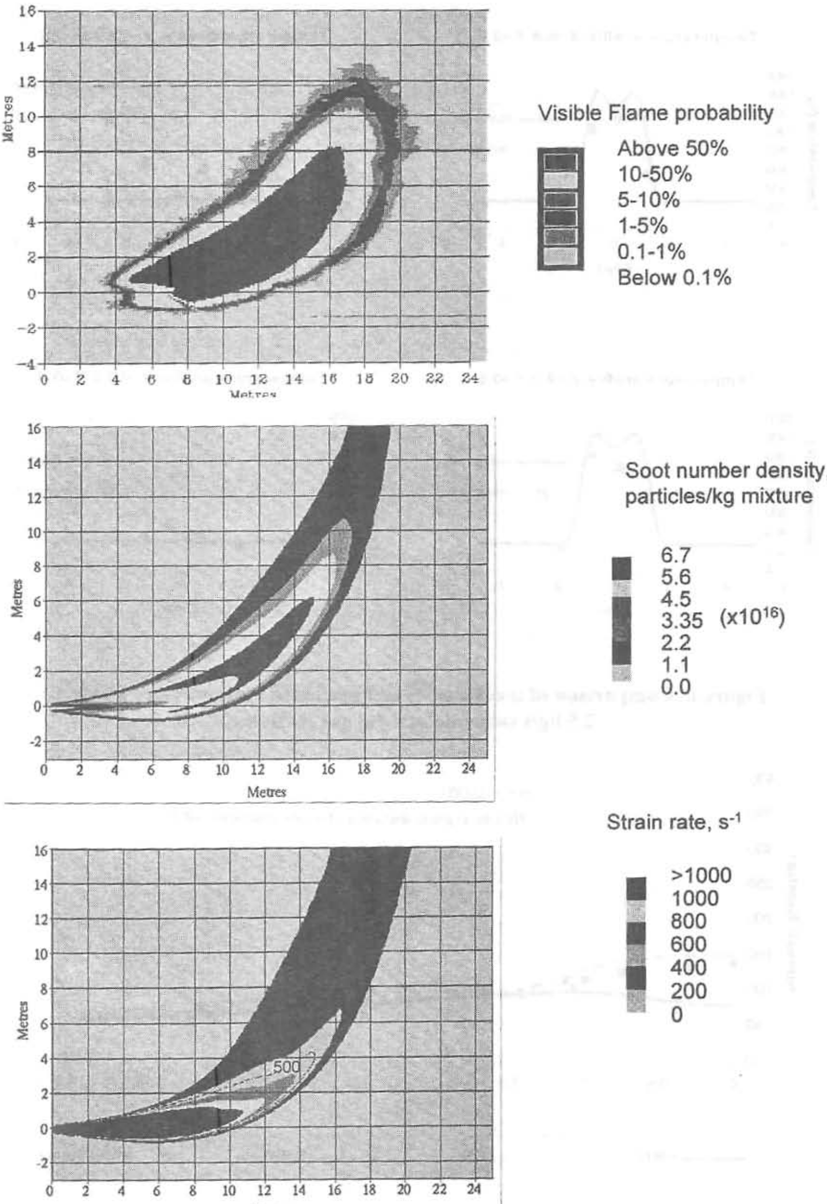


Figure 5. Comparison of measured[22] and predicted properties of a 2.5 kg/s subsonic natural gas jet flame.

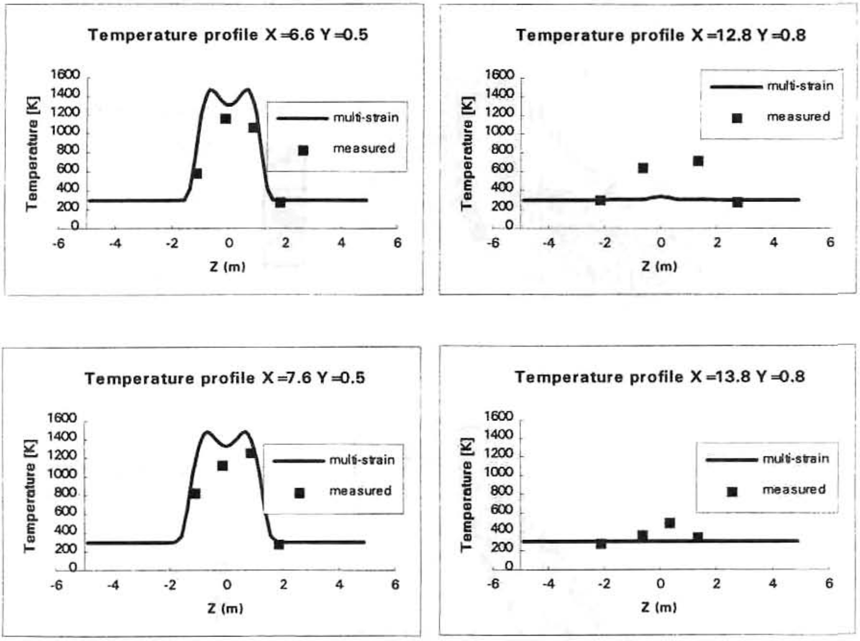


Figure 6. Comparison of measured[22] and predicted temperatures inside a 2.5 kg/s subsonic natural gas jet flame.

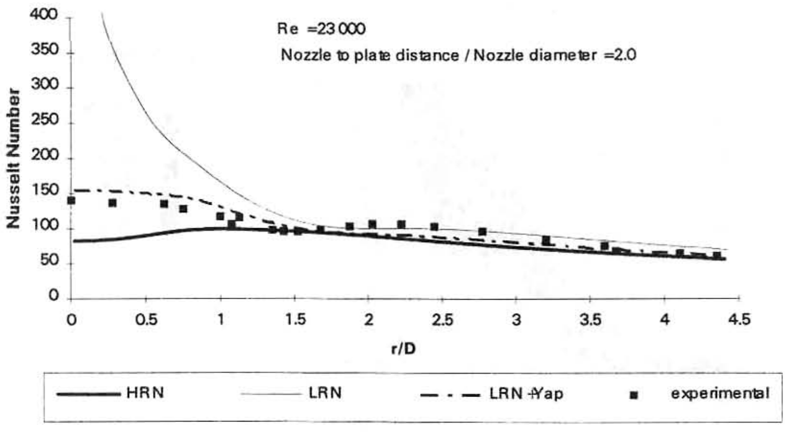


Figure 7. Comparison of measured[25] and predicted heat transfer for a round isothermal jet impinging on a heated plate.

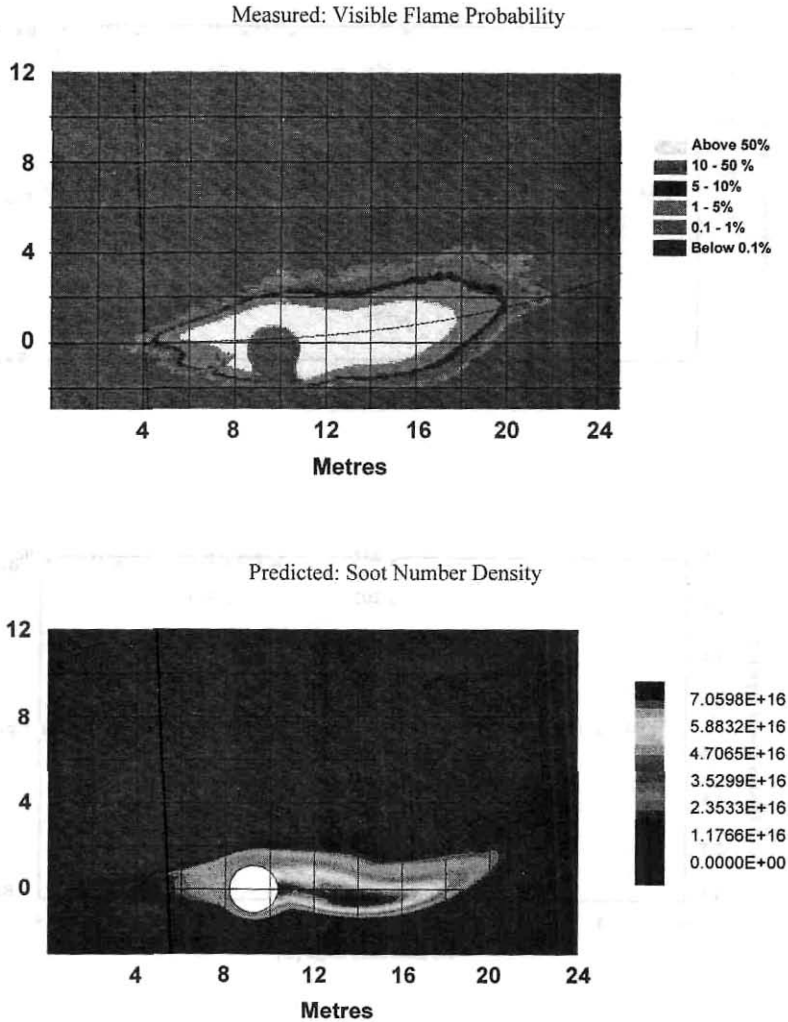
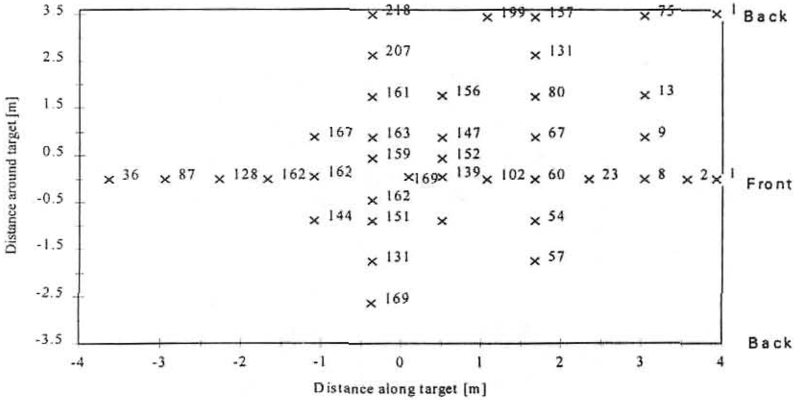


Figure 8. Comparison of measured[26] and predicted properties of a 2.5 kg/s subsonic natural gas jet flame, impinging on a 2m diameter tank.



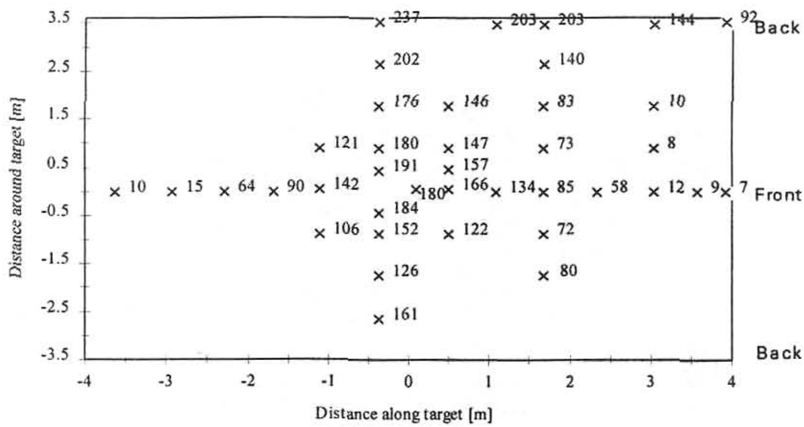


Figure 9. Heat fluxes on the surface of a 2m diameter tank impinged by a 2.5 kg/s subsonic natural gas jet flame. CFD predictions using a 500 s^{-1} flamelet.