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# CFD CALCULATION OF INITIAL DILUTION

**Graham A. Watt<sup>(1)</sup>, Christopher T. Mead<sup>(2)</sup>**

## Summary

Initial dilution is typically calculated using simple models, such as those implemented in the CORMIX and PLUMES packages, or even more basic formulae such as that of Lee and Neville-Jones. Even the more advanced of these models suffer severe limits to their applicability. As diffuser designs become increasingly complex, and regulators' requirements more stringent, there is a need to look for more sophisticated and general methods for calculating the dilution of discharges from such diffusers. Computational fluid dynamics (CFD) offers the flexibility to meet this challenge.

This study has compared results calculated using CFX with those obtained from CORMIX and a physical model for a simple outfall. The results are encouraging, and suggest that CFD may prove useful and practical in more complex initial dilution applications.

A benchmark test was carried out, modelling an outfall for which physical model data was available. This was a very simple outfall consisting of a single round port discharging horizontally into a co-flowing ambient. The effluent was positively buoyant, having a temperature of 76°C in an ambient of 12°C, these values having been selected so as to replicate the relative densities of a freshwater discharge into the sea.

The CFX model was set up in accordance with the experimental setup. Water densities were matched to the lab values. Mesh controls were applied to optimise mesh resolution near the outfall, and mesh adaption was used to refine the mesh further in regions of strong temperature gradients. The model was run with various turbulence formulations.

Simulations were carried out with different mesh and solver parameters, the physical situation being the same in all cases.

CORMIX was used to calculate the initial dilution for the same discharge configuration, and the CFX results were compared against each other, and with the CORMIX and laboratory results.

In this simple case, the results for initial dilution calculated by CFX are comparable to those from CORMIX. Given uncertainties in the experimental results, satisfactory agreement existed between these and the results of the CFX and CORMIX calculations. There would seem to be no advantage in using CFX in a situation where a relatively simple mixing zone model, such as CORMIX, can be applied with confidence.

Setting up a CFD model is currently very much more onerous than using CORMIX. More complicated situations would quickly become very processor-intensive and time-consuming.

Investigations are continuing to improve HR Wallingford's understanding and capability of using CFD code in this application, and in particular the applicability of CFD to more complex situations.

**Keywords:** initial dilution, computational fluid dynamics, CFD

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## Introduction

Outfall studies frequently require analysis of the near-field behaviour of discharges, either as an explicit requirement or to assist the introduction of discharges into mid- and far-field dispersion models. This analysis is usually conducted using models such as CORMIX [1]. However, all dedicated initial dilution models have limitations, both in terms of the situations where they can be applied and in terms of the accuracy of the results they produce.

For this reason, the present study was undertaken to explore the potential benefits of using Computational Fluid Dynamics (CFD) methods to calculate initial dilution, specifically using the package CFX [2]. As a first step, a simple case was modelled, based on a previous physical model experiment, so that the results could be compared. If the CFD model could be shown to reproduce the main features of the experimental results for this simple case, there would clearly be some benefit in progressing to an assessment of the suitability of the technique in more complex applications.

## Previous Studies

A number of relevant studies have been reported in the proceedings of a NATO workshop held in 1993 [3]. In particular, Gosman *et al.* [4] have shown good agreement between an experiment and a CFD simulation of a buoyant jet in cross-flow, slightly better with a Reynolds stress turbulence model than with a  $k-\varepsilon$  model. Laurence and Simonin [5] described the details of a specific turbulence model, concluding that one must be very careful in the choice of turbulence model. None of the authors gave details of the actual formulation of the problem from the perspective of a CFD user, and these practical aspects were an important focus of the present investigation.

Some more recent studies have investigated rather sophisticated outfall designs using CFD techniques (e.g. [6] and [7]). These have tended to compare CFD results against results from other models, rather than experimental data.

## Test Case

A benchmark test was carried out, modelling an outfall for which physical model data were available. This was a very simple outfall consisting of a single round port discharging horizontally into a co-flowing ambient. The effluent was positively buoyant, with a temperature of 76°C in an ambient of 12°C, these values having been selected so as to replicate the relative densities of a specific freshwater discharge into the sea. The laboratory study was undertaken in 1994, and the full data are not available, but this was a convenient choice of simple first case.

The ambient velocity was a steady 0.7m/s, and the port exit velocity was 1.23m/s. The water depth was 2.76m, the port diameter was 0.338m, and its centre-line was raised 0.8m above the bed. All dimensions given in this paper refer to the prototype scale.

## CFX Model

The CFX model was set up in accordance with the details of the laboratory experiment, as summarised above. Water densities were matched to the laboratory values. Mesh controls were applied to maximise mesh resolution near the outfall, and automatic mesh adaptation was used during the run to refine the mesh further in regions of strong temperature gradients. The model was run with Reynolds stress turbulence formulation and a rigid-lid approximation at the free surface. All 'walls' were modelled initially with free slip. Two separate simulations were carried out, with the second using a finer mesh than the first, and the results are presented in the following sections. The physical situation being modelled was the same in both cases.

## Base Case Results

CFX predicted the highest temperature at the water surface to be 2.7°C above ambient, which corresponds to a minimum surface dilution (MSD) ~24, at a distance of 15m downstream of the point of discharge; the shape of the plume is illustrated in Figure 1. These values are compared (as 'CFX I') with

the experimental data and results from a CORMIX simulation in Table 1, below. It is difficult to measure MSD experimentally, and it is likely that the measured MSD value is somewhere between the actual minimum and the average value on the surface.

**Table 1 Simulation results**

	MSD	distance downstream (m)
experimental	71	30
CORMIX	30	11
CFX I	24	15
CFX II	12	25 (offset either side)

It may be seen that the results from CFX are comparable to those from CORMIX in this simple case. The experimental MSD was around twice as great, which is consistent with the uncertainty in its measurement. It is evident (as discussed below) that there is significantly less ambient turbulence in the CFX model than in the laboratory flume. This lack of turbulence would contribute to reducing the MSD.

In terms of predicting the surfacing point, both CFX and CORMIX gave distances a factor of 2-3 less than that measured in the lab.

The CFX mesh used in this simulation was not particularly fine in the region where the plume impinged on the surface, as is evident from the slightly chequered nature of the plume margins in the plot of the surface temperature shown in Figure 1. The mesh resolution in the surfaced plume was approximately 50cm. Since the plume width at the surface was around 2m, this gave only four elements across.

### Improved Resolution Results

For the second simulation, the basic mesh was refined in the plume region, both along the rising path and at the surface. This was achieved by hand, implementing additional mesh controls along the plume trajectory indicated by the Base Case result.

The refined mesh contained just over one million elements, with a maximum edge length of 1m near the downstream boundary, and a fixed resolution of 0.05m on the diffuser. At the surface, the resolution was some 7cm, which provided about 30 elements across the plume.

The results are shown in Figure 2, which shows that the plume has bifurcated on surfacing. Although this is a well-documented characteristic of buoyant plumes under conditions where the plume buoyancy is strong ([8] – [12]), it was not observed in the laboratory test. The ambient flow in the laboratory had a high level of turbulence, since it was driven by a pump and only rudimentary efforts were made to stabilise the flow across the channel. Therefore it is likely that the effects of turbulence dominated those of buoyant spreading, preventing the formation of the bifurcated pair.

In contrast to the laboratory experiment, this initial CFX model has very little turbulence in the flume, as the channel walls and bed have free slip, the inflow is distributed evenly across the channel and the ‘free’ surface is constrained. The numerical result is consistent with that of the laboratory experiment of Rodi and Weiss [11] who produced conditions of low turbulence in their channel and observed bifurcation at the surface.

The results from this test are included as ‘CFX II’ in Table 1. The MSD has reduced to half the previous value. However, the position of the surfaced, bifurcated plume is in good agreement with the experiment.

### Conclusions

In the simple applications described in this paper, the results for initial dilution calculated by CFX are reasonably comparable to those from CORMIX. There is clearly no advantage in using CFX in a situation where CORMIX is fully applicable.

Setting up a CFD model is very much more onerous than using an initial dilution model such as CORMIX, and it is necessary, to

some extent, to estimate the answer before beginning, as the mesh must have sufficient spatial extent and resolution to contain and represent the plume. More complicated situations would quickly become very processor-intensive and time-consuming. Whereas an initial dilution model can be set up and run in a few minutes, defining the geometry for CFX for the test described here took some hours. Iteratively refining the mesh and adjusting the run parameters would yield optimum CFD results, but could make a CFD study a very long process. This is a significant limitation of the technique, but is expected to diminish over time with the advent of increasingly powerful computer processors.

On the other hand, the results encourage the hope that CFD models may prove useful in more complex situations where the use of CORMIX, and other initial dilution models, is less routine. These include multi-port diffusers of complex geometry, large

discharges into relatively shallow water and situations where the ports are not deeply submerged. This conclusion is in agreement with previously reported studies (e.g. [6]).

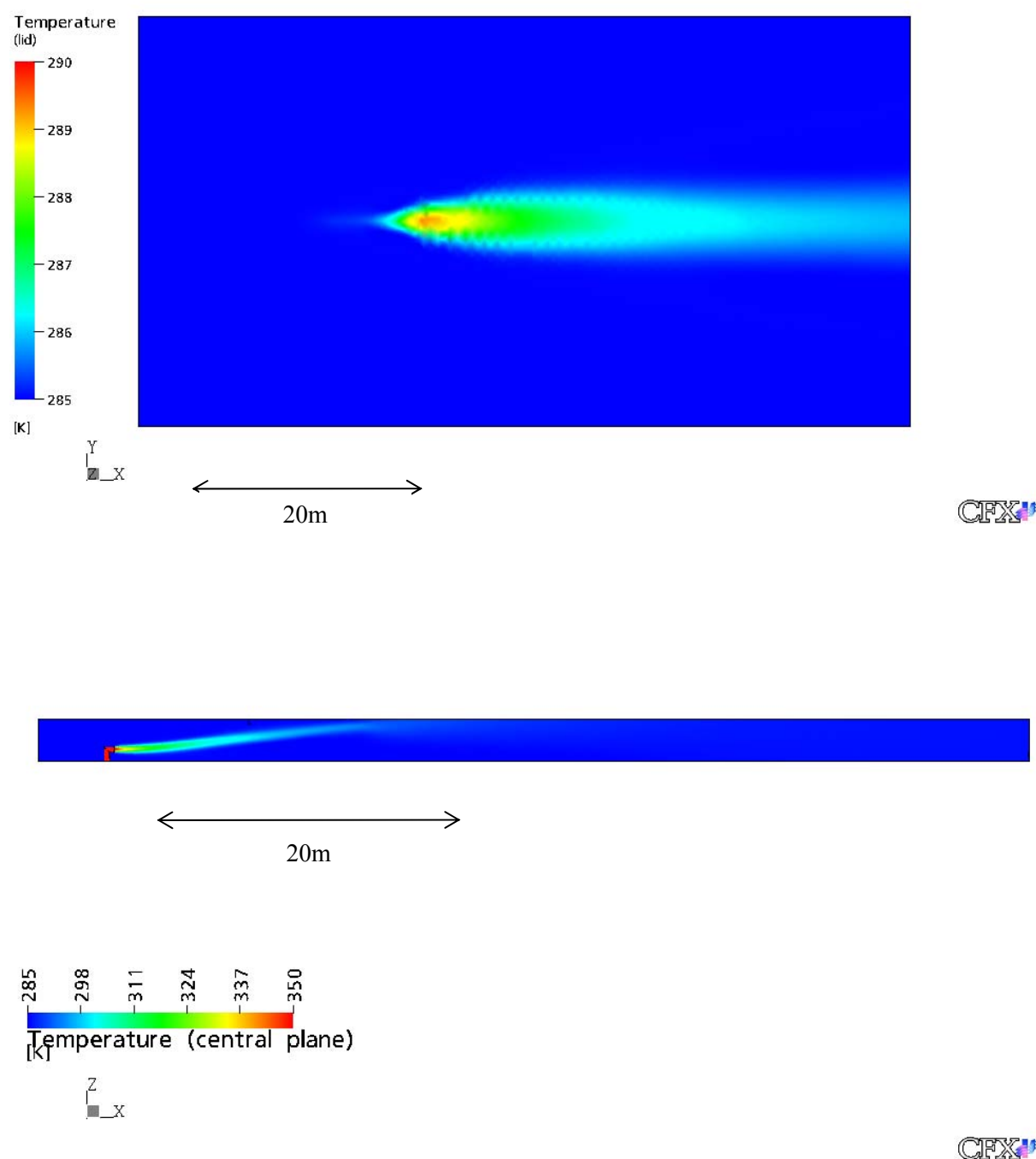
This paper has described initial results for a very simple test case. It is clear that many aspects of the use of CFD in this application require further investigation, including the turbulence models and wall parameters. In due course, it is hoped to model more complicated outfall configurations with CFX, and to validate the results using comprehensive experimental or field data.

### Acknowledgements

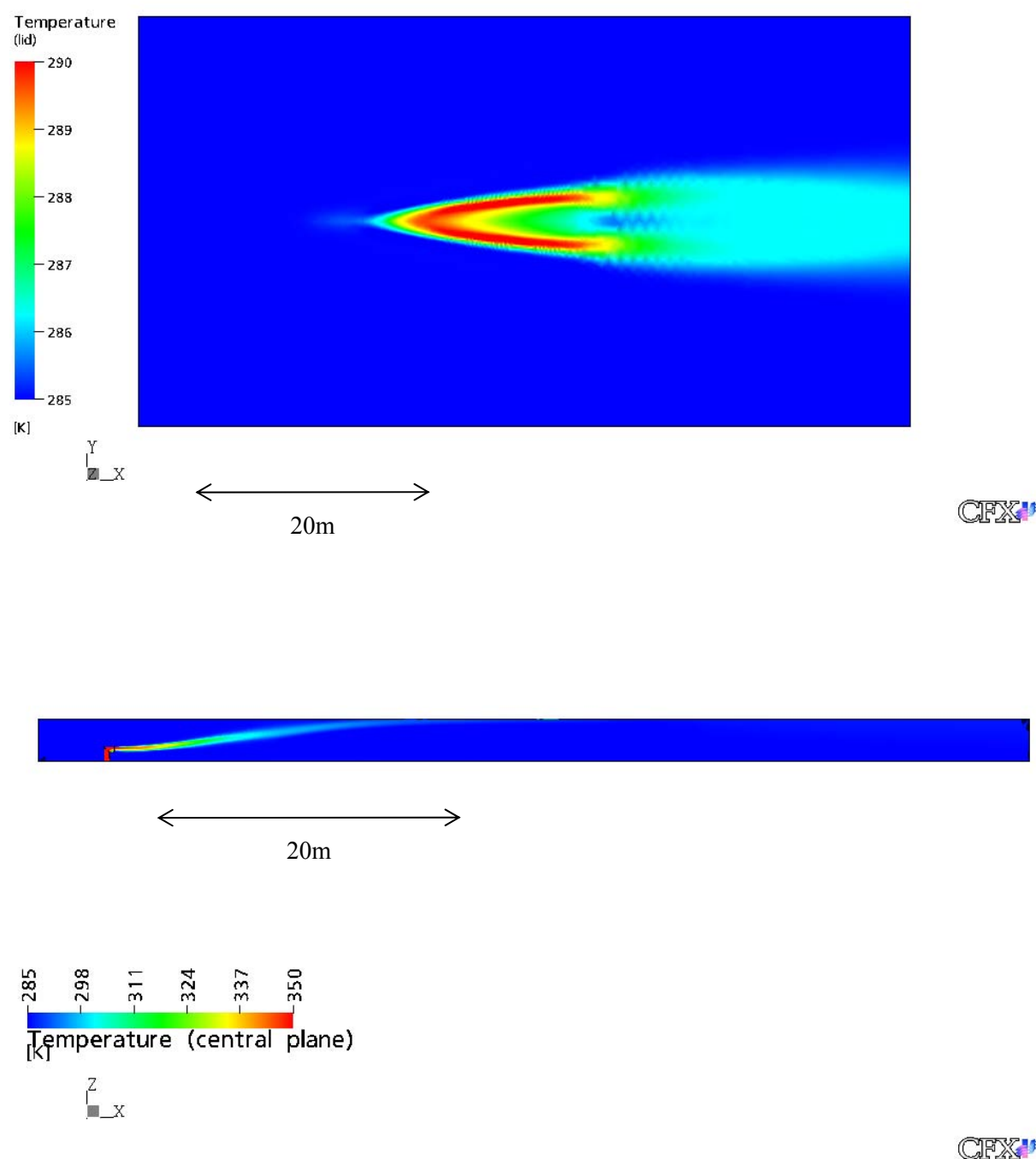
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**Figure 1** Results from Simulation 1 (top and side view)



**Figure 2** Results from Simulation 2 (top and side view)



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