

# **QNET-CFD WIKI KNOWLEDGE BASE**

**APPLICATION CHALLENGE DOCUMENT TEMPLATE**

# APPLICATION CHALLENGE (AC) DOCUMENT

## ABSTRACT

Provide a summary of the AC test case submitted.

## 1. DESCRIPTION

### 1.1 INTRODUCTION

Brief description and overview of the Application Challenge (AC). Enough information for the reader to get a good idea of the fluid engineering issues and type of flow regimes involved, and why this makes a good AC. Brief overview also of the experimental and CFD results and of experimental methods, computational domain and turbulence models used.

### 1.2 RELEVANCE TO INDUSTRIAL SECTOR

An assessment of the relevance of the AC to the Industrial Sector. In particular, is it a test case by which the competency of CFD for the sector can be judged? An indication of the level at which the AC is understood should also be given (in terms of data/insight available, and overall quality).

### 1.3 DESIGN OR ASSESSMENT PARAMETERS

The design or assessment parameters (DOAPs), are those which will be used to judge the competency of CFD calculations. These must be fully defined (e.g. the lift, drag and pitching moment of a wing; the pressure recovery in a diffuser; the species concentration at a given location downstream from a building, etc).

### 1.4 FLOW DOMAIN GEOMETRY

The flow geometry associated with the AC should be fully described including clear diagrams or illustrations (preferably, the geometry should also be specified in digital form).

This description should include

- geometrical features of the domain and their dimensions, locations of all boundaries
- conventions (e.g. coordinate system used, sign conventions etc)

### 1.5 FLOW PHYSICS AND FLUID DYNAMICS DATA

The key aspects of the flow physics (e.g. laminar/turbulent, compressible/incompressible, heat transfer/isothermal, etc) and the governing non-dimensional parameters (GNDPs) (e.g Reynolds, Mach, Grashof numbers, etc.) should be identified clearly. The physics of other key processes (such as chemical kinetics, flow through porous media, etc) must also be discussed. All the fluid dynamics data (except boundary conditions) which are necessary in order to set up a CFD simulation must be described. The properties of the working fluid(s) must be specified or readily deducible (e.g a statement that it is air is sufficient, however if the fluid is non-newtonian, the appropriate constitutive law(s) must be given).

## 2. TEST DATA

### 2.1 OVERVIEW OF TESTS

Provide an overview of the scope of the tests and the experimental approach used. This should cover the main aspects of the experimental set up and the measurement techniques used (LDV, hot wire, pressure tappings etc).

If a scaled model was used, due consideration should be given to model scaling issues. Any model simplifications/idealisations of the AC geometry should also be described (e.g. 2D instead of 3D, omission of detailed features, simplification of complex features, i.e. porous media, use of roughness elements). If important details of the geometry representation are uncertain then the impact of these uncertainties on the DOAPs should be discussed, including possible ways for managing their effect.

Sampling/averaging times, and their effect on quantities measured and on DOAPs in particular, should also be discussed.

Identify all experimental tests for which data is available. In order to minimise the number of test descriptions, it is suggested that, as far as possible, experimental data from various runs or experimental conditions be grouped together under a single test case, if variations to experimental setup can be clearly defined in terms of:

- the governing non-dimensional parameters (GNDPs defined above in 1.5), or
- problem definition parameters (PDPs), such as wind direction, angle of attack, aspect ratio, source rate etc.

It is left to the discretion of each author to decide the most appropriate way for structuring and summarising the test case results, within the broad framework suggested above.

A summary table for all tests should be included as shown below in Table EXP-A. The variables measured in each test should also be clearly identified, (e.g. UVW, k, concentration, etc). A distinction should be drawn between detailed local data (e.g.  $p(x,y,z)$ ) and data relating to DOAPs which are likely to be global/summary parameters (e.g. coefficient of lift,  $C_L$ ).

All available detailed data should be stored in separate electronic datafiles (according to the Data Submission Guidelines of the Library section of the Wiki). These should be summarised as shown below in Table EXP-B, with links to each of the datafiles. If the experimental data are available from established external databases, a link should be provided.

<i>NAME</i>	<i>GNDPs</i>		<i>PDPs (problem definition parameters)</i>			<i>MPs (measured parameters)</i>	
	Re	Fr	Wind direction	Source rate (kg/s)	Release density (kg/m <sup>3</sup> )	detailed data	DOAPs
<b>EXP 1</b> (dense gas dispersion)	10 <sup>5</sup> -10 <sup>6</sup>	0.2-10	0, 30, 45, 90,180	1 -3	1.22 -3.00	C, U	C/Co
	Re		Wind direction	Building geometry		detailed data	DOAPs
<b>EXP2</b> (passive gas releases)	10 <sup>5</sup> -10 <sup>6</sup>		0, 30, 45	A, B,C,D		C, U,V,W, k	C/Co

Table EXP-A Summary description of all test cases

	MP1 U V W (ms <sup>-1</sup> )	MP 2 k (m <sup>2</sup> s <sup>-2</sup> )	MP 3 C (kg/m <sup>-3</sup> )	DOAPs, or other miscellaneous data
EXP 1	✓ ✗ ✗ <a href="#">exp11.dat</a>	✗	✓ <a href="#">exp13.dat</a>	-
EXP 2	✓ ✓ ✓ <a href="#">exp21.dat</a>	✓ <a href="#">exp22.dat</a>	✓ <a href="#">exp23.dat</a>	<a href="#">exp24.dat</a>

Table EXP-B Summary description of all measured parameters and available datafiles

## 2.2 TEST CASE EXP1

### 2.2.1 Description of experiment

Quantify the parameters that define this particular set of experiments (GNDPs and PDPs). Describe which parameters were measured (MPs), where in space and time (state units in SI). Conventions for presenting data in each of the datafiles should be simple, and clearly stated.

### 2.2.2 Boundary Data

Specify in detail the conditions pertaining at all boundaries on all dependant variables (data need not be quantified here if included as a dataset). The boundaries should include inflows, symmetry surfaces, walls, far-fields, free surfaces and outflows. If the walls are rough, roughness heights should be specified. Are the turbulent stresses and length scale measured at inflows? If not give advice on how these should be set up. If any boundary data is uncertain then discuss the sensitivity of DOAPs to this uncertainty. Is there any reasonable way of managing this uncertainty if the sensitivity is appreciable?

### 2.2.3 Measurement Errors

A realistic estimation of the accuracy of the data (crucially important for the DOAPs) employing one or more of the following:

- Appraisal of the accuracy of the measured quantities arising from the given instrument/technique (error bars are desirable)
- Repeated or reference measurements, and calibration checks.
- Demonstration of consistency in the measurement of different quantities
- Checks on the global conservation of physically conserved quantities.

### 2.2.4 Measured Data

List all measured quantities and provide links to all data files if these are provided. Describe the data storage format used, and specify measurement positions (preferably on a diagram of the flow domain).

For example:

**EXP1** Dense gas release measurements: mean and RMS measurements of each of the three wind components (U along-wind, V lateral and W vertical), at 4 heights and 7 locations downstream of the building. Ground level concentrations at 7 locations downstream of the building.

[exp11.dat](#) (ASCII file; headers: Re, Fr, wind direction, source rate, release density; columns: x, y, z, <U>, <V>, <W>, u'<sub>RMS</sub>, v'<sub>RMS</sub>, w'<sub>RMS</sub>)

[exp13.dat](#) (ASCII file, headers: Re, Fr, wind direction, source rate, release density; columns: x, y, z, <C>)

### 2.2.5 References

Any references in the scientific literature that are relevant; if possible use references that can be accessed via the web and add hyperlink.

## **2.3 TEST CASE EXP2**

**(as per EXP1)**

## **3. CFD SIMULATIONS**

### **3.1 OVERVIEW OF CFD SIMULATIONS**

Provide a brief overview of the CFD simulations of the AC that have been performed. This should cover the scope of the calculations and the main aspects of the modelling strategy e.g. equations solved, turbulence and other physical models employed). All computational domain simplifications/idealisation, and the treatment of subgrid features should also be identified (e.g. imposed symmetry plane, omission of detailed features, simplification of complex/small scale features, i.e. porous media, use of equivalent wall roughness). If important details of the geometry representation are uncertain then the impact of these uncertainties on the DOAPs should be discussed, including possible ways for managing their effect.

It is left to the discretion of each author to decide the most appropriate way for structuring and summarising the CFD results. Ideally, the data structures used should be consistent with those used for the test data.

A summary table for all CFD simulation results should be included, as shown below in Table CFD-A. Available data should be clearly identified, (e.g. UVW,  $k$ , concentration, etc). As with test data, a distinction should be drawn between detailed local data (e.g.  $p(x,y,z)$ ) and data relating to DOAPs which are likely to be global/summary parameters (e.g. coefficient of lift,  $C_L$ ).

All available detailed data should be stored in separate electronic datafiles (not mandatory) according to the Data Submission Guidelines of the Library section of the Wiki. These should be summarised as shown below in table CFD-B, with links to each of the datafiles.

<i>NAME</i>	<i>GNDPs</i>		<i>PDPs (problem definition parameters)</i>			<i>SPs (simulated parameters)</i>	
	Re	Fr	Wind direction	Source rate (kg/s)	Release density (kg/m <sup>3</sup> )	detailed data	DOAPs
<b>CFD 1</b> (dense gas dispersion)	10 <sup>5</sup> -10 <sup>6</sup>	0.2-10	0, 30, 45, 90, 180	1 -3	1.22 -3.00	C, U	C/Co

  

	Re	Wind direction	Building geometry	detailed data	DOAPs
<b>CFD 2</b> (passive gas releases)	10 <sup>5</sup> -10 <sup>6</sup>	0, 30, 45	A, B,C,D	C, U,V,W, k	C/Co

Table CFD-A Summary description of all test cases

	SP1 U V W (ms <sup>-1</sup> )	SP 2 k (m <sup>2</sup> s <sup>-2</sup> )	SP 3 C (kg/m <sup>-3</sup> )	DOAPs, or other miscellaneous data
<b>CFD 1</b>	✓✓✓ <a href="#">cfd11.dat</a>	✓	✓ <a href="#">cfd13.dat</a>	<a href="#">cfd14.dat</a> , <a href="#">cfd15.dat</a>
<b>CFD 2</b>	✓✓✓ <a href="#">cfd21.dat</a>	✓ <a href="#">cfd22.dat</a>	✓ <a href="#">cfd23.dat</a>	<a href="#">cfd24.dat</a> , <a href="#">cfd25 dat</a> , <a href="#">cfd 26.dat</a>

Table CFD-B Summary description of all available datafiles, and simulated parameters.

## 3.2 SIMULATION CASE CFD1

### 3.2.1 Solution strategy

A self-contained description of the solution strategy employed. This should include:

- the name of the code (including version number)
- the basic equations solved, the turbulence model, and any other physical model used (e.g. chemistry, pollutant transport). Except for standard models, describe the main features and provide a reference to the full description.
- the numerical discretisation scheme used in both space and time (this may depend on the equation set solved, e.g. momentum equations may be different from the turbulence equations)
- the solution algorithm used

### 3.2.2 Computational Domain

Describe the geometry of the computational domain including the location of all boundaries. Does this domain coincide with the test geometry or does it represent a simplification? Discuss the impact of any simplification on the DOAPs. In particular justify any 2-D idealisation. Describe in detail the mesh (or meshes) used, including the total number of cells/grid points and mesh density distribution.

### 3.2.3 Boundary Conditions

Describe the numerical boundary conditions at all boundaries including inflows, symmetry surfaces, walls, far-fields, free surfaces and outflows. In each case, comment on how these replicate conditions in the test rig (e.g. inflow conditions based on measured data taken at a rig measurement station?). Have sensitivity tests been carried out to explore the effect of uncertainties in boundary conditions (e.g. turbulence data at inflow, position of far field boundaries, etc.)

### 3.2.4 Application of physical models

Describe the details of how turbulence models, and any other physical models, were applied. For example if RANS turbulence models have been used what is the near wall set-up? What is  $y^+$  at the first grid point from the wall ( $y$  is normal distance to the wall) and how many grid points lie in the wall boundary layer? (the type of wall treatment employed, i.e. wall functions or low Reynolds number turbulence model is described in 3.2.3 above).

### 3.2.5 Numerical Accuracy

What steps have been taken to estimate or demonstrate the numerical accuracy of the results (e.g. mesh and time-step refinement studies, increasing the order of accuracy of the scheme)? What measure of iteration convergence was used, and was this achieved?

### 3.2.6 CFD Results (not mandatory)

List data included, with links to all data files. Describe the data storage format used, and specify conventions (define reference coordinate system, and state if data are vertex, cell-centered, or interpolated).

For example:



**CFD1** Dense gas release simulation: RANS calculations, standard k- $\epsilon$ , coordinate system as per experiments, cell-centered data

[cfd11.dat](#) (binary file; headers: Re, Fr, wind direction, source rate, release density; columns: x, y, z, U, V, W)

[cfd13.dat](#) (binary file; headers: Re, Fr, wind direction, source rate, release density; columns: x, y, z, C)

### 3.2.7 References

Any references in the scientific literature that are relevant; if possible use references that can be accessed via the web and add hyperlink.

## 3.3 SIMULATION CASE CFD2

(as per CFD1)

## 4. EVALUATION - COMPARISON OF TEST DATA AND CFD

Comparison of CFD with Test data. Comparison may be qualitative (e.g. scatter plots, contour plot comparison) or quantitative (statistical measures, e.g. mean bias and variance). Particular note on agreement between measured and calculated DOAPs. Discussion, conclusions and recommendations.

## 5. BEST PRACTICE ADVICE

### ***GUIDANCE NOTES FOR COMPLETING THIS SECTION***

*The advice should concentrate on the prediction of the design or assessment parameters (DOAPs) since, by definition, these are the quantities of prime interest to the analyst. This does not preclude consideration of the detailed flow structure (i.e higher order parameters) if this is both possible and deemed to add value to the advice. The BPA should constitute a synthesis of the data contained within this AC document. It is important to stress that the advice set down should be supported by the evidence presented in this document. Personal prejudice and judgements based on personal experience must be avoided.*

*If the author's final conclusion is that the detail and quality of the AC data is not sufficient for drawing out reasonably well-founded BPA, then this should be stated, the BPA left open, and recommendations made for further remedial work.*

### 5.1 KEY FLUID PHYSICS

Briefly describe the key fluid physics/flow regimes which exert an influence on the DOAPs.

### 5.2 APPLICATION UNCERTAINTIES

List any uncertainties which make a high fidelity CFD model difficult to assemble. Typical examples might include:

- a gas leakage between two components which is difficult to resolve on practical meshes, and even if it is resolved, the leakage flow conditions may not be known.
- flow conditions at inlet to the AC (or indeed other boundaries) which may be complex and not precisely known.
- fine details of the geometry are imprecise.

Briefly discuss the sensitivity of the DOAP predictions to these uncertainties and their impact on the BPA. In particular, can clear, unequivocal BPA be given or is it necessary to introduce appropriate caveats.

### **5.3 COMPUTATIONAL DOMAIN AND BOUNDARY CONDITIONS**

- State any restrictions on simplifications to the geometry (e.g. three dimensional effects are important and thus 2-D idealisation must not be used; wind tunnel blockage effects are significant and thus the wind tunnel geometry must be modelled; the flow displays transient un-symmetric behaviour and thus a geometric symmetry element cannot be used etc.).
- Advise on the extent of the computational domain in order to capture all flow features and minimise uncertainties in the setting of boundary conditions.
- At each boundary of the computational domain provide advice on which boundary condition to use and how to set it up.

### **5.4 DISCRETISATION AND GRID RESOLUTION**

- Provide advice on the order of the numerical scheme which is necessary to resolve the main flow features (controlling the DOAPs) on practical grids.
- Provide clear advice on the level of grid resolution (at walls and across shear layers and dominant flow structures) which is required in order to predict the DOAPs with reasonable accuracy.
- If possible, provide advice on the level of grid resolution which is required to capture more detailed (higher order) aspects of the flow (e.g. velocity profiles, turbulent stresses etc.). This is not mandatory.

### **5.5 PHYSICAL MODELLING**

- Provide advice and recommendations on which models are capable of delivering accurate predictions of the DOAPs, provided the advice in 3 and 4 is heeded.
- If possible, provide advice and recommendations on which models are capable of delivering accurate predictions of higher order flow parameters.

### **5.6 RECOMMENDATIONS FOR FUTURE WORK**

Provide recommendations for work which, if undertaken, will improve significantly the quality of the BPA. Typical examples might include:

- Calculations of the AC should be repeated using contemporary turbulence models.
- Calculations of the AC should be performed on finer grids and/or with higher order schemes.