# QNET-CFD WIKI
# KNOWLEDGE BASE

## APPLICATION CHALLENGE DOCUMENT TEMPLATE

# APPLICATION CHALLENGE DOCUMENT

## 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. All available experimental and CFD results should be briefly described (i.e. 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 guidelines set out by the Knowledge Base team at the University of Surrey). These should be summarised as shown below in Table EXP-B, with links to each of the datafiles.

| *NAME* | *GNDPs* | | *PDPs (problem definition parameters)* | | | *MPs (measured parameters)* | |
|---|---|---|---|---|---|---|---|
| | Re | Fr | Wind direction | Source rate (kg/s) | Release density (kg/m$^3$) | detailed data | DOAPs |
| **EXP 1** (dense gas dispersion) | $10^5$-$10^6$ | 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 |
| **EXP2** (passive gas releases) | $10^5$-$10^6$ | | 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$^{-1}$) | MP 2 k (m$^2$s$^{-2}$) | MP 3 C (kg/m$^{-3}$) | DOAPs, or other miscellaneous data |
|---|---|---|---|---|
| EXP 1 | ✓ ✗ ✗ exp11.dat | ✗ | ✓ exp13.dat | - |
| EXP 2 | ✓ ✓ ✓ exp21.dat | ✓ exp22.dat | ✓ exp23.dat | exp24.dat |

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 data measured, with links to all data files. 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>, $u'_{RMS}$,$v'_{RMS}$ ,$w'_{RMS}$)

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

If CFD simulations of the AC have been performed then provide a brief overview. 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/idealisations, 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 (according to guidelines set out by the Knowledge Base team at the University of Surrey). These should be summarised as shown below in CFD-B, with links to each of the datafiles.

| *NAME* | *GNDPs* | | *PDPs (problem definition parameters)* | | | *SPs (simulated parameters)* | |
|---|---|---|---|---|---|---|---|
| | Re | Fr | Wind direction | Source rate (kg/s) | Release density (kg/m$^3$) | detailed data | DOAPs |
| **CFD 1** (dense gas dispersion) | $10^5$-$10^6$ | 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 |
|---|---|---|---|---|---|
| **CFD 2** (passive gas releases) | $10^5$-$10^6$ | 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$^{-1}$) | SP 2 k (m$^2$s$^{-2}$) | SP 3 C (kg/m$^{-3}$) | DOAPs, or other miscellaneous data |
|---|---|---|---|---|
| **CFD 1** | ✓ ✓ ✓ cfd11.dat | ✓ | ✓ cfd13.dat | cfd14.dat , cfd15.dat |
| **CFD 2** | ✓ ✓ ✓ cfd21.dat | ✓ cfd22.dat | ✓ cfd23.dat | cfd24.dat , cfd25 dat , cfd 26.dat |

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)
- all equations solved, including the turbulence model, and any other physical model used (e.g. chemistry, pollutant transport)
- 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

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-ε, 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 Best Practice Advice (BPA) for Application Challenges (ACs) follows the same format as that adopted for UFR BPA . However, 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 with that in the associated UFRs (as formalised in the UFR BPAs ). Guidance on how to make this synthesis is set out below. It is important to stress that the advice set down should be supported by the evidence presented in these documents. Personal prejudice and judgements based on personal experience must be avoided.*

*The DOAPs may not be well predicted in the AC study because the UFR-BPA, based on strong high quality evidence, has not been followed in the AC calculations (e.g. insufficient grid, low order numerical scheme, incompetent turbulence models etc.). Under such circumstances the AC-BPA advice should be based upon the UFR-BPA and appropriate recommendations made for further AC studies.*

*The evidence embodied within the AC-Document may not be consistent with the associated UFR-BPA. There may be various reasons for this:*

*1) There are no UFRs presently within the knowledge base which are relevant to this AC.*

2) *The UFR test cases which have been studied are not sufficiently well aligned with the flow conditions encountered in the AC. For example the flow parameters/conditions controlling the UFR test-case may not be as severe as the AC case (e.g. pressure gradient, level of streamline curvature, Grashof number etc.), or perhaps the UFR test case features several interacting flow regime of which only one is relevant to the AC.*

*Under such conditions, you should base the BPA solely on the AC evidence (provided this is of sufficient detail and quality) and then make appropriate recommendations for the identification and analysis of UFR test cases.*

*The reasons for the (marked) inconsistency may be none of the above and may not be easily identifiable. The inconsistency could be due to AC application uncertainties. Once again, under such circumstances you should base your AC-BPA solely on the AC evidence (providing this is of sufficient detail and quality) whilst embodying appropriate caveats.*

*If, in the last analysis, 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. Ideally this should draw together into a coherent picture the associated UFR descriptions together with any important interactions which are AC specific. Mention the UFRs associated with this AC that you have considered in drafting your best practice advice. *Access the Knowledge Base to find the UFRs associated with your AC.*

## 5.2 APPLICATION UNCERTAINITIES

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.
- The advice should be consistent with the BPA for the associated UFRs whilst not contradicting the evidence in the AC document. If this is not the case give reasons why.

## 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 (this is not mandatory).
- The advice should be consistent with the BPA for the associated UFRs whilst not contradicting the evidence in the AC document. If this is not the case give reasons why.

## 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 both the AC and perhaps some of the associated UFRs should be repeated using contemporary turbulence models.
- Calculations of the AC should be performed on finer grids and/or with higher order schemes in order to establish consistency with the UFR BPA.
- Further UFR test cases, which are better aligned with the flow conditions encountered in the AC, should be identified and analysed.