

Steve Howell – 27 September 2022

Dr Steve Howell

Steve studied in Newcastle upon Tyne and is a chartered engineer. He has 25+ years experience in the application and development of CFD, founding Abercus in 2010 to provide specialist simulation and modelling services, initially to the energy sector.

Steve is an active member of the CFD (Chair) and SGM* working groups at NAFEMS, the international organisation for engineering simulation.

Disclaimer: Steve has been employing CFD for fire applications for 20+ years. This material reflects his own thoughts and experience and may not reflect those of the respective NAFEMS working groups.

* Simulation governance and management

Abercus

Abercus is an **independent**, privately-owned consultancy specialising in **advanced engineering simulation** – CFD, FEA, bespoke software tools and teaching/training.

Agenda

- [CFD for fire applications](#page-4-0)
- [A framework for verification and validation](#page-18-0)
- [Confidence in CFD for fire applications](#page-46-0)
- [In conclusion](#page-57-0)

Kings Cross fire (1987)

- Harwell Laboratory used CFD to model the fire event and identified the so-called trench effect, where the flames and hot combustion products are confined in the trench of the escalator, which were wooden.
- HSL subsequently undertook one-third scale experiments and confirmed the existence of the trench effect.
- This was essentially a successful blind test of the CFD code for fire simulation.

Personal experience (built environment)

Underground stations (CFX)

Personal experience (built environment)

Underground stations (CFX)

Personal experience (built environment)

- My first exposure to Fire Dynamics Simulator (FDS) coincided with these CFX studies of the underground stations – first impression of FDS:
	- Impressive, free to download CFD code.
	- Verification and validation manual.
	- Democratisation anyone can download FDS and use it on a project.
- Within the company, CFD was restricted to a small team of PhD qualified experts.
- Colleagues from outside the CFD team: *We're going to make CFD a non-PhD tool!*
- Democratisation is a double-edged sword there was clearly a need to make CFD a more widely available tool within the company, but this should really be controlled by SQEP individuals.

Personal experience (built environment) Smoke impairment of hotel atrium (FDS)

Personal experience (built environment)

Smoke impairment of hotel atrium (Fluent)

5 minutes 6½ minutes

Personal experience (built environment)

Smoke impairment of hotel atrium

- The predicted time to impairment was significantly different for Fluent and FDS.
- Different turbulence modelling approaches were used:
	- FDS uses LES.
	- In this case, Fluent used uRANS.
- Following the comparison of the FDS and FLUENT predictions, a review found that the FDS mesh had a spacing of 0.25 m, but the door connecting the hotel room to the atrium was only 1 m wide, so there were only four cells across the door.
- A mesh sensitivity study in FDS showed the impairment time within the atrium to be reduced with further mesh refinement.

Personal experience (oil and gas)

Fire and smoke assessment for an offshore platform (general-purpose CFD vendor)

Jet fire represented by a fixed cone, with uniform smoke/heat sources within the cone.

Personal experience (oil and gas)

Fire and smoke assessment for an offshore platform (general-purpose CFD vendor)

Temperature

Personal experience (oil and gas)

Fire and smoke assessment for an offshore platform (general-purpose CFD vendor)

- A lot of effort had gone into surface wrapping the congested geometry across the topsides of the platform, leading to a +60M cell mesh that required an HPC facility to solve.
- Very little thought had gone into thinking about the physics relevant to the fire application, or the scenarios to consider.
- **This case study is not a good advert for CFD! It is very easy to create colourful nonsense with a CFD code.**
- Abercus updated the assessment five years later using KFX, an application-specific CFD code for fires that is widely used in the oil and gas sector.

Personal experience (oil and gas)

Fire and smoke assessment for an offshore platform (updated by Abercus with KFX)

Personal experience (oil and gas)

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Personal experience (oil and gas)

Fire and smoke assessment for an offshore platform (updated by Abercus with KFX)

- The previous study predicted completely unrealistic behaviour, with fire temperatures of only around 80 °C in the region around the decks, and a maximum temperature of 200-300 °C occurring at a height of around 100 m above the deck (at the top of the *fixed* fire cone).
- Based upon this CFD assessment, the fire scenarios considered were not thought to pose a significant risk to the facility.
- The updated study by Abercus (with KFX) predicted realistic fire temperatures of ~1000 °C in the region around the deck, which does pose a significant risk to the facility. By the time Abercus updated the study, the facility had already been built.

- Question: how can we have confidence in CFD for fire simulation?
	- Through rigorous verification and validation:
		- This requires significant effort that should not be underestimated.
	- Widespread adoption in industry:
		- Develop mature processes embed best practice within a workflow approach.
		- Competence training and accreditation for both CFD users and CFD codes/workflows.
		- . Improve confidence in the CFD process through blind benchmarking.
		- How to interpret the CFD predictions absolute or relative criteria.
		- Standard templates for fire reports using CFD.

ASME V&V 10 diagram

- ASME and NAFEMS have published a *What is?* guide that is freely available for download: http://www.nafems.org/publications/browse_buy/browse_by_topic/qa/verification_and_validation/
- NAFEMS has also published the Engineering Simulation Quality Management Standard (ESQMS), which interprets quality standard ISO 9001:2015 in the particular context of the engineering simulation process: https://www.nafems.org/publications/resource_center/esqms-01/

What is C Verification and Va

www.asme.org www.nafems.org

ASME V&V 10 diagram

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- Verification is:
	- the process of determining that a computational model accurately represents the underlying mathematical model and its solution.
- Validation is:
	- the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.

ASME V&V 10 diagram

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- Verification is:

```
-\text{ the } process of determining that a computational model
accuration and Mathematics and underlying mathematics
mod Are we solving the equations correctly?
```
• Validation is:

ASME V&V 10 diagram (Derived from) ASME V&V 10-2019

• What is verification?

Code verification

Are the numerical algorithms correctly implemented in the computer code? Are they functioning as intended? Does the code correctly solve the underlying equations, as intended?

Calculation verification

Are the simulation errors sufficiently small? (Round-off error, iterative error, discretization error, stochastic error.)

Uncertainty quantification

Are the simulation results sensitive to the simulation inputs?

UQ margins of uncertainty accumulate on top of any errors due to code and calculation verification.

Experimental branch

Similar quality assurance and UQ activities mirrored along the experimental branch.

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Validation

Quantitative comparison of simulation outputs with experimental outputs. Is the prediction within the required bounds?

Not a comparison of single point data, but of predictive/experimental bounds.

Conceptual model Experiment design Validation experiment Experimental results **Experimental** outputs Mathematical model Computational model Simulation results **Simulation** outputs Modelling and simulation Physical experimentation Validation case in hierarchy (Reality of interest) Abstraction Satisfied? **Quantitative** compariso Next validation case in hierarchy (Reality of interest) Yes No Revise model or simulation or experiment • Selecting an appropriate mathematical model (turbulence) **ASME V&V 10 diagram** (Derived from) ASME V&V 10-2019 LES/DES uRANS

ASME V&V 10 diagram (Derived from) ASME V&V 10-2019

• Selecting an appropriate mathematical model (turbulence)

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Validation case in hierarchy (Reality of interest) Abstraction

ASME V&V 10 diagram (Derived from) ASME V&V 10-2019

• Selecting an appropriate mathematical model (turbulence)

No

Conceptual

Validation case in hierarchy (Reality of interest) Abstraction

Revise model or simulation or experiment

ASME V&V 10 diagram (Derived from) ASME V&V 10-2019

• Selecting an appropriate mathematical model (turbulence)

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Validation case in hierarchy (Reality of interest)

ASME V&V 10 diagram (Derived from) ASME V&V 10-2019

- Selecting an appropriate mathematical model (radiation)
	- Is impairment due to radiation a quantity of interest? Pyrolysis?
	- If so, this should be modelled accurately. If not, it may suffice to reject radiative energy from the fire plume using a simple radiation model if it is the subsequent dispersion that is of interest.
	- To model radiative transfer accurately, need to capture the directionality of radiative transfer, which can be computationally intensive.
	- Also need to quantify the radiative absorption coefficient within the fire, since this describes the emissivity of the flame – should this be prescribed (OSRAMO, for example) or predicted from first principals looking at concentration of combustion products?

- Calculation verification
	- Need to demonstrate that the CFD predictions are converged, and are independent of the mesh discretisation and time-step.
	- Finer mesh and time-step refinement is required for LES/DES compared to uRANS.
	- It can be difficult to achieve mesh independence with LES/DES, partly because the mesh edge length is usually taken as the LES filter length, so as the mesh is refined, the model is changed.
	- Turbulence-radiation interactions (TRI) can cause difficulties with mesh sensitivity – a simple, more stable prescription of absorption coefficient may help.
	- Present evidence of mesh/time-step sensitivities in the report.

ASME V&V 10 diagram (Derived from) ASME V&V 10-2019

- Uncertainty quantification
	- Don't simulate one single fire case super-accurately. Having a quick running CFD model that can be used to explore multiple fire scenarios can provide a more complete understanding of the associated fire risk.
	- Consider probability of occurrence for each simulated consequence to give an understanding of risk.
	- Comparison of a single CFD prediction with a single experimental result does not constitute robust validation.

- What is validation?
	- From ASME V&V 10 2019: Validation is the process of determining the degree to which the model is an accurate representation of *corresponding physical experiments* from the perspective of the intended uses of the model.
- Often have to rely on experimental data already in the public domain rather than undertake new validation experiments – make sure comparisons are undertaken by the CFD user, even if the code developer has provided a rigorous validation manual.

ASME V&V 10 diagram (Derived from) ASME V&V 10-2019

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ASME V&V 10 diagram (Derived from) ASME V&V 10-2019

- What is validation?
	- From ASME V&V 10 2019: Validation is the process of determining the degree to which the model is an accurate representation of *corresponding physical experiments* from the perspective of the intended uses of the model.
	- The 2019 definition of validation is really focused upon the quality and management aspects of validation identified in the bottom part of the V&V 10 diagram. The quantitative comparison constituting the validation step in line with this definition is between the outputs of the simulation model and of corresponding physical experiments,

both of which derive from the conceptual model.

- What is validation?
	- From ASME V&V 10 2019: Validation is the process of determining the degree to which the model is an accurate representation of *corresponding physical experiments* from the perspective of the intended uses of the model.
- How can we be confident that our simulation predictions are an accurate representation of reality?
	- Are our experiments an accurate representation of our reality of interest?
	- Just like a computer simulation, a physical experiment is merely a simulation of our reality of interest, it is not the actual reality.

- How can we be confident that our physical experiments are an accurate representation of our reality of interest?
	- If the **abstraction** process misses out some important physics, **the outcomes of the simulation and validation experiment might agree well with each other, but not necessarily with the reality of interest.**

- How can we be confident that our physical experiments are an accurate representation of our reality of interest?
	- If the **abstraction** process misses out some important physics, **the outcomes of the simulation and validation experiment might agree well with each other, but not necessarily with the reality of interest.**
- NAFEMS VVUQ 2021 undertake a PIRT analysis to formally identify the important physical phenomena for any particular validation case. * Phenomena Identification and Ranking Technique

(Derived from) ASME V&V 10-2019

ASME V&V 10 diagram (Derived from) ASME V&V 10-2019

- Examples:
	- Bouncing F1 cars (see NAFEMS Benchmark magazine, July 2022)
	- Natural displacement ventilation of buildings*
	- $-$ Atmospheric dispersion within the built environment*
	- $-$ Fires in ship compartments*
	- Thermal cooldown/hydrate avoidance*.

* Discussed in detail in my NWC 2021 paper – please email me at steve.howell@abercus.com for a copy

On the importance of abstraction validation for fluid flow applications

Steve Howell (Abercus)

 $*$ NWC 2021 paper – Please email me at steve.howell@abercus.com for a copy

- • Need to have mature simulation processes – embed best practice within a workflow approach.
- Competence training and accreditation for both CFD users and CFD codes/workflows.
- Improve confidence in the CFD process through blind benchmarking.
- How to interpret the CFD predictions absolute or relative criteria.
- Standard report templates for regulatory compliance.

Mature processes through the workflow approach Capability maturity model integration (CMMI)

Accreditation for CFD users and CFD codes/workflows

Precedent for built environment – dynamic simulation models (DSM) for energy use

Accreditation of the software

TAS (EDSL) ApacheSim (IESVE) EnergyPlus (Bentley/DesignBuilder)

Accreditation of the user (CIBSE Certification)

Low **Carbon Energy** Assessor

Low Carbon Consultant

Accreditation for CFD users and CFD codes/workflows

Precedent for built environment – dynamic simulation models (DSM) for energy use

Accreditation of the software

MHCLG approved national calculation methodologies and software programs for buildings other than dwellings
For use in connection with the calculation of the energy performance of building for the purposes of:

-
- (a) regulations 24 of the Building Regulations 2010 and
(b) calculating the asset ratings that are included in Energy Performance Certificates, and
- (c) operational ratings that are included in Display Energy Certificates and air conditioning inspection report software approved as fit for commercial use in its current state and form.

Approved versions (2018)

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 $\frac{1}{4}$ within a workflow with standard inputs/outputs. APP The DSM codes are analogous to stand-alone CFD codes. When accredited for Part L, they are embedded

Accreditation for CFD users and CFD codes/workflows

Precedent for built environment – why not for fire CFD?

Accreditation of the software

FLUENT CFX STAR-CCM+ OpenFOAM

FDS FLACS Fire KFX/Exsim FireFOAM **SmartFire**

Accreditation of the user (CIBSE Certification?)

Accreditation for CFD users and CFD codes/workflows

Precedent for built environment – why not for fire CFD?

How to interpret the CFD predictions – absolute or relative criteria

- National calculation method (NCM) for energy use in buildings is based on a relative target – a fictional reference building is created and the energy use for the actual design must improve on that for the reference building by some percentage.
- This is, in part, in recognition that predictions from the various dynamic simulation tools do not generally agree:
	- The simulation code is used for calculating the energy use of both the reference building and the actual building.
	- Having a relative target means that any error in the simulation code is present in the prediction for both the reference building and the actual building, so that when they compared they, to some degree, cancel out.

Loss of confidence in CFD

- Use of CFD for atmospheric dispersion in France.
- CFD-based probabilistic explosion studies in the oil and gas sector.
	- The user inconsistencies in the probabilistic approach have been known about for many years but have not been addressed – PROBABLAST JIP (FABIG, 2021).

- In Norway, the RISP project has yielded a new non-CFD tool for determining explosion risk in future, this may displace CFD-based studies in the Norwegian sector altogether.
- In the UK, IMechE has issued guidance against the use of probabilistic methods (September 2021), although this has now been removed as the IMechE are engaging with key stakeholders to revise it and publish a second edition.

Regaining confidence in CFD

- In France, blind benchmarking for atmospheric dispersion has been undertaken:
	- It demonstrated differences in CFD predictions between different parties.
	- This is the start of the process of regaining confidence in CFD-based methods by acknowledging issues of variation and inconsistency.
- Blind benchmarking is the true test of a simulation code:
	- Most blind benchmarking exercises show that there can be significant variation in simulation predictions when the process is blind, even if participants are using the same simulation code.
	- Of course, these variations can be reduced once the comparison data has been released and participants have the chance to modify their simulation model to improve agreement, but this in itself demonstrates the value of blind benchmarking.
- **It is important to recognize and acknowledge such variations, because then we're in a much better position collectively to address the issue**.

Regaining confidence in CFD

- For probabilistic explosion studies, perhaps a move to relative targets could address much of the concern about user inconsistency.
- This is also in line with the ALARP approach essentially a probabilistic approach with relative targets is *comprehensive ALARP*.
	- Note that the criticism of probabilistic methods in the IMechE guidance of 2021 may not necessarily be aimed directly at CFD-based methods, it is perhaps more how the CFD predictions are captured into a probabilistic framework using absolute criteria.

In conclusion

- CFD is a powerful tool that when used successfully, can deliver detailed understanding of dynamic fire event. On the other hand, when CFD is mis-used, predictions can be misleading. General-purpose CFD codes, in particular, should not be used as *out-of-the-box* solutions.
- In order to improve confidence, it is important to undertake rigorous verification and validation, but the effort involved should not be underestimated. If there are relevant physics missing from the conceptual model, the outcomes of a simulation model and physical validation experiment can agree very well with each other, but not necessarily with the reality of interest.

In conclusion

- For widespread adoption of CFD for fire simulation, the suggested approach is:
	- Develop mature simulation processes embed best practice within a workflow approach.
	- Competence training and accreditation for both CFD users and CFD codes/workflows.
	- Improve confidence in the CFD process through blind benchmarking.
	- Consider how to interpret the CFD predictions absolute or relative criteria.
	- Standard templates for fire reports using CFD, requiring sections on calculation verification, for example.

Contact us

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