Verification and Quality Assurance in the Simulation Analysis Process

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Quality & Reliability of CFD Simulations

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NAFEMS

Who We Are

MMI provides scientific, engineering, safety and risk management consulting services

Service areas

- Safety & Risk Management
- Major Hazards Modelling
- Major Hazards Engineering
- Structural Analysis, Design and Integrity
- Fluid System Modelling and Design

Sectors

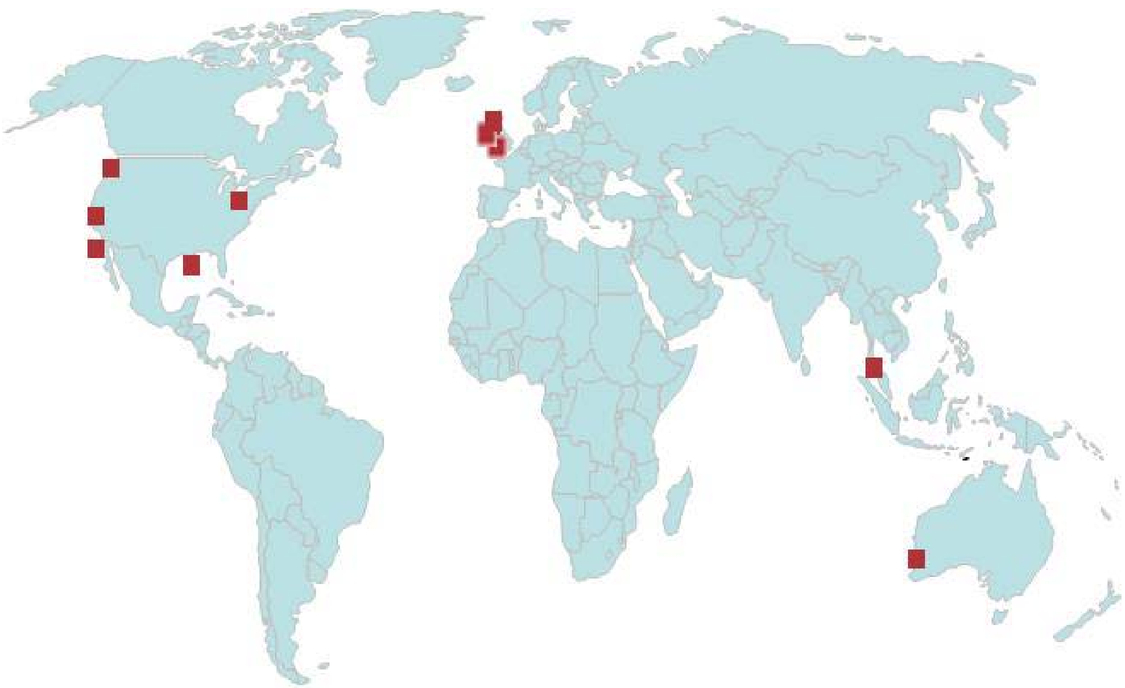
- Oil and Gas/Petrochemical
- Clean Energy (Wind, Tidal, Waste-to-Energy, Carbon CS, Geothermal)
- Nuclear (Decommissioning, New Build, Transport, Fusion)
- Utilities (Water and Power generation industry)
- Security & Defence

MMI Today

- More than 100 Personnel
  - 30 in US, 65 in UK, 7 in AUS
- Engineers
  - Structural, mechanical, safety, electrical, process, chemical, fire protection
- Scientific
  - Physicists, chemists, mathematicians
- Support
  - Graphics and AV media

- Approximately 30% qualified to PhD level, majority of remainder MSc
- Close relationships with Regulators
- Research initiatives – Industry wide developments, JIP’s, TSB
- Design, construction and operational experience
- Comprehensive analytical capability
  - Finite Element Analysis
  - Computational Fluid Dynamics
  - Hazard Modelling
  - System Analysis

MMI Engineering Locations



- **USA** – started Feb 2001
  - Houston, San Francisco, Los Angeles, Boston
- **UK** – started May 2002
  - Warrington, Aberdeen, Bristol, Northern Ireland, York, London
- **Malaysia**
  - Kuala Lumpur, Ipoh
- **Australia** – started 2008
  - Perth WA

Covering major time zones

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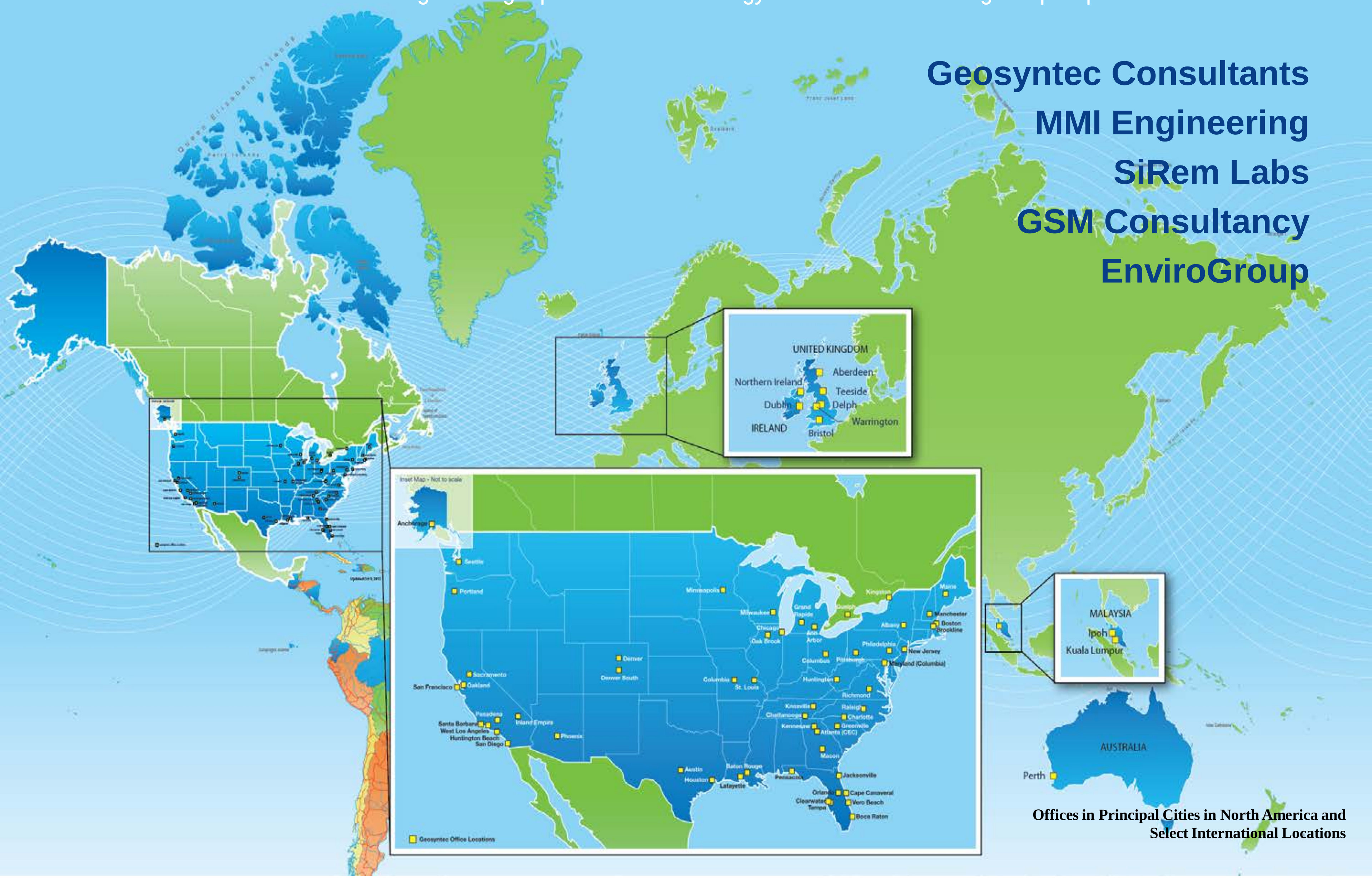

Offices in Principal Cities in North America and Select International Locations

Tools

- **Structural/Stress Analysis**
  - ABAQUS, ANSYS , DYNA USFOS, CAP, SACS, STAAD, Code-Aster
- **Dispersion, Ventilation & Fire Modelling**
  - FRED, PHAST, CIRRUS, CFX, Kameleon KFX
- **System Analysis**
  - FlowMaster, RELAP5, MELCOR, ICARE/CATHARE, Aspen

- **Fluids Engineering**
  - CFX, Fluent, FLACS, openFOAM, Code-Saturne
- **Explosion Modelling**
  - CAM, PHAST, CEBAM, FLACS, AutoReaGas
- **Risk Management**
  - BowtieXP, FaultTree+ RiskVu, SPAR-H

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- Project and analysis objectives
- Input control
- Process quality assurance
- Client communication and conclusions

Introduction

Simulation analysis process is used increasingly in the engineering world to complement experimental and testing programmes or even to substitute them.

The reasons for this are economic as the simulation techniques offer

- greater flexibility in managing ‘testing’ environment,
- a faster turn-around time,
- more comprehensive post-processing options,
- lower costs.

In some cases, safety considerations make physical testing impractical all together (e.g. fire engineering, nuclear safety, space equipment design).

Introduction

Despite all these advantages, it is important to recognise that the simulation process is fundamentally different from physical experimentation and testing.

- In the world of numerical simulations, most of the effort is focused on recreating reality in a digital environment.
- Once the created virtual reality is representative of the analysed environment, capturing relevant data is often much simpler than during physical testing.

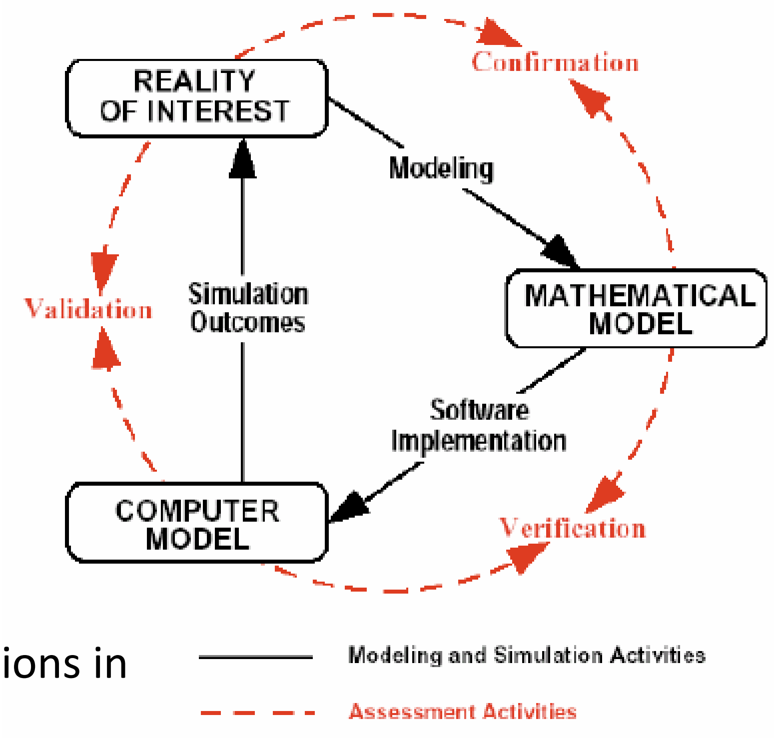


Figure 1: Concept relations in modelling analysis [1]

Introduction

Although, the simulation analysis approach offers much larger flexibility, it also allows much larger errors to be incorporated in the development process much faster.

To avoid mistakes and to mitigate their impact (some of them will inevitably stay undetected), suitable quality assurance (QA) processes need to be set up and implemented with full rigor.

Such QA processes are well established part of the engineering design and manufacturing procedures, but they do not always extend to the engineering analysis although the related requirements have been defined (ISO-9001, 10CFR50 Appendix B, 10CFR21and NQA-1).

Project and analysis objectives

The analysis objectives must be clearly defined and agreed between all stakeholders. Such definitions shall be qualitative and quantitative (as much as possible).

- The analysis output; its content as well as its form.
- Clear separation between the design process and analysis objectives.
- The analysis objectives have be propagated from top to bottom. The executing analyst/engineer has to understand the analysis objectives (i.e. what had been sold).

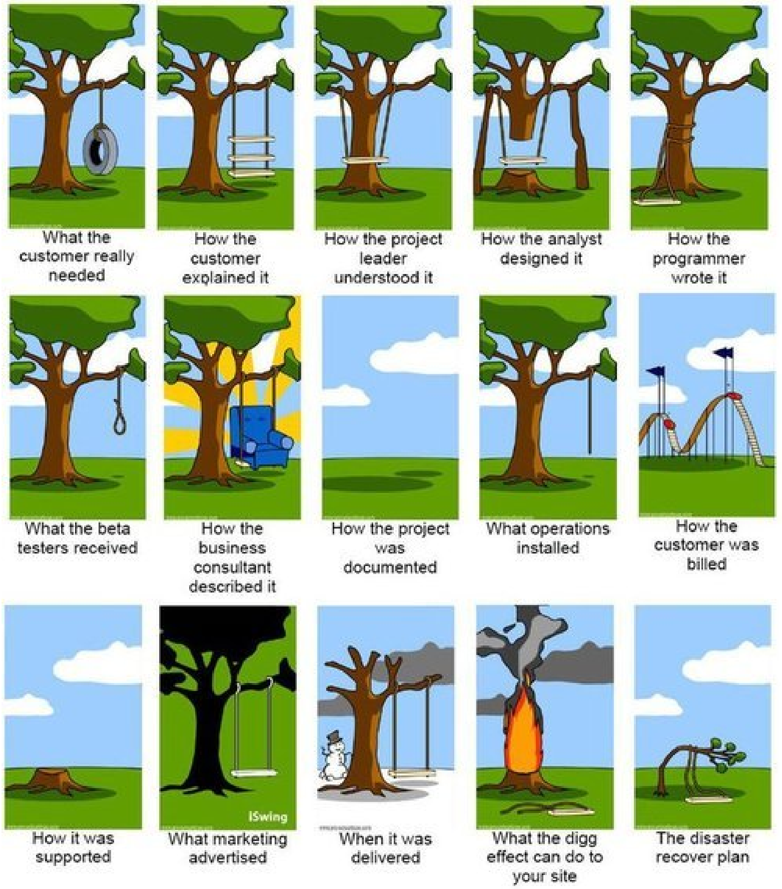


Figure 2:

Project and analysis objectives

Quality parameters (e.g. modelling uncertainty, numerical errors, results variability and sensitivity) shall be an integral part of the analysis objectives.

Input control

The input control process consists of

- Toolset control (e.g. knowledge base, hardware, software)
- Personnel (e.g. suitable degree level, skills and experience)
- Analysis and quality control procedures (e.g. lumped parameter modelling, CFD)
- Project specifications and requirements

Most of these activities are generic and applicable to different projects. They are time consuming and therefore have to be accomplished prior to the analysis task start-up.

Validation and verification of the declared software capabilities is an integral part of the input QA control, which **may be shared** with software vendors.

Input control

Well documented cases (i.e. benchmarks) with understood physics and high accurate predictions shall be used to independently **validate** and **verify** the declared software capabilities.

- 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 [2].

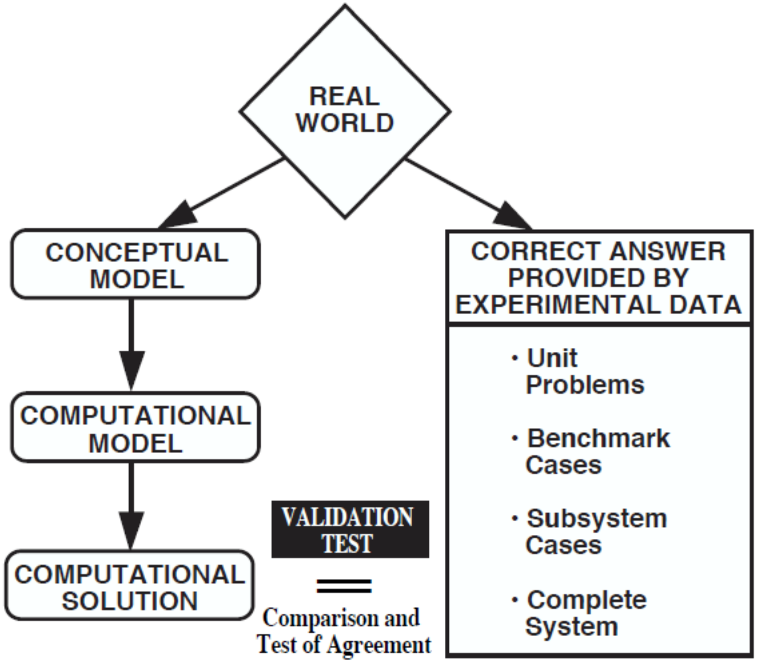


Figure 3: Validation process [2]

Input control

- Verification is the process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model.

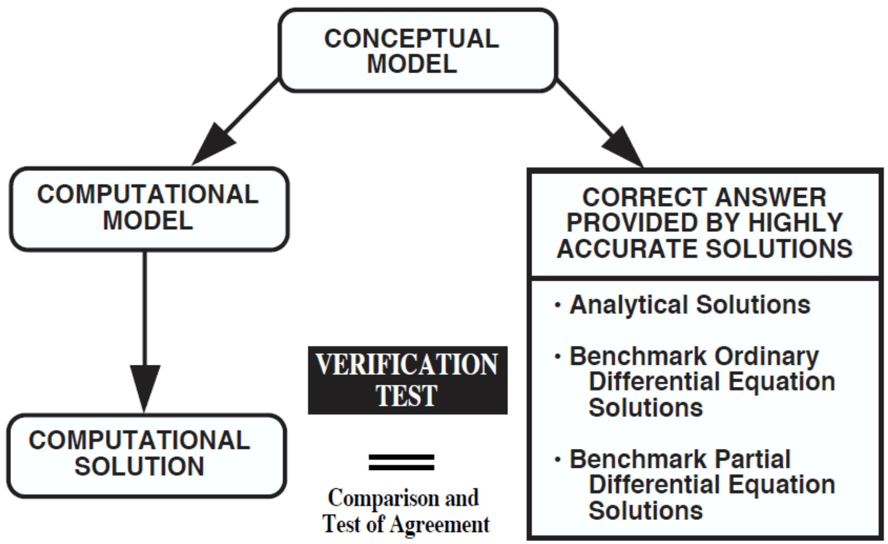


Figure 4: Verification process [3]

Input control

CFD community started to look into validation and verification problems some time ago. First papers started to appear in 1970s [4].

At present, the discipline is well defined. The methodology and the associated terminology have been accepted [5].

A number of online resources (e.g. ERCOFTAC, NASA, Uni. Manchester) are available specifically for validation of software tools offering experimental databases, conferences and periodic exercises.

The available pool of experimental data is strongly focused on turbulence modelling problems.

As the modelling is becoming increasing complex and coupled (e.g. turbulence, multiphase, combustion, structural mechanics, electro-magnetics etc), the supporting experimental data and theoretical investigations are simply missing.

Input control

Commercial software vendors may assist in the validation and verification process; they should not be a primary source of it.

It is important to assure independence of the software validation and verification and/or to preform in-house testing (which also includes the user-component).

Certain degree of modelling analysis “prototyping” will always be required on individual project basis.

Input control

Recent EFDA sponsored 3PT project [8] examined readiness of available modelling software tools for coupled analyses in fusion technologies taking into account:

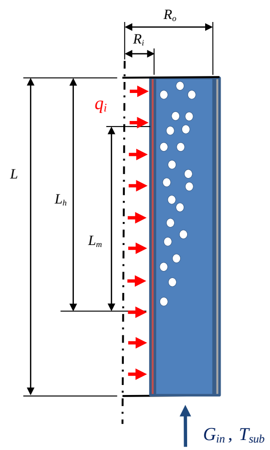
- Pre-processing capabilities
- Simulation methods
- Fluid mechanics
- Heat transfer
- Multiphase modelling
- Structural mechanics
- Multibody mechanics
- Electromagnetics
- Neutronics
- Parallel processing
- Post-processing and visualisation

A number of benchmark cases have been defined covering some of the relevant analysis areas.

Input control

CCFE CULHAM CENTRE FUSION ENERGY	WALL BOILING	TEST NO 7	DATE / ISSUE 2013/07/26
ORIGIN	PPPT project		
ANALYSIS TYPE	Multiphase, boiling analysis		
OBJECTIVES	Testing of vapour volume fraction distribution		

GEOMETRY



Annular domain height (L) is 2.376 m
Heating section height (L_h) is 1.670 m
Distance to the measuring plane (L_m) is 1.610 m
Outer radius of the inner tube (R_i) is 0.0095 m
Inner radius of the outer tube (R_o) is 0.01875 m

MATERIAL PROPERTIES	Material properties of water - vapour mixture covering the pressure range between 1 and 2 bar, and the temperature range between 30°C of subcooling and the saturation conditions.
LOADING	A limited set of experimental cases [2] is selected with • inlet mass flux G_{in} = 715.2, 714.4, 716.4 kg m^{-2} s^{-1} • inner wall heat flux q_i = 139.1, 197.2, 232.4 kW m^{-2}
INITIAL CONDITIONS	Due to the steady-state nature of the boiling heat transfer case, initial conditions are not important. They should be used to enhance stability of the solution procedure.
BOUNDARY CONDITIONS	At the inlet, the following mass flux values and subcooling temperatures used in the experiments [2] are prescribed: • G_{in} = 715.2, 714.4, 716.4 kg m^{-2} s^{-1} • T_{sub} = 12.0, 13.8, 14.9 °C At the outlet, a fix pressure should be set. It has to be adjusted to meet the requested inlet subcooling conditions. Due to pressure dependence of the boiling location, it may be more suitable to imposed fix total pressure conditions at the inlet and mass flux at the outlet. At the inner wall, fix heat flux values are prescribed: q_i = 139.1, 197.2, 232.4 kW/m^2 The external wall can be kept adiabatic.

MESH ELEMENTS

Such multiphase simulations in simple geometries are most often performed using a hexahedral mesh although other mesh types are not discouraged.

Maximum grid spacing should be below 0.01 m in the vertical direction, and below 0.0004 m in the radial direction. In the tangential direction, a finite volume should not cover an angle that is larger than 3°.

It is expected that mesh independency of the simulation results is demonstrated.

OUTPUT	The experimental results cover the radial distribution of water vapour volume fraction, liquid and vapour velocity at the plane elevation L_m. They are shown below. The modelling results should be compared with the experimental data for the above listed sets of parameters (i.e. inflow max flux G_i, subcooling temperature T_{sub} and the wall flux q_i).

Figure 5: Benchmark case for boiling flow (just a couple of pages) [8]

Input control

Periodic review of available personnel / analysts, their skill sets and capabilities shall not be forgotten.

The problems are related to

- Frequent and significant software changes (e.g. each year)
- Frequent career changes (internal and external)

Process quality assurance

In most cases, a suitable analysis process has to be identified prior to the start of the project.

This means that the commercial, design and analysis teams need to work together in preparation of the analysis specifications.

Key performance indicators need to be defined. They can be

- **commercial** (hourly rate, profit level),
- **technical** (method implementation, results accuracy),
- **scientific** (novel approach),
- **client satisfaction**.

Process quality assurance

The process plan needs to be **simple as possible** and to allow feedback as the analysis work progresses.

STAGE 1: Specification Review, CAD prep	5 days	Mon 02/01/12	Fri 06/01/12
Kick off meeting	1 day	Mon 02/01/12	Mon 02/01/12
Review of specification	2 days	Tue 03/01/12	Wed 04/01/12
CAD simplifications	2 days	Thu 05/01/12	Fri 06/01/12
Stage 2: CFD Analysis	46 days	Mon 09/01/12	Mon 12/03/12
Geometry discretisation	1 day	Mon 09/01/12	Mon 09/01/12
Engineering analysis of load cases	8 days	Tue 10/01/12	Thu 19/01/12
Meshing	3 days	Thu 19/01/12	Mon 23/01/12
CFD model setup	4 days	Tue 24/01/12	Tue 14/02/12
QA process and related meetings	2 days	Thu 26/01/12	Fri 02/03/12
Simulation of load cases	25 days	Fri 27/01/12	Thu 01/03/12
Post-processing and results analysis	2 days	Fri 10/02/12	Mon 05/03/12
Simulation time contingency	5 days	Tue 06/03/12	Mon 12/03/12
Stage 3: Report preparation	5 days	Tue 13/03/12	Mon 19/03/12
Report	3 days	Tue 13/03/12	Thu 15/03/12
Final Meeting	2 days	Fri 16/03/12	Mon 19/03/12

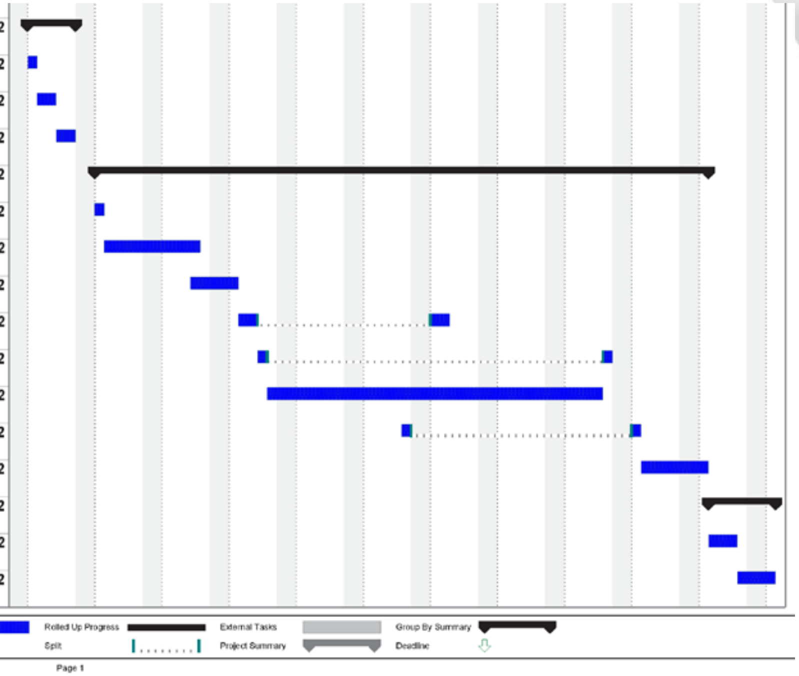


Figure 6: Typical Gantt diagram for CFD analysis

Process quality assurance

Task ownership has to be established, associated project interfaces agreed and set up.

Personal preference to **task lists** (e.g Excel or on-line) that allow instant feedback.

CFD Analysis of Particle Sampling in [redacted] MEMS [redacted]

	Stage 1: Preparation stage	**Completed**
1	(AH – 2014/03/30) Discuss and define operating conditions.	
2	(AH – 2014/03/30) Define appropriate meshing strategy (AH – 2014/03/30) AH & PW discussed: (a) the extent of the simulation domain, (b) how to split the domain, (c) where to use tets or hexas	(AH – 2014/03/30)
3	(AH – 2014/03/30) Clean both CAD for both geometries	
4	(AH – 2014/03/30) Prepare the starting statement.	
5	(AH – 2014/03/30) Send to the client the starting statement and the clean CAD models.	
6	(AH – 2014/03/30) Mesh CAD models	
	Stage 2: CFD analysis of particle distribution for 2 inlet design variations	**Completed**
7	(AH – 2014/03/30) CFX setup – steady-state fluid only analysis. This has to be performed for 2 models.	
8	(AH – 2014/03/30) Perform CFX simulation for 2 geometries and a single operating condition	

Figure 7: Interactive task list

Process quality assurance

Quality control plan needs to be established. It controls **if**, **how** and to **what extent** the key performance indicators are met.

On the technical level, **analysis check lists** can importantly contribute to clarity of the inspection categories and the related qualitative and quantitative analysis parameters:

General

- Analysis information
- Review information
- Analysis report
- Analysis files

CFD analysis

- Analysis objectives
- Geometry
- Meshing
- Model selection & strategy
- Model preparation
- Analysis results
- Analysis validation
- Data archiving

Analysis report

- Front sheet
- General
- Introductory section
- Main section
- Final section

Review notes

- Review 1
- Review 2

Process quality assurance

required. The ordinary 'Thermal Model' would suffice.	
Is the analysis interested in steady-state or transient behaviour	Status: Steady-state
Symmetry flow conditions expected	Status: Yes
Vertical pressure variation considered Reviewer (2014/01/18): The analysis is interested in heat transfer. Even when pressure distribution is required, the vertical hydrostatic contribution will be small.	Status: Not required
MODEL PREPARATION	
Units (especially in the expressions and the additional model code) are consistent	Status: Yes
Material properties and related models are well defined and appropriate Reviewer (2014/01/18): The CFD analysis is isothermal (i.e. all wall boundaries are adiabatic). Therefore, the temperature level is unknown as well as its effect on the material properties.	Status: Cannot be determined
All important thermal effects are represented or their omission explained Reviewer (2014/01/18): There is no source of thermal energy in the simulation domain. Therefore, no thermal effects are actually simulated and, consequently,	Status: No

Figure 8: Section of an example CFD checklist

Process quality assurance

Quality control plan tracks all phases of the project execution.

In helps in recording evolution of quality concerns and eventually resolving the problems. It needs to be a **living document**.

After completion, **project performance** review helps improving efficiency and quality (e.g. accuracy) of the overall analysis process.

Its findings have to be fed back to update the analysis processes and the corresponding quality plans.

Client communication and summary

- Principles of quality assurance process applied to the engineering analyses does not only improve the quality of the output (i.e. higher results accuracy, less variability, better repeatability), but also **reduces the commercial risks** associate with analysis complexity.

- Technical aspects of the quality assurance plan need to be communicated to the client (either internal or external).

- It is important that the client understands the accuracy of the analysis results and possible impact of the input parameter variations.

- Overstating the accuracy of the analysis results may have serious consequences. The results uncertainty is an integral part of the deliverable.

- Although, available computational resources may allow, a more detailed picture shall not become a substitute for results accuracy and/or their variability.

Thank you

References

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