PAUL SCHERRER INSTITUT

Wir schaffen Wissen – heute für morgen

Paul Scherrer Institut

B. L. Smith, Thermal Hydraulics Laboratory

On the Use of Computational Fluid Dynamics (CFD) in Reactor Technology

OUTLINE OF FIRST PART OF TALK

- What is CFD?
- Origins
- Commercial CFD Packages
- Navier Stokes Equations
- Building Blocks of CFD: Mesh Construction
- Capabilities of CFD Codes: Nuclear and Non-Nuclear
- Summary

What is CFD?

Universal truism of science and technology

Everyone believes an experiment…except the guy who ran it
And no one believes a calculation…except the guy who made it.

What actually is CFD?
And can it influence these beliefs?

Various Definitions

Officially stands for…	Computational Fluid Dynamics
Is accused of being…	Colourful Fluid Dynamics
Is often (ab)used as…	Colours For Directors
Or worse…	Colourful Fantasy Dreams
Begins to be…	Credible Fluid Dynamics
But is not always…	Cost-effective Fluid Dynamics

Could add one more… Commercial Fluid Dynamics WHY?

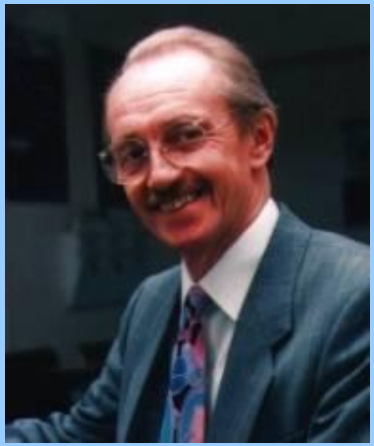
Origins

With the advent of fast, digital computers in the 1960s, it became possible to attempt the numerical solution of the Navier-Stokes equations, the governing equations of fluid dynamics.

In the early days, the general policy was to write specific codes for specific tasks, and universities, research laboratories and industry all followed this trend.

The result was a myriad of special-purpose codes, with each code almost exclusively operated by the person, or group of persons, who wrote it. Documentation was usually poor, and often non-existent. There was almost always one key, central person, who was the ultimate source of knowledge of the software.

In 1974, Prof. D. B. Spalding of Imperial College, London founded a spin-off company called CHAM (Concentration, Heat And Momentum). Initially, CHAM followed the general trend of special-purpose software, but in 1980 adopted a single-code policy, with a central, robust solver, and then concentrated on model development. This new code system, PHOENICS, could be regarded as the first, genuinely multi-purpose CFD code, and a role model for those that followed.



Exploitation of the commercial potential of this concept also began.

For these reasons, Brian Spalding is often referred to as the "Father of CFD"

The new era of CFD: led by PHOENICS

Modular design: central solver, pre-processor (mesh generator), post-processor (graphical display of results) and modules to link in, as needed for the particular application.

This strategy is now followed by all the main commercial CFD vendors.

CFD Software Packages

Commercial

CFX — originally developed by AEA Technology, Harwell, UK;
acquired by ANSYS Inc. in 2003

FLUENT — originally developed by Creare Inc., USA, Sheffield Univ., UK and FDI, Chicago, USA;
acquired by ANSYS Inc. (mainly involved in structural mechanics) in 2006

STAR-CD, STAR-CCM+ — originally developed at Imperial College, London in the group headed by David Gosman,
then by Computational Dynamics Ltd (UK),
marketed by the CD-adapco group (USA)

PHOENICS — originally developed at Imperial College, London, then by CHAM Ltd (UK)

Freeware

OpenFOAM — originally developed by Henry Weller and colleagues at Imperial College, London, then by
Nabla Ltd, but then made freely available by OpenCFD in 2004.
Unique feature: source code access (written in C++)
but difficult to program one's own models into the code, and slow running.

Navier-Stokes Equations: The Foundation of CFD

There are many ways of writing the governing equations, at different levels of complexity. As a starting point, those reproduced here are the basis set for single-phase, laminar flow, written in conservative form. Later, turbulent flow and multi-phase effects will be discussed.

Body force

Summation over repeated indices

Mass continuity: $$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho u_j\right) = 0$$

Momentum transfer: $$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_i u_j) = B_i - \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\sigma_{ij}$$

Energy transfer: $$\frac{\partial(\rho H)}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j H) - \frac{\partial}{\partial x_j}\left(\lambda \frac{\partial T}{\partial x_j}\right) = \frac{\partial p}{\partial t}$$

in which $\boldsymbol{\sigma}$ is the viscous stress tensor. For a Newtonian fluid, this is linearly related to the rate of strain tensor, according to:

$$\sigma_{ij} = \mu D_{ij} + \left(\varsigma - \tfrac{2}{3}\mu\right)\frac{\partial u_k}{\partial x_k}\delta_{ij} \qquad D_{ij} = \tfrac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

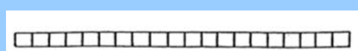
and where μ and ζ are the shear and bulk viscosity coefficients

Also, H is the total enthalpy: $H = h + \frac{1}{2}u_j u_j$

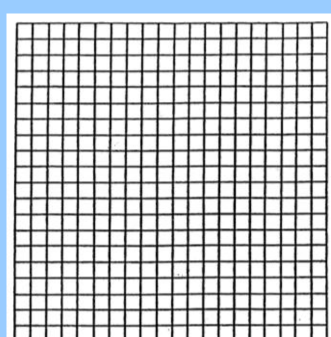
Other symbols have their usual meanings

Discretization

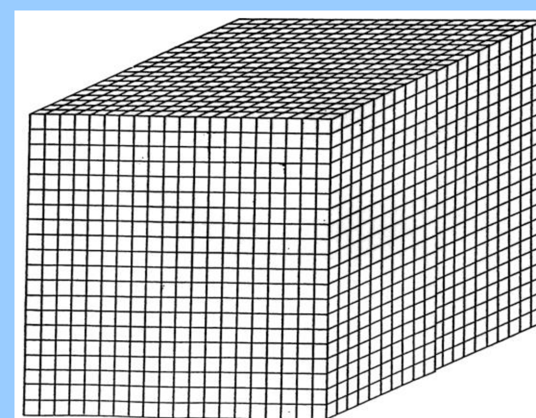
The differential forms of the equations are far too complex to be solved analytically, except in the very simplest of cases, so the equations have to be discretized and then solved numerically. The most common procedure among the commercial CFD codes is the finite volume method, which involves integrating (actually averaging) the equations over a large number of small cells or meshes making up the entire flow domain.



1D: 20 cells



2D: 400 cells



3D: 8000 cells

In 1-D, 20 mesh points would often be considered a very crude level of discretisation. In 3-D, 8000 mesh cells is considered likewise!

The data structures are very large in 3-D CFD!

Data Structures are VERY LARGE in CFD

A 1-D Situation

This is a Japanese "Bullet Train", similar to the TGV in France.

The seating capacity is 1327 (16 carriages)…

… which is here used to represent our 1-D "system code" type discretization, as used in RELAP5, for example.

Imagine the infrastructure needed to support the passengers on this train during its "transient": i.e. ticketing, seat allocation, information desk, announcements, escalators to the platform, snack bars and restaurants, washroom facilities, station staff, taxis, etc.

In a 3-D representation, as used in CFD, the number of seating places required would be: 2'336'752'783 (~2.4 billion).

This is close to twice the population of China.

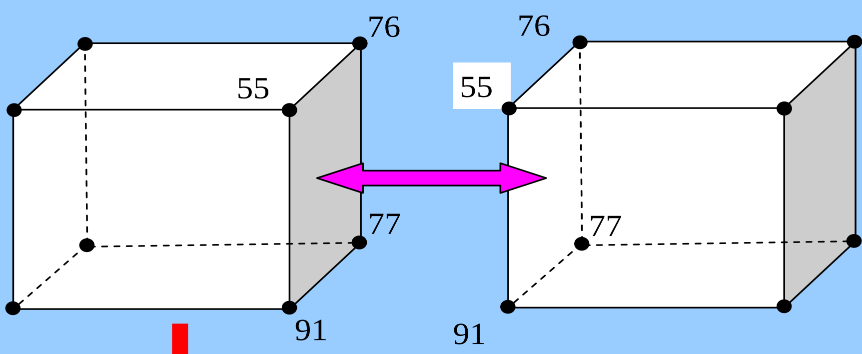
Now imagine the infrastructure needed to support this number of passengers during its "transient": communication networks, data storage, etc.

The data structures are VERY LARGE in 3-D CFD!

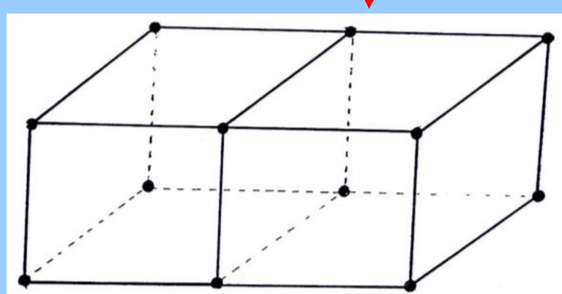
Multi-Block Strategy

The problem geometry may be built up using blocks; these may be hexahedral, tetrahedral, prism, pyramid, etc.

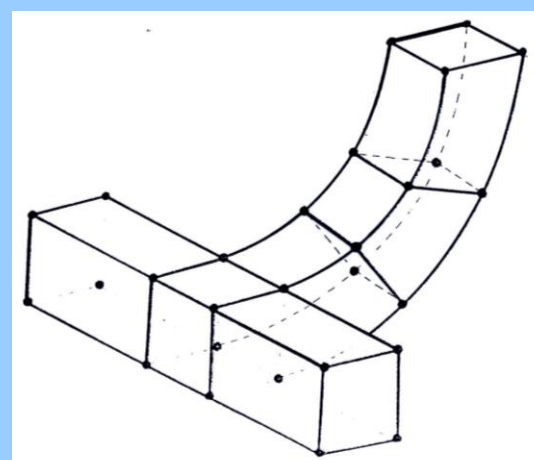
Global Node Numbering



The joining of the E and W faces of adjacent (hexahedral) blocks is accomplished using the concept of shared nodes; i.e. nodes have the same number in the global node numbering system.



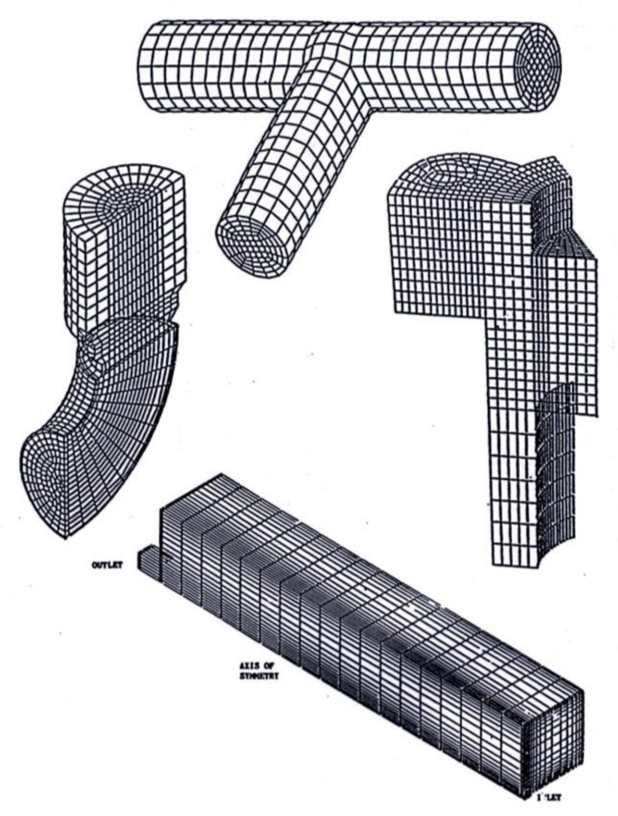
Blocks are joined

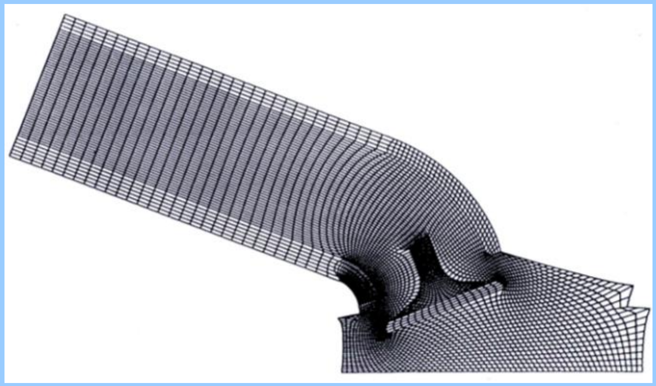


The blocks can have curved edges, to fit the problem geometry, but must remain topologically equivalent to a rectangular block

Blocks are subdivided into as many computational cells as needed to resolve the flow. In principle, the exact problem geometry may be represented in this way, however complex.

Examples of Mesh Construction





CFD is widely used in the aerospace and automotive industries. The concept of moving meshes, for example to represent the motion of engine exhaust valves, has been introduced. As the valve moves, the meshes in the vicinity are adapted to the new flow geometry.

Traditionally, the major CFD vendors offered custom-built mesh generators with their CFD solvers. More recently, stand-alone mesh generators, with built-in interfaces to different commercial CFD packages, have become popular.

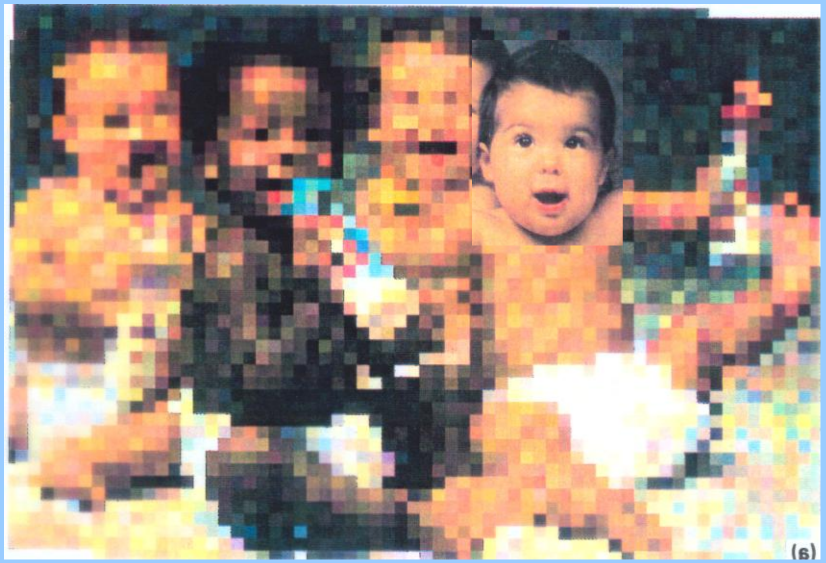
Today, the number of meshes used in CFD simulations often exceeds 1 000 000 000.

Discretization

The discretization process itself an art form. Too fine a mesh, and the computation can take a very long time.

Too coarse a mesh, and there is a danger of washing the baby out with the bath water, meaning important information is being lost

Fine-Mesh Simulation



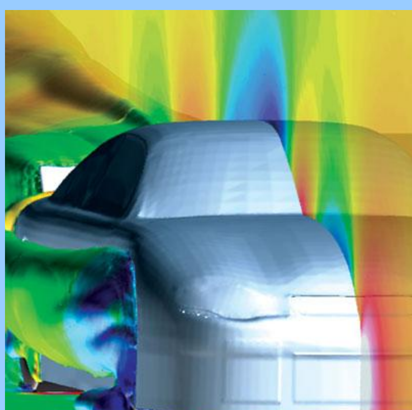
Coarse-Mesh Simulation

To economise on the number of meshes, but still retain all relevant information, modern grid generators have the capacity to refine the mesh in places where more detail is required.

But…an efficient algorithm is needed for interactive mesh adjustment!

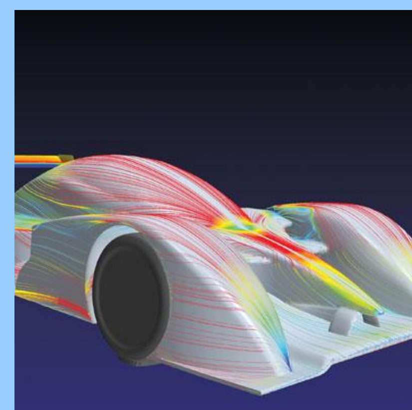
Illustration of CFD Capability (Non-Nuclear)

The rapid growth in the industrial use of CFD in the last 30 years, accompanied by spectacular improvements in computer hardware, has come at a time of stagnation in the nuclear industry. The nuclear accidents at Three Mile Island (1979), Chernobyl (1986) and recently at Fukushima (2011) have stunted growth in the nuclear domain. Consequently, the principal driving force for the development of physical models for use in CFD codes has come from, and for the time being at least remain in, the non-nuclear area.

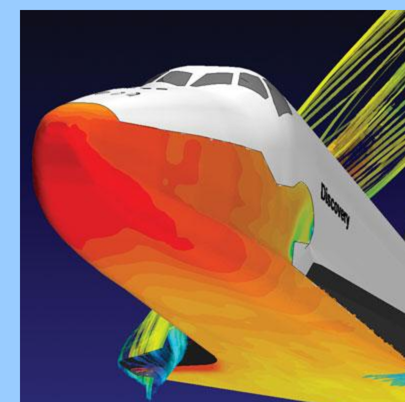


CD-adapco (STAR-CD)
Jacobs
Flow performance of a full NASCAR

CD-adapco (STAR-CCM+)
Aerodynamic analysis of a competition bicycle



CD-adapco (STAR-CD)
Epsilon Euskadi & METCA
Aerodynamic analysis of eLMP1 Automobile



CD-adapco (STAR-CD)
STAR-CCM+
Simulation of a high-altitude re-entry vehicle

Illustration of CFD Capability (Non-Nuclear)

Actual incident at the Petit Le Mans race in the US

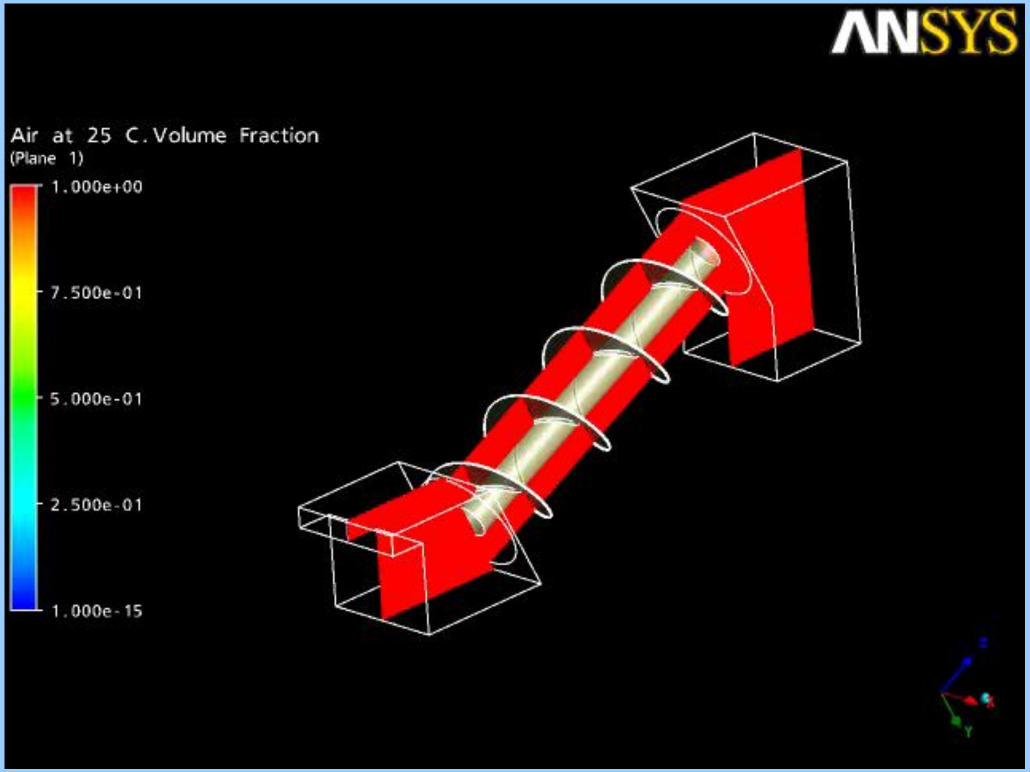
The problem arose because there was a relaxation in the rules regarding maximum power of the cars.

However, no one had studied thoroughly the air flow over the car, and more particularly the flow underneath it!

These days, this type of accident should not happen on the F1 circuit , because CFD is now used to study the aero-dynamics of the flow over the car shape, and the design modified accordingly.

Message: accidents occur in other industries too!

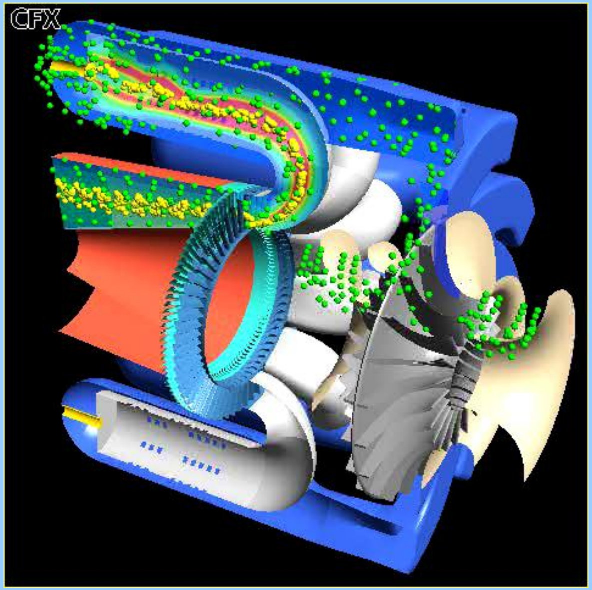
Illustration of CFD Capability (Non-Nuclear)



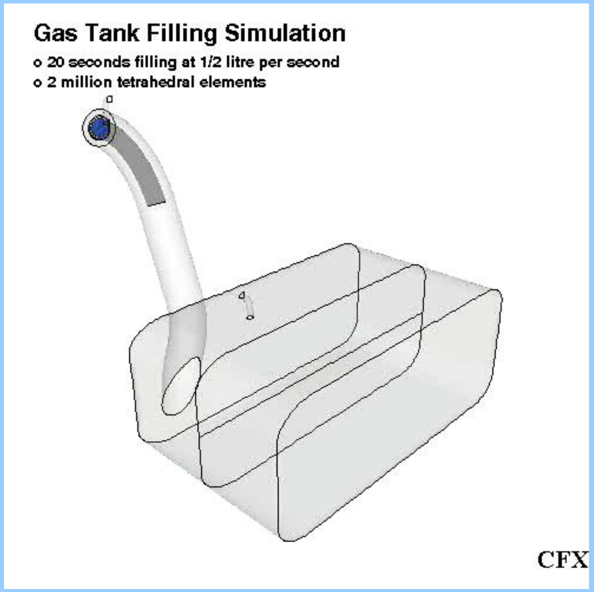
Archimedean screws at the
Kinderdijk in Holland
Capacity: 1.35 million litres/day

ANSYS-CFX
Flow performance of an Archimedean screw

Illustration of CFD Capability (Non-Nuclear)



ANSYS-CFX
Simulation of gas turbine

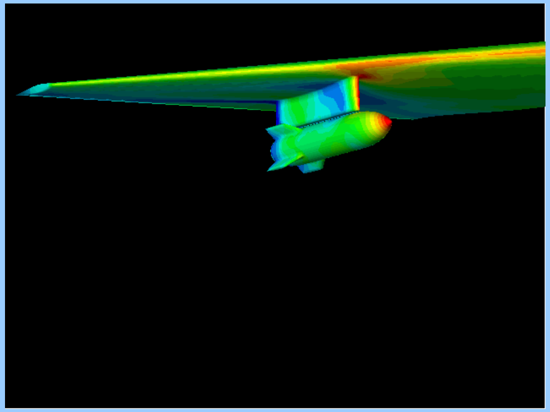


ANSYS-CFX
Simulation of fuel tank filling

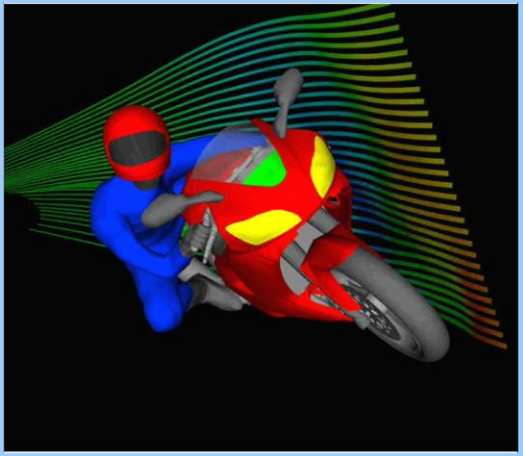
Illustration of CFD Capability (Non-Nuclear)

The use of CFD is widespread in the automotive and aerospace industries

ANSYS FLUENT
Aerodynamics of a F1 racing car



ANSYS FLUENT
Simulation of missile launch from an attack aircraft



ANSYS FLUENT
Aerodynamics of a racing bike

ANSYS FLUENT
Aerodynamics of a F1 airbox intake

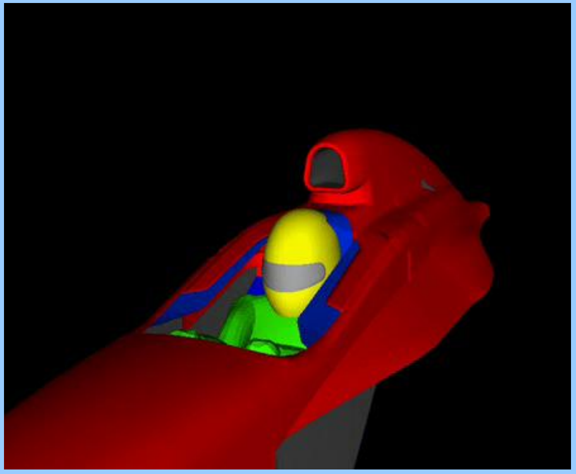
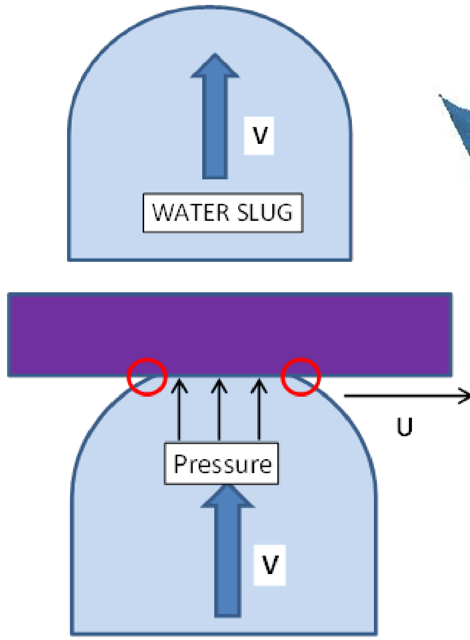
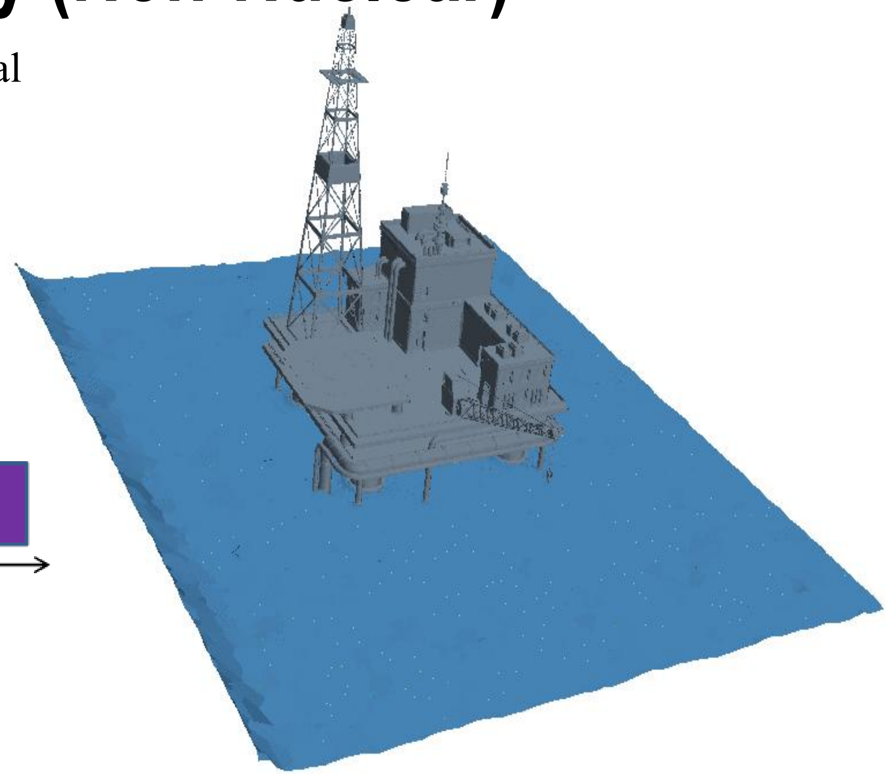


Illustration of CFD Capability (Non-Nuclear)

Oblique versus normal water slug impact



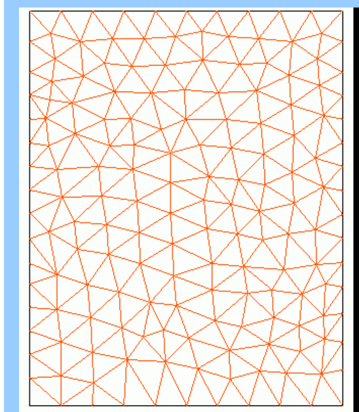


STAR-CCM+
Wave breaking over an off-shore oil platform to test water impact loads

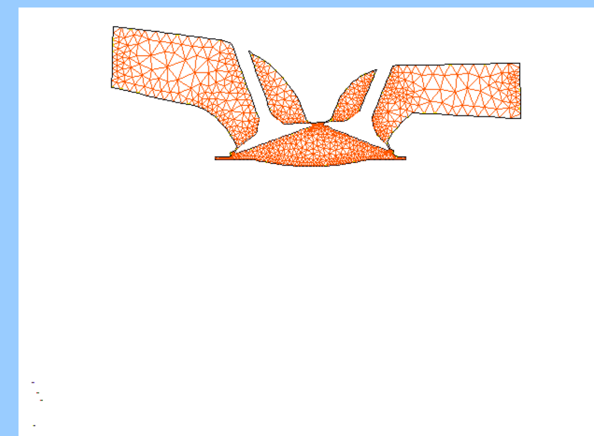
Oblique impact (U<c): $\Delta p = \frac{1}{2} \rho v^2$	e.g. v = 10m/s	Δp = 0.50 bar
Normal impact (U>c): $\Delta p = \rho c v$	e.g. v = 10m/s	Δp = 150 bar

This pressure, integrated over the impact area, can amount to a very destructive force. Crucial to know the shape and hence dynamics of the surface at impact to estimate the structural load. Only CFD can do this.

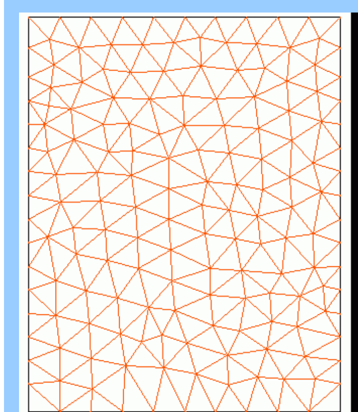
Illustration of CFD Capability (Non-Nuclear)

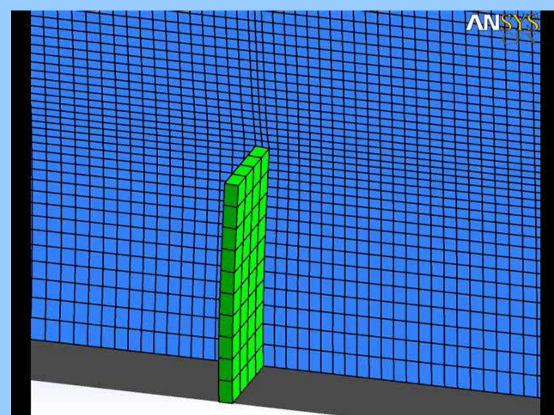


ANSYS FLUENT
Mesh adaptation for small movement of boundaries



ANSYS FLUENT
Mesh adaptation for large movement of boundaries, (mesh removal and generation)





ANSYS-CFX
An example of fluid-structure interaction

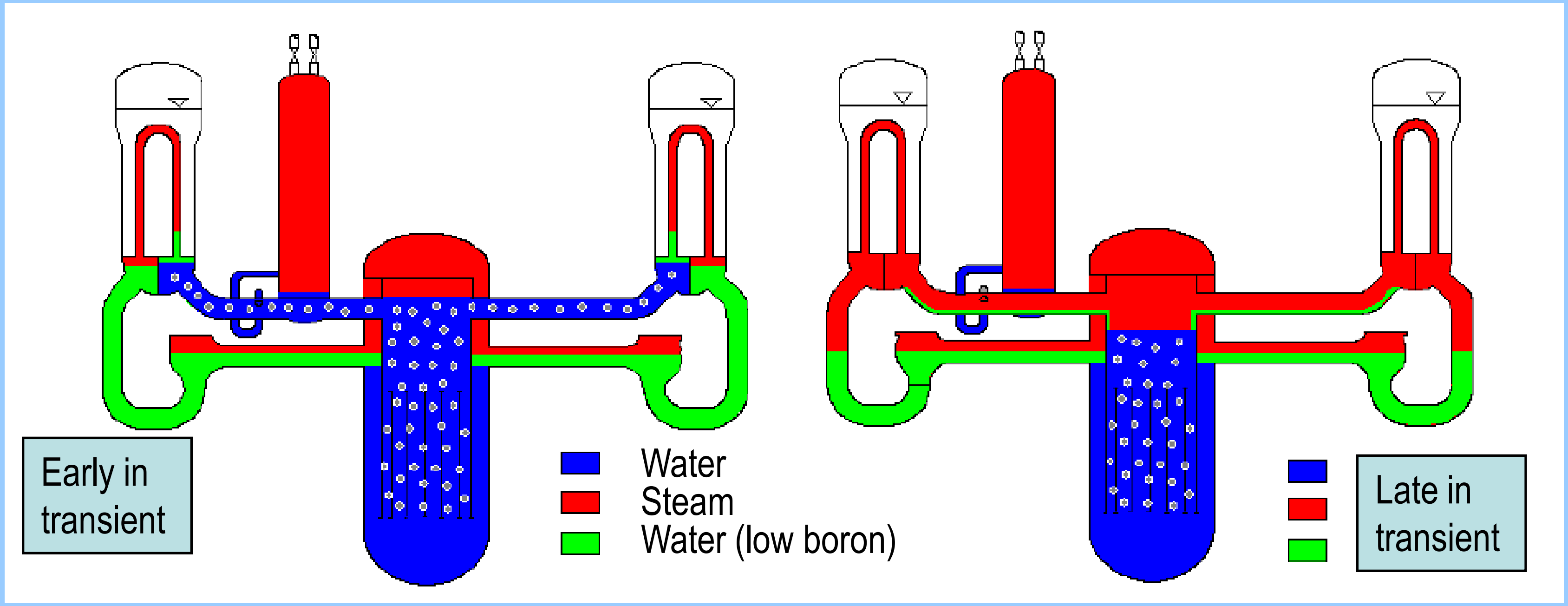
FLUENT
Mesh adaptation for simulation of valve motion in a diesel engine

Automatic mesh adaptation is now a regular feature of CFD simulations

Illustration of CFD Capability (Nuclear)

Boron Dilution

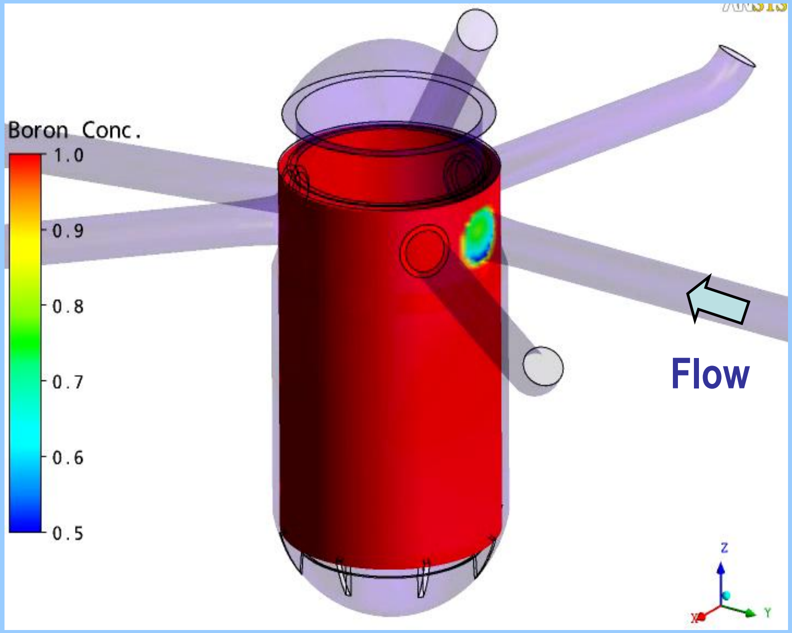
The scenarios of concern start with a Small-Break Loss-Of-Coolant Accident (SB-LOCA). If the event leads to boiling in the core and then the loss of natural circulation, boron-free condensate can accumulate in the cold legs.



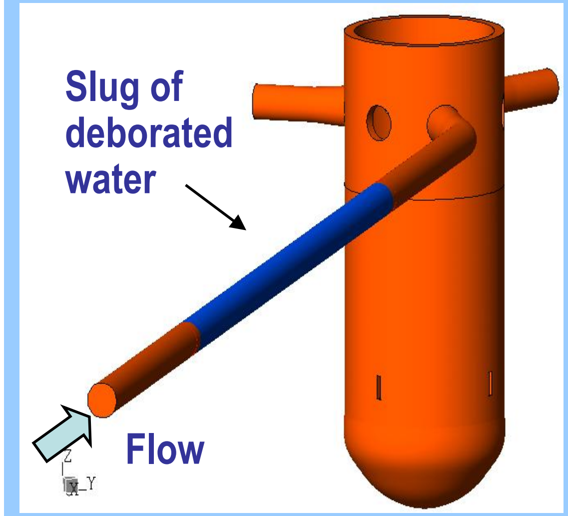
The dilution event occurs when natural circulation is re-established or a reactor coolant pump (RCP) is restarted. The low-borated water, if it remains unmixed, could be transported to the core and produce a power excursion.

Illustration of CFD Capability (Nuclear)

Boron Dilution
Example of pump start-up transient for a 3-loop PWR



ANSYS-CFX
Development of mixing process



ANSYS-CFX
Concentration at core inlet

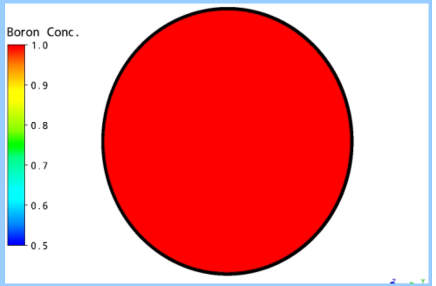
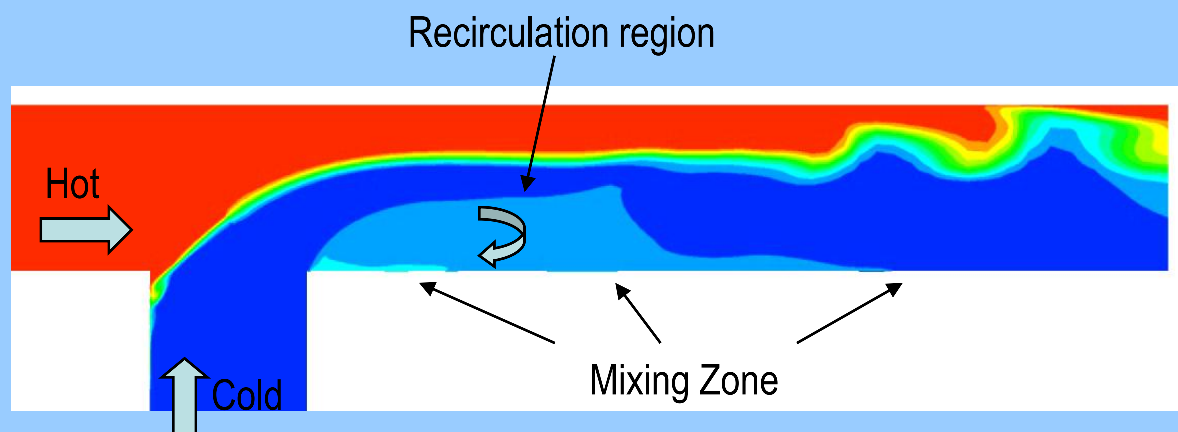


Illustration of CFD Capability (Nuclear)

Mixing in T-Junctions

Critical parameters:
1. frequencies (ω);
2. temperature differences (ΔT);
3. number of cycles (N);
4. material properties

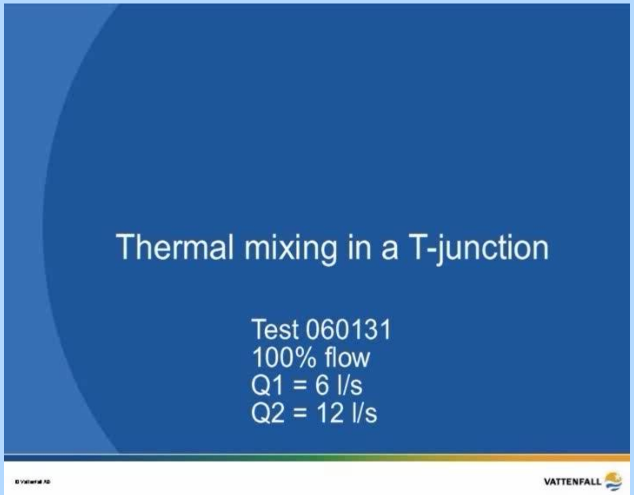


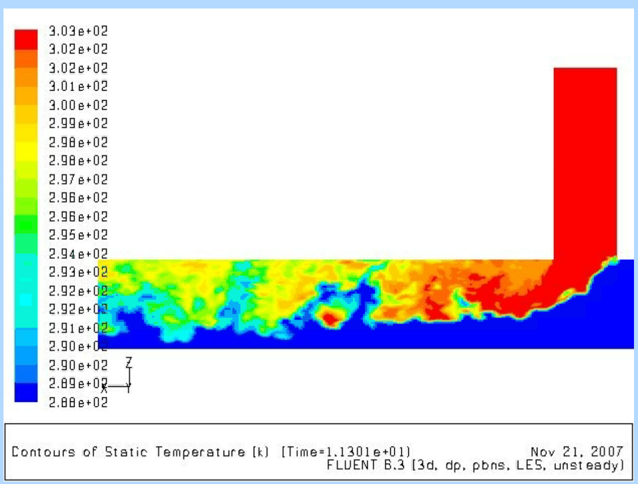
Most damaging thermal loads appear to be due to large-scale turbulent fluctuations; i.e. identification and quantification of non-steady phenomena of low frequency (1-10 Hz) are important.

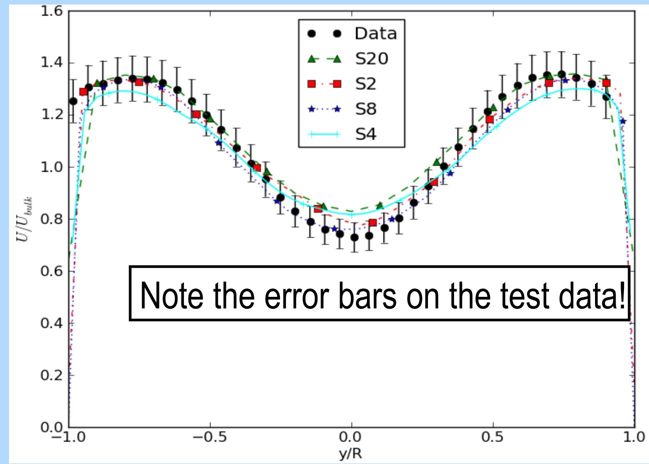
The recirculation region immediately behind the tee plays a crucial role in determining the frequency and amplitude of the thermal (and consequently mechanical) loads to the pipe wall.

The data required from the thermal hydraulics (ΔT, ω) can be obtained from empirical laws derived from mock-up experiments and/or using CFD. In the latter case, serious consideration has to be given to the modelling of turbulence .

Vattenfall T-Junction Tests

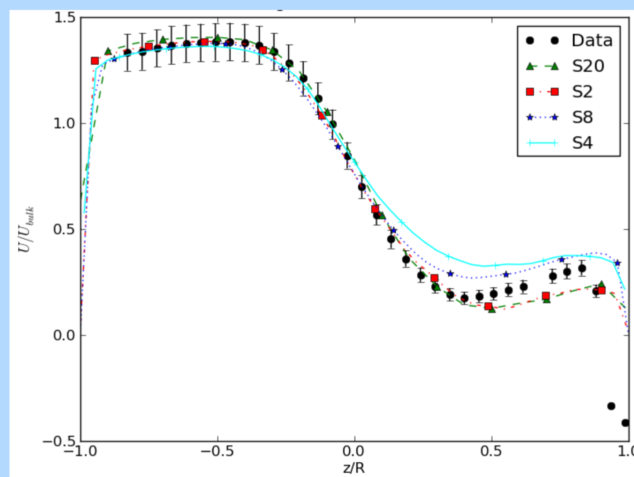






Time-averaged U
at 1.6D
downstream
in horizontal plane

Best results obtained
using LES
turbulence model

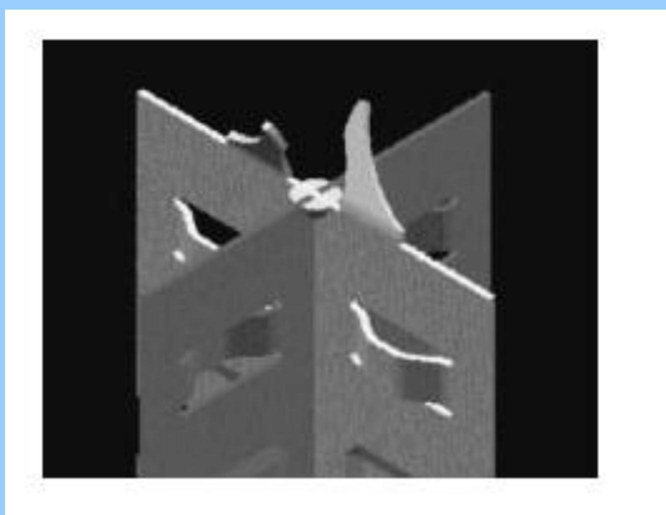


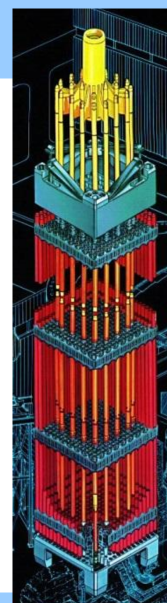
Time-averaged U
at 1.6D
downstream
in vertical plane

Illustration of CFD Capability (Nuclear)

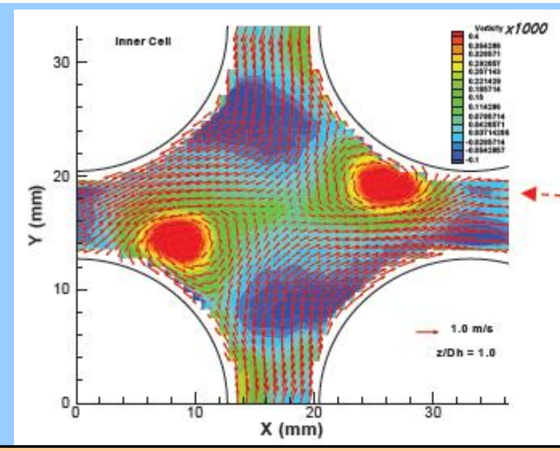
Fuel Rod Spacers

CFD provides an efficient engineering tool to aid the design of fuel rod spacers (enhanced heat transfer – higher power).



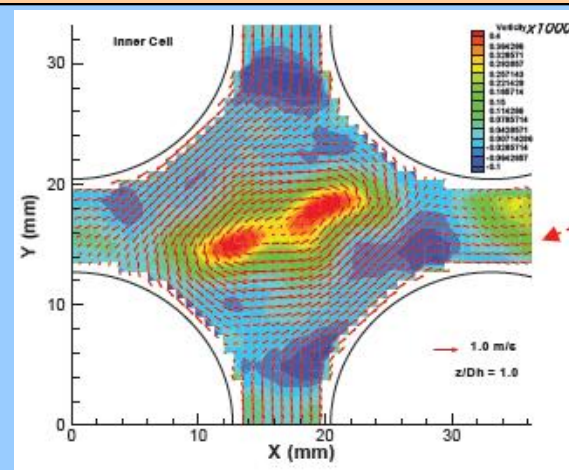


Spacers are often of very intricate design to promote "flow mixing" and improve fuel rod cooling.



Split-type spacer
$L/D_h = 1$

Vorticity Concentrations

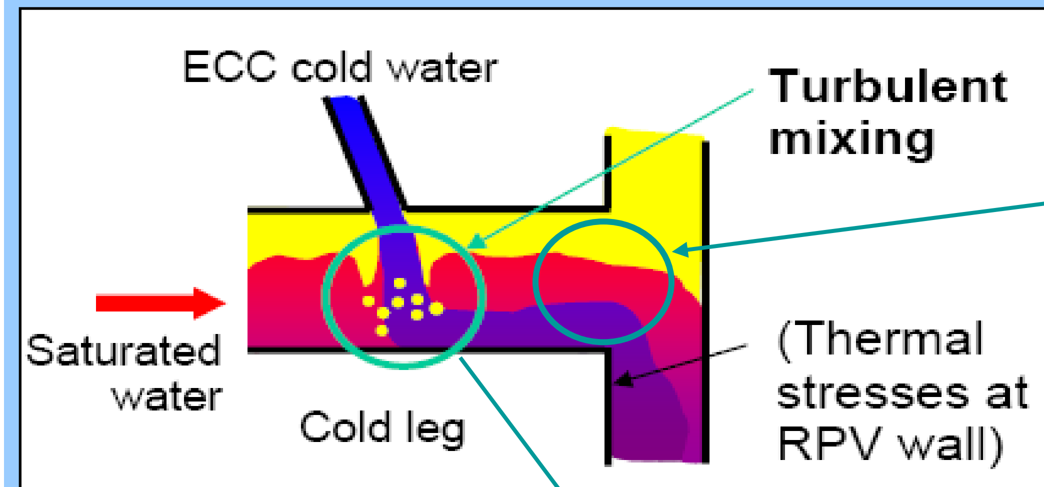


Swirl-type spacer
$L/D_h = 1$

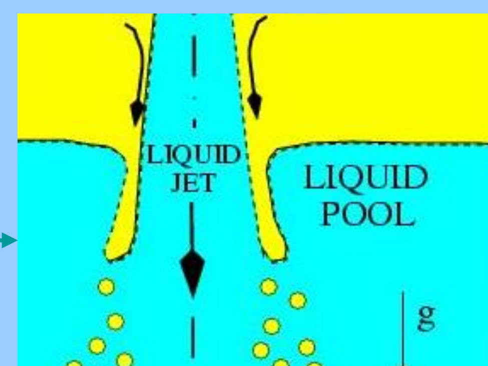
The Use of CFD in the Nuclear Industry

Beginnings of two-phase CFD modelling for **Pressurized Thermal Shock (PTS)**

Following SB-LOCA, cold-legs can be become partially filled with hot water. Cold water (ECC) injection could produce high stresses in the RPV if there is insufficient mixing



Free-Surface Flow
Thermal Stratification
Mixing in Shear Layers



Idealised physical situation

Illustrative Example: Single-Phase PTS Event

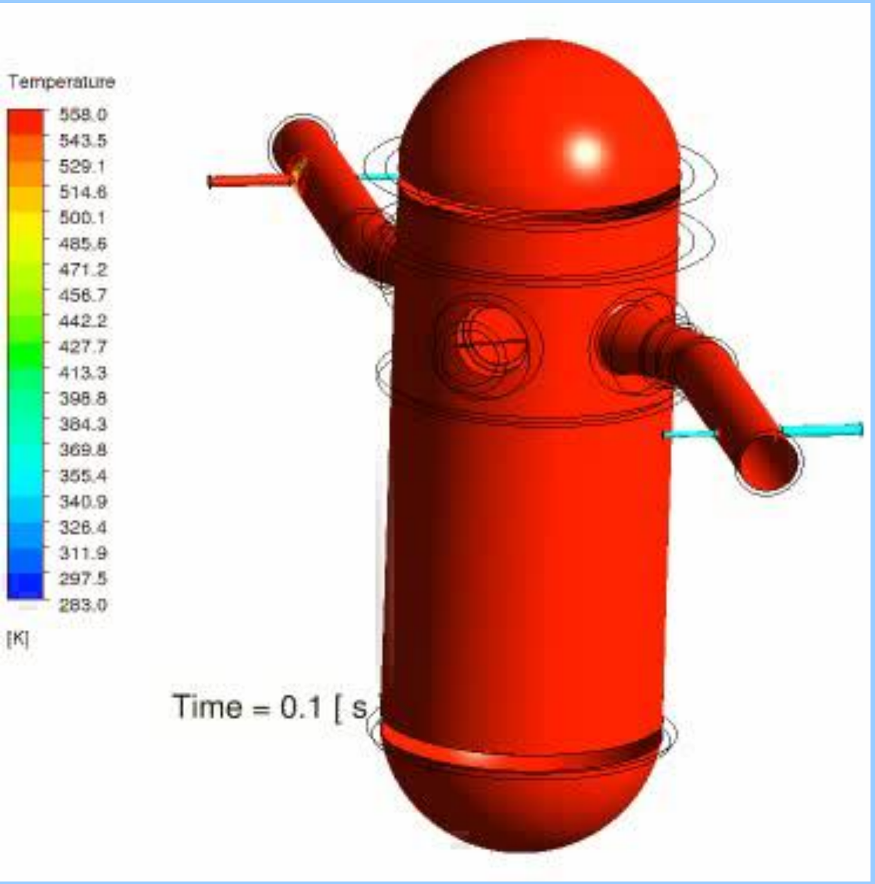
CFD simulation of Emergency Core Cooling (ECC) injection in a typical two-loop PWR following a postulated SB-LOCA.

In this design, cold-leg injection occurs in a horizontal injection mode.

The analysis here is based on boundary conditions obtained from a previous Relap5 system simulation for a break in the hot-leg of area 70 cm^2.

The CFD simulation runs for 100s following initiation of ECC injection.

In this calculation, 4M cells were used for the fluid domain and 0.7M for the RPV wall structure.



Total run-time ~ 800 hrs (5 weeks) on 32 processors.

Material provided by M. Sharabi, PSI

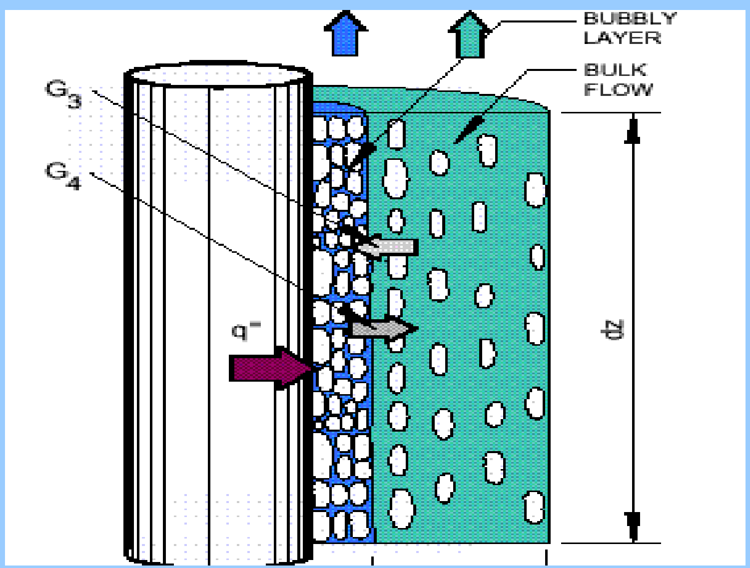
The Use of CFD in the Nuclear Industry

Beginnings of two-phase CFD modelling for **Critical Heat Flux (CHF)**

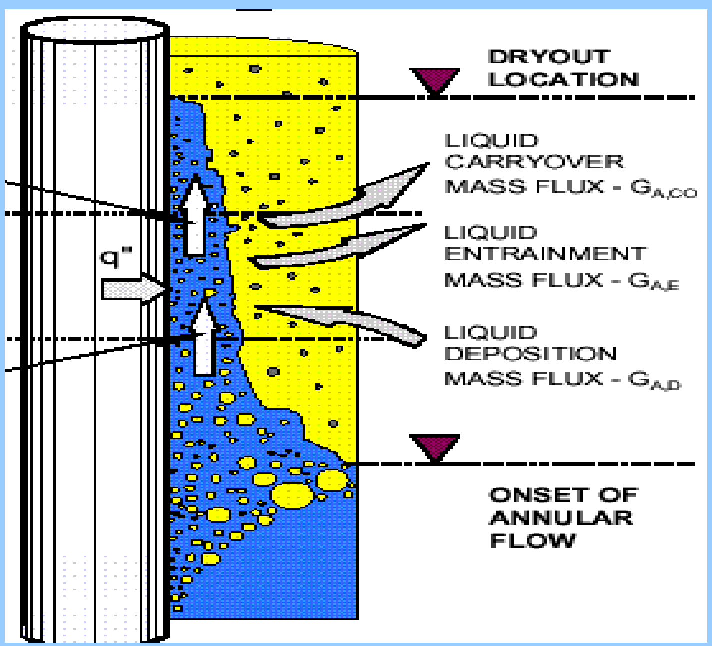
Surface temperatures of fuel rods can increase dramatically and even burn through if liquid contact with the surface is lost

Dry-out (high steam quality)

DNB (low steam quality)



Can track bubble growth/coalescence using CFD



Can track liquid film using CFD

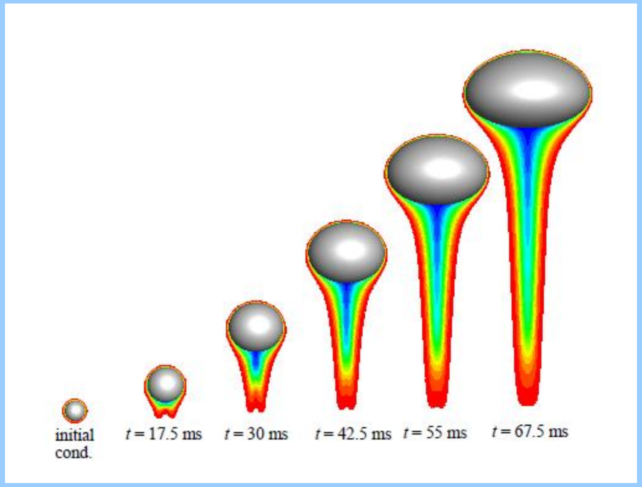
The Use of CFD in the Nuclear Industry

Pool Boiling Modelling

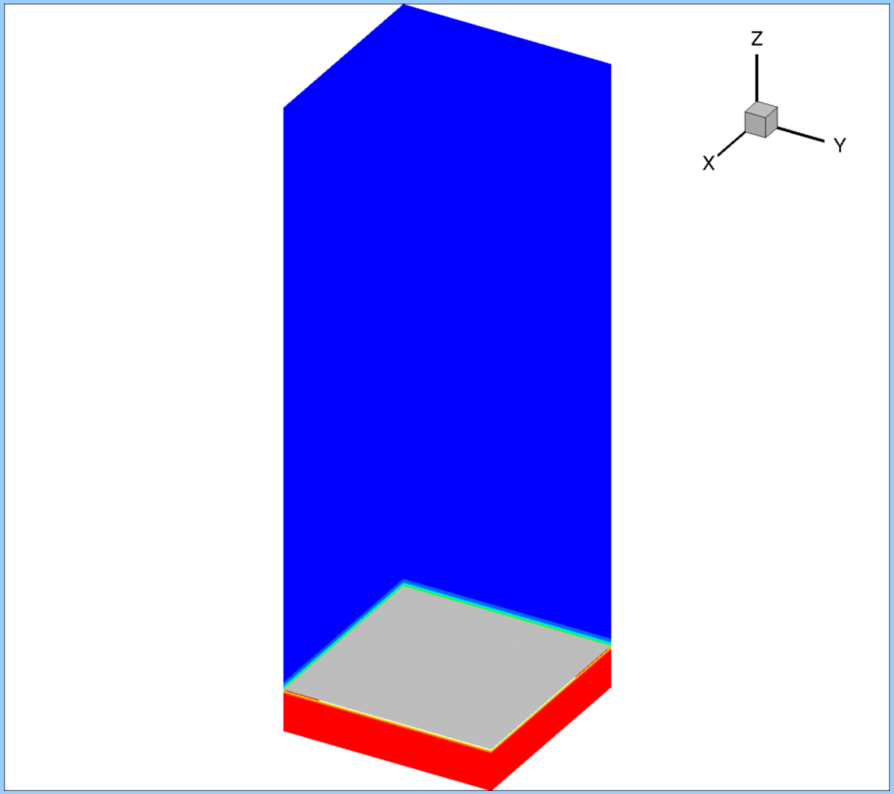
The phase indicator:
$\phi = 1$ in the liquid,
$\phi = 0$ in the vapour

The sharp transition at the liquid/vapour interface can be followed using a phase-field model within an existing CFD code.

Fundamental studies for single bubble growth…



…are developed into multi-bubble configurations for the testing of bubble break-up and coalescence.



Material provided by A. Badillo, PSI

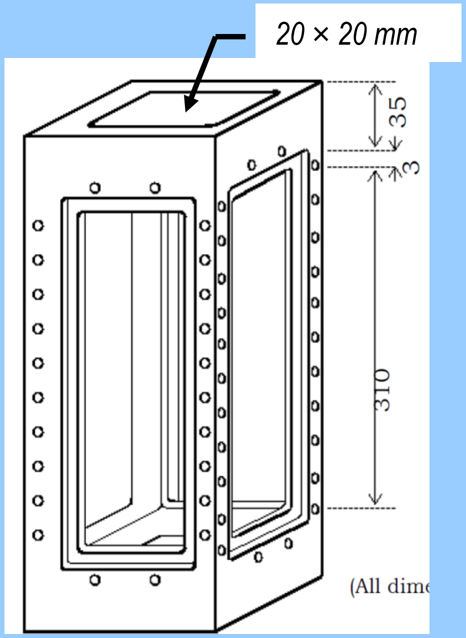
The Use of CFD in the Nuclear Industry

Convective Boiling Modelling

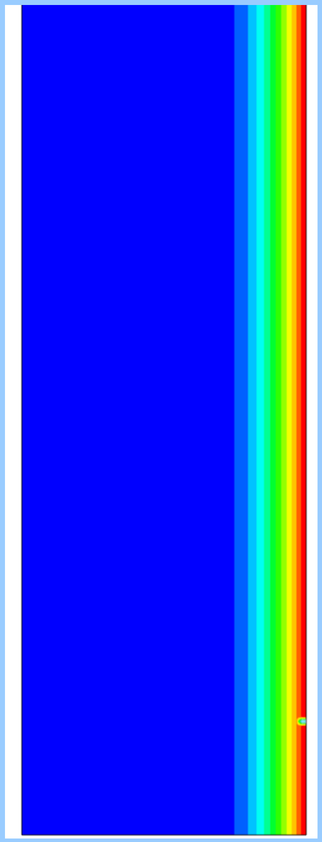
Fundamental studies for single bubble growth…

The CIP-CSL2 interface tracking method, with surface sharpening incorporated into the in-house CFD code: PSI-Boil.

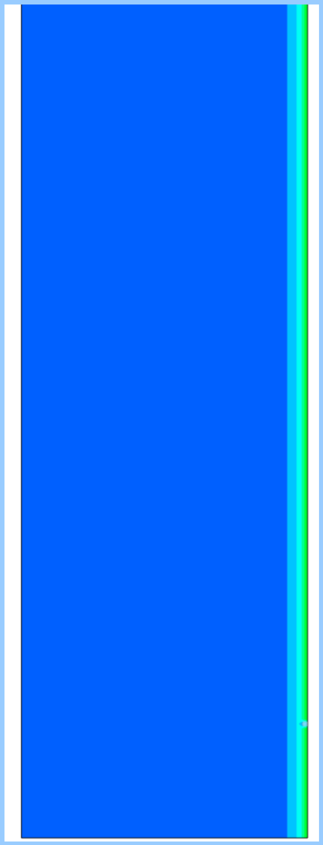
Comparisons against data of Dhir, UCLA



U = 0.077 *m/s*



U = 0.15 *m/s*



Material provided by Y. Sato, PSI

Summary of CFD Capabilities

CFD is a well-established numerical tool in a multitude of diverse engineering disciplines.

All major CFD codes have in-built links to industrial-standard CAD/CAM packages to accelerate the mesh-generation process, state-of-the-art solvers for running on parallel-architecture machines, sophisticated modules for post-processing of data (including the use of animations), and automatic links to FEM software packages for performing the associated stress analysis (and now there are corporate links between CFD and FEM).

It is unthinkable that nuclear engineering will remain outside of this technology advance. However, public perception of safety in regard to nuclear power is more highly charged than in other areas, and great care must be taken to ensure that results obtained using new methods can be trusted.

Proper user guidelines on how to perform reliable CFD simulations have been formulated.

Demonstration of the reliability of sample calculations in terms of validated cases has been established for single-phase applications .

Advances have been made in the application of two-phase CFD, though this remains an area of active research, and needs further development and validation.

Work of the OECD Writing Groups on CFD 2003 → 2007

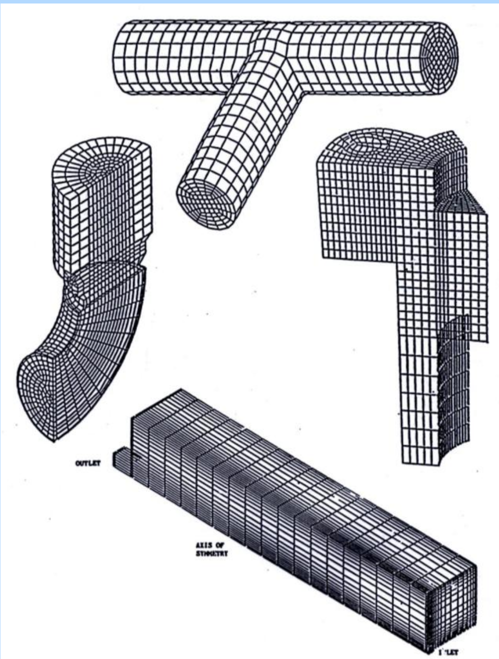
CFD does not aspire to replace system codes like RELAP5, TRACE, CATHARE and ATHLET, but to complement them in certain situations which are strongly 3D in nature.

Always in safety analysis, care must be taken to evaluate uncertainties to ultimately give margins of safety.

OUTLINE OF SECOND PART OF TALK

- What can CFD do?
- How to Run a CFD Code: Best Practice Guidelines
- How to Run a CFD Code: Sources of Error
- Verification and Validation Procedures
- Role of OECD/NEA Writing Groups
- New IAEA Initiative in CFD
- Summary

What can CFD do?
Discretization

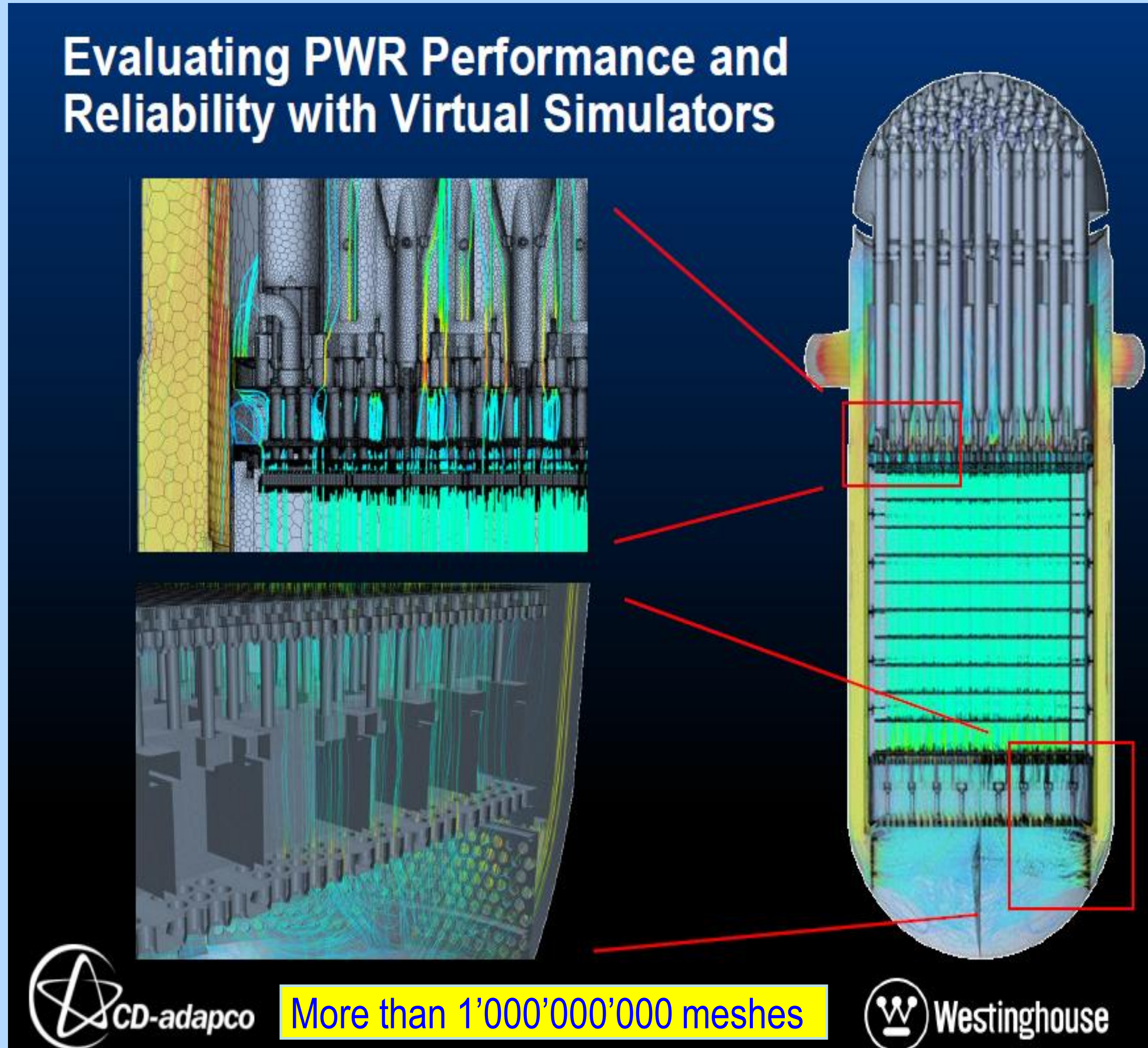


Complex shapes can be built up:

3-D geometry is exactly represented.

The potential for realism is LARGE

Question: how much machine power is available for the simulation?



Origin of OECD Writing Groups on CFD

Joint OECD/NEA — IAEA Sponsored Meetings:

Exploratory Meeting of Experts to Define an Action Plan on the Application of Computational Fluid Dynamics (CFD) Codes to Nuclear Reactor Safety Problems, Aix-en-Provence, 15-16 May, 2002.

Use of Computational Fluid Dynamics (CFD) Codes for Safety Analysis of Reactor Systems including Containment, Pisa, 11-14 November, 2002.

Action Plan: Set Up 3 Writing Groups under the sponsorship of OECD/NEA/WGAMA

WG1: Chairman J. H. Mahaffy (PSU)
Provide a set of guidelines for the application of CFD to NRS problems
(Concluded: December 2006. Document: NEA/CSNI/R(2007)5)

WG2: Chairman B. L. Smith (PSI)
Evaluate the existing CFD assessment basis, and identify gaps that need to be filled
(Concluded: December 2007. Document: NEA/CSNI/R(2007)13)

WG3: Chairman D. Bestion (CEA)
Summarise the extensions needed to CFD codes for two-phase NRS problems
(Concluded: December 2009. Document NEA/CSNI/R(2010)2)

WGAMA: Working Group on the Analysis and Management of Accidents

Overall Strategy

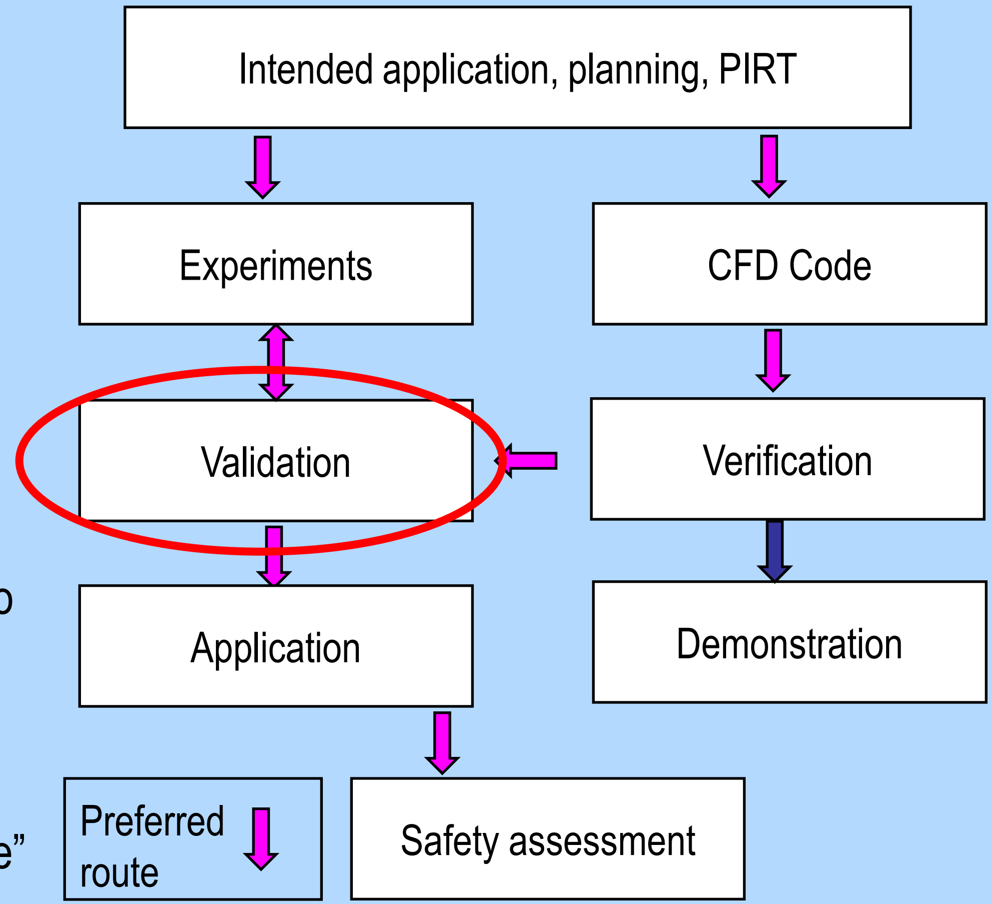
Computer simulation is much more than generating input data, running a calculation, and plotting results.

In a nuclear reactor safety assessment, for which trusted results are essential, these activities do not even occupy the majority of the staff time expended.

A set of well-defined procedural steps have to be followed, starting with a clear definition of what is to be expected from the study.

This is commonly defined in terms of a PIRT: "Phenomena Identification and Ranking Table"

And ends with the safety assessment itself.



Note that without the validation step (comparison of numerical predictions against measured data) only a <u>demonstration</u> of code capability can be made.

Best Practice Guidelines

Quality Assurance

The verification procedure will give some assurance against the code developer leaving errors in the code that can sometimes be very difficult to detect otherwise.

The software vendors will have followed and documented a V&V procedure to ensure that the models built into the code are error free and represent physical reality (if used properly).

However, it is extremely important to have some quality assurance (QA) procedure in place for a CFD project, part of which is a review of existing V&V procedures relevant to all the models being used.

Also, analysts must always be aware of their own ability to introduce errors into their input data.

Rigorous adherence to international standards for a QA programme is generally not possible —it is just too time consuming.

Nonetheless, the four primary components of a QA procedure should be followed:

- documentation of the work;
- development procedures for input models and the code;
- testing;
- review of all the work done.

The WG1 document (NEA/CSNI/R(2007)5) contains extended discussion of all these QA aspects.

Best Practice Guidelines

Adhering to a set of step-by-step instructions in performing a CFD simulation will greatly increase quality and trust in the numerical predictions.

The following steps were defined by WG1, building on experience from other areas: namely, ERCOFTAC, ECORA 5th EU FWP, MARNET, AIAA.

1. Initial Preparation

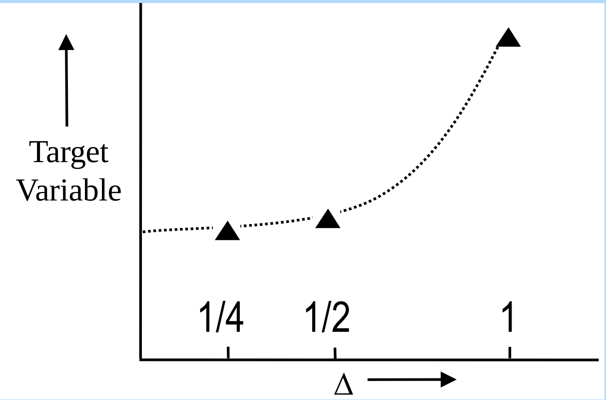
2. Geometry Preparation

3. Selection of Physical Models

4. Grid Generation

5. Numerical Method

6. Sources of Error



- Follow quality assurance procedures to limit and locate user errors.
- Check for round-off errors. Generally, try to run on a 64-bit machine.
- Check for errors associated with selection of iteration convergence criteria.
- Check for errors associated with discretization of space and time: demonstrate mesh/time-step independence.

How to Obtain Good Results?

Eliminate, or at least minimize, errors

Sources of error

User errors	— Control by Quality Assurance (QA) of input data — Perform basic consistency checks: mass, momentum and energy conservation — Check on convergence criteria — Check grid quality (distortion, skewness, etc.)
Programming errors (i.e. bugs in the code)	— Control by **Verification** Procedures
Modelling errors	— Control by **Validation** Procedures
Numerical errors	— Control by **Best Practice Guidelines**
Machine (round-off) errors	— Control by choosing correct machine precision

User errors probably account for more than 80% of all errors made in CFD calculations!

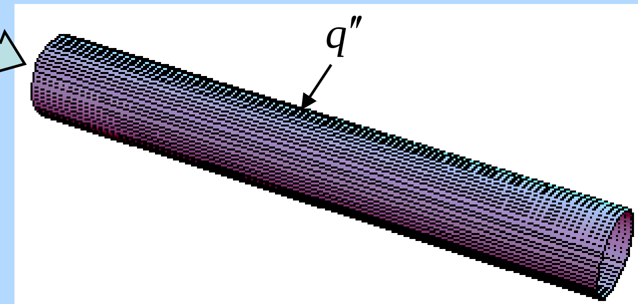
Verification

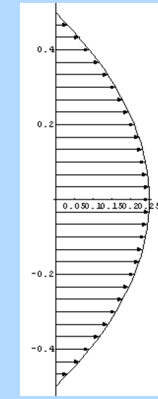
1. Laminar Viscous Flow through a Circular Pipe

For fully-developed flow, the axisymmetric solution gives a parabolic velocity profile:

$$\frac{u}{U} = 1 - \frac{r^2}{R^2}$$

where U is the centerline velocity and R is the pipe radius.





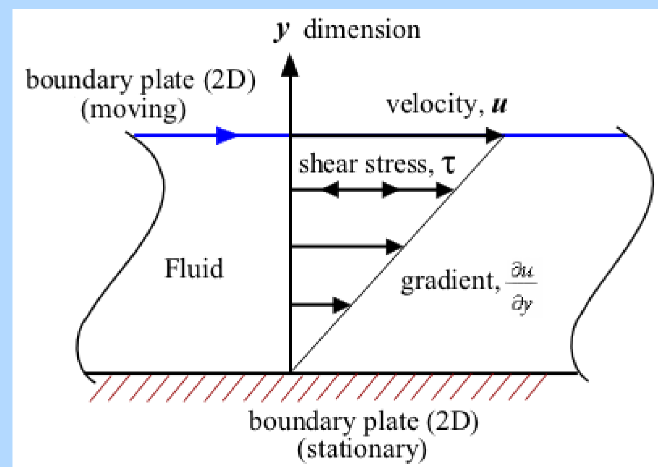
In the case of heat transfer due to a constant heat flux applied to the external surface, the temperature profile is quartic:

$$T(r) = T_w - \frac{Rq''}{4\lambda}\left(1 - \frac{r^2}{R^2}\right)\left(3 - \frac{r^2}{R^2}\right)$$

2. Plane Couette Flow

This is viscous, laminar flow between a fixed and a moving boundary. Again for fully developed flow, the velocity profile is linear in terms of height:

$$\frac{u}{U} = y$$



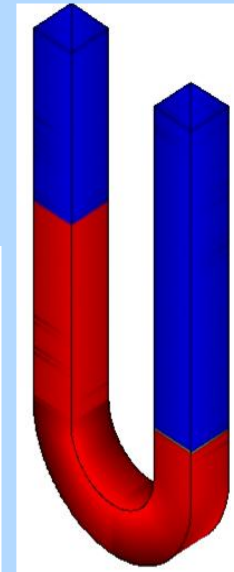
Some temperature profiles can also be derived for simple heating arrangements.

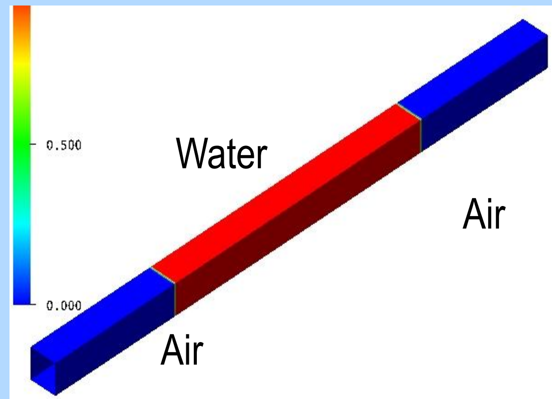
In all cases, code predictions are compared against exact results, and bugs traced, as necessary

Verification

3: Manometer Oscillation

In the real case, the motion is 2-D (or even 3-D) due to the different flow paths around the U-bend, but if the problem is considered 1-D, there is an analytical solution for laminar, inviscid flow conditions.

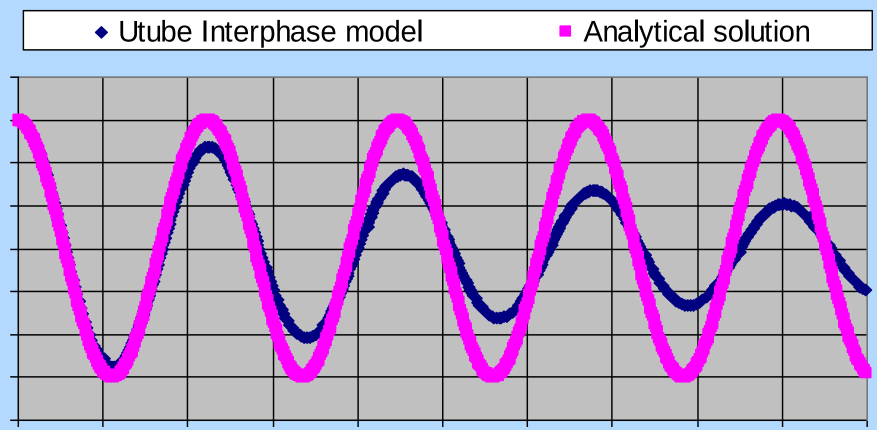




It is possible to ensure 1-D motion by bending the tube straight, and compensating for the U-bend by appropriately modifying gravity:

$$g = g' \cos[\frac{\pi}{5}(z - 7.5)]$$

The two situations are then mathematically equivalent.



Some complications are introduced by the presence of the two water/air interfaces. In the case shown here, there is clearly too much numerical diffusion: the amplitude is decaying, though the period is calculated accurately, with very little phase shift.

Validation: Work of the OECD WG2 Writing Group

Objectives

- Provide a classification of NRS problems requiring CFD analysis;
- Identify and catalogue existing CFD assessment bases, both nuclear and non-nuclear;
- Identify any gaps in the CFD assessment bases;

These items are documented in the final written report of the WG2 group: NEA/CSNI/R(2007)13

An updated version of this document is due to appear during 2013.

Follow-up activities (described below)

NRS problems for which CFD analysis brings real benefits (1)

	NRS problem	System classification	Incident classification	Single- or multi-phase
1	Erosion, corrosion and deposition	Core, primary and secondary circuits	Operational	Single/Multi
2	Core instability in BWRs	Core	Operational	Multi
3	Transition boiling in BWR/determination of MCPR	Core	Operational	Multi
4	Recriticality in BWRs	Core	BDBA	Multi
5	Reflooding	Core	DBA	Multi
6	Lower plenum debris coolability/melt distribution	Core	BDBA	Multi
7	Boron dilution	Primary circuit	DBA	Single
8	Mixing: stratification/hot-leg heterogeneities	Primary circuit	Operational	Single/Multi
9	Heterogeneous flow distribution (e.g. in SG inlet plenum causing vibrations, HDR expts., etc.)	Primary circuit	Operational	Single
10	BWR/ABWR lower plenum flow	Primary circuit	Operational	Single/Multi
11	Waterhammer condensation	Primary circuit	Operational	Multi

The safety items are grouped into issues concerning the core, primary circuit and containment

NRS problems for which CFD analysis brings real benefits (2)

	NRS problem	System classification	Incident classification	Single- or multi-phase
12	PTS (pressurised thermal shock)	Primary circuit	DBA	Single/Multi
13	Pipe break – in-vessel mechanical load	Primary circuit	DBA	Multi
14	Induced break	Primary circuit	DBA	Single
15	Thermal fatigue (e.g. T-junction)	Primary circuit	Operational	Single
16	Hydrogen distribution	Containment	BDBA	Single/Multi
17	Chemical reactions/combustion/detonation	Containment	BDBA	Single/Multi
18	Aerosol deposition/atmospheric transport (source term)	Containment	BDBA	Multi
19	Direct-contact condensation	Containment/ Primary circuit	DBA	Multi
20	Bubble dynamics in suppression pools	Containment	DBA	Multi
21	Behaviour of gas/liquid surfaces	Containment/ Primary circuit	Operational	Multi
22	Special considerations for advanced (including Gas-Cooled) reactors	Containment/ Primary circuit	DBA/BDBA	Single/Multi

Illustrative Example: Boron Dilution

What is the issue and what is the relevance to NRS?

Boron concentration aims at controlling the power and subcriticality for shutdown conditions in a PWR. Mechanisms supposed to lead to boron-diluted water are known (consequence of small break, SG leakage, etc.) The safety problem concerns the possible transport to the core of a diluted slug of water, and the related power excursion.

Why is CFD Needed?

The entire phenomenon requires modelling at two steps: (i) knowledge of the concentration of boron at the core entrance, and (ii) thermal-hydraulics/ neutronics calculations for the core region. The first step (covered by CFD) thus provides the initial and boundary conditions for the second. Main CFD inputs are: (i) pump start-up, or (ii) natural circulation after water inventory restoration. Relevant part of the reactor for flow modelling concern at least the downcomer, the lower plenum, and possibly the pipework related to the transportation of the slug.

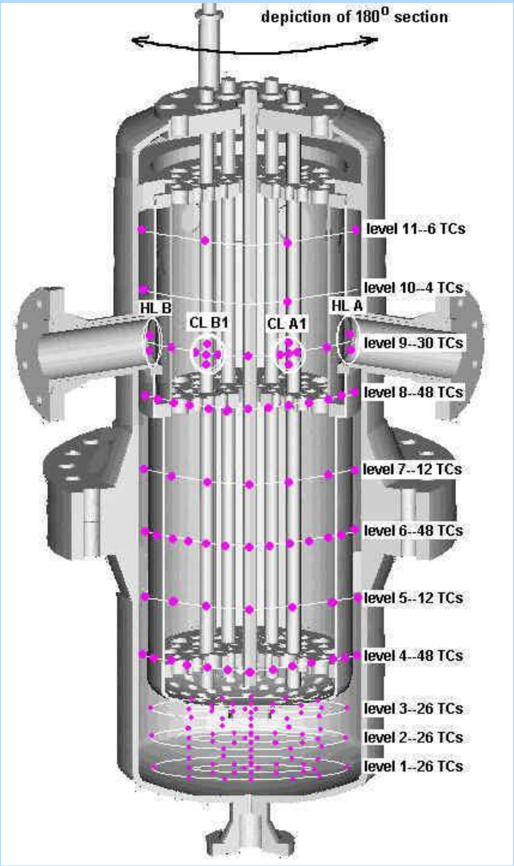
Example of what has been done

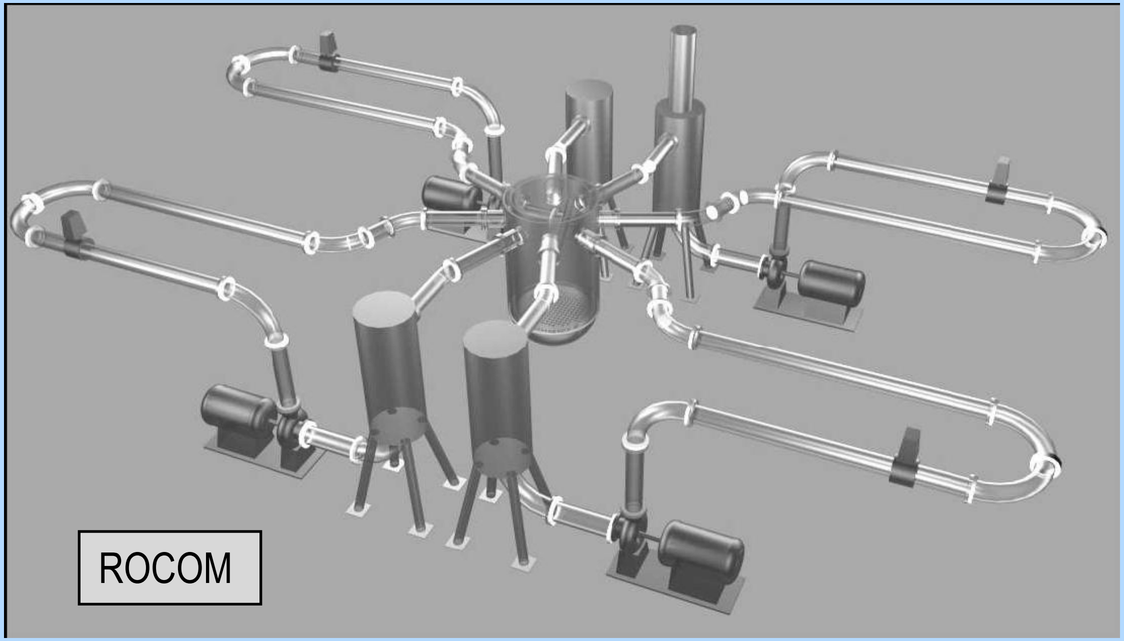
There are a number of experiments and simulations: e.g. University of Maryland (basis of ISP-43), ROCOM (HFZR), Vattenfall 1:5 scale tests in Sweden. Also, boron dilution and in-vessel mixing have been the subject of the EU-funded programmes EUBORA and FLOWMIX-R.

Existing Databases (Nuclear)

Boron Dilution

ROCOM Test Facility (Germany)
OKB GIDROPRESS (Russia)
VATTENFALL (Sweden)





University of Maryland Tests (US)

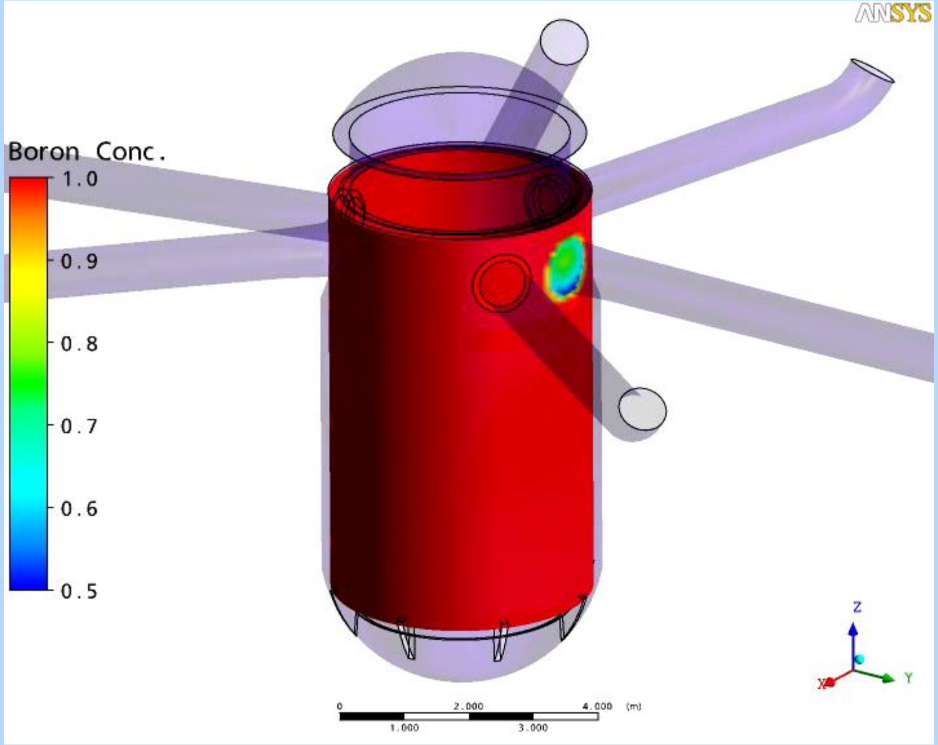
Basis of OECD/NEA ISP-43

Test data released within the EU
5th FWP FLOWMIX-R

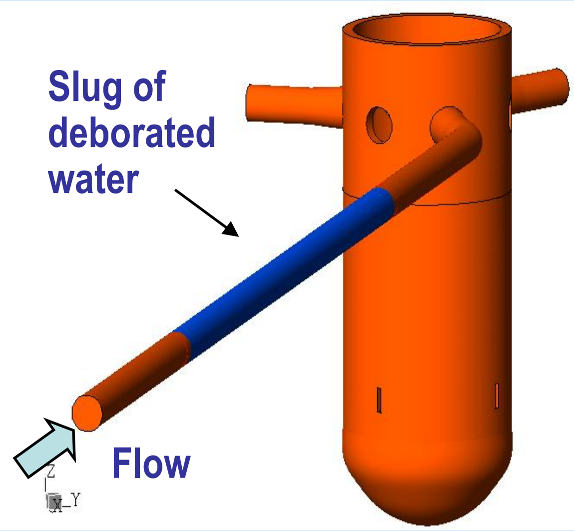
What has been done using CFD?

Sample Calculation

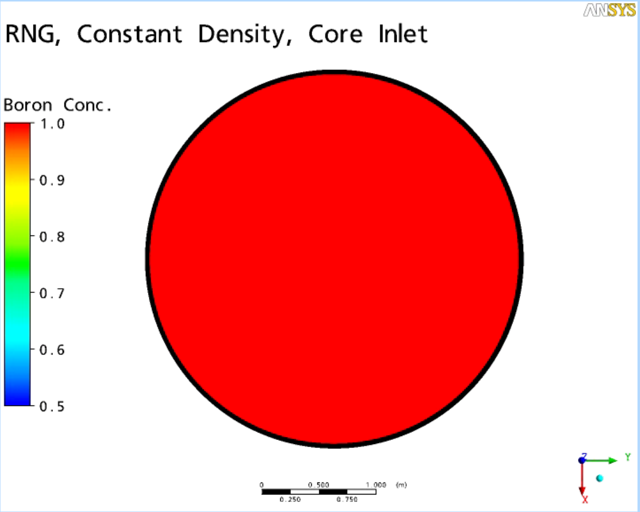
Pump start-up transient for a 3-loop PWR



Development of downcomer mixing



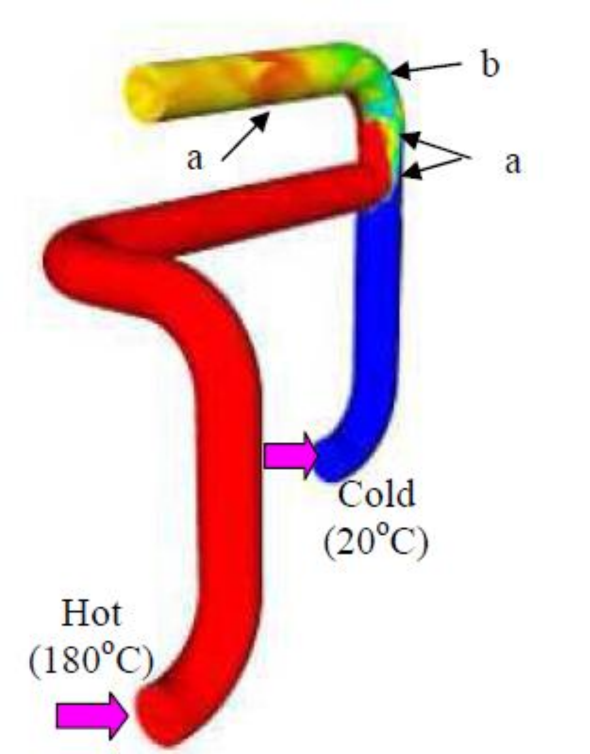
CFD model



Concentration at core inlet

Illustrative Example: Thermal Fatigue

What is the issue and what is the relevance to NRS?
Fluid dynamic mixing of coolant streams is a common phenomenon in reactor circuits. An example is the thermal striping phenomena in piping mixing tees where hot and cold streams join, which can result in large (~ 160°C) temperature fluctuations near the pipe walls. The associated wall temperature fluctuations can cause cyclical thermal stresses and perhaps fatigue cracking.



Why is CFD Needed?
The mixing processes are 3-D, and depend on the associated turbulence intensities and scales. The geometric details (flow obstacles, changes in flow direction, etc.) themselves have a strong influence ont he levels of turbulence. CFD is needed to model this.

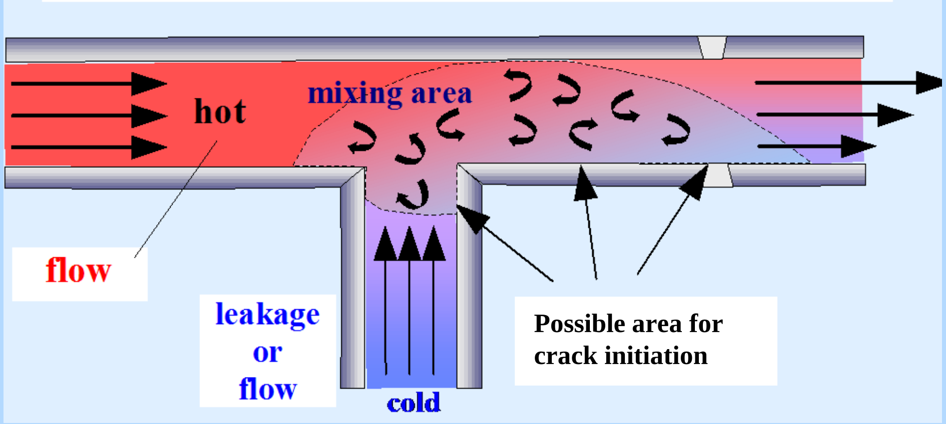
What has been done to date (an example is given here as illustration)
Schematic of part of the piping geometry in the Civaux-1 RHR system where both (a) circumferential and (b) longitudinal cracks appeared after only 1500 hrs of plant operation. The longitudinal crack was 180 mm long on the exterior of the pipe elbow.
S. Chapuliot et al., Nucl. Eng. Des. **235**, 575–596 (2005)

RHR: Residual Heat Removal

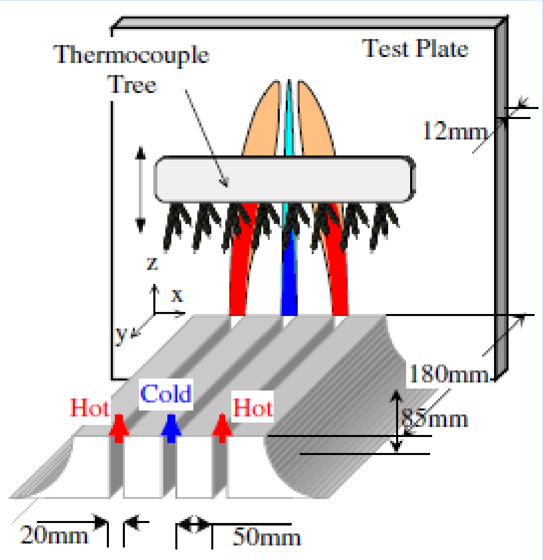
Existing Databases (Nuclear)

Thermal Fatigue

Most studied configuration: a straight-through main pipe and inlet branch pipe.



Can also occur as a result of thermal striping caused by alternate hot/cold jets.



Thermal striping experiment at O-arai Engineering Center, Japan

Data Bases (T-Junctions)

SPG	(Germany)
FATHERINO	(France)
PSI	(Switzerland)
VATTENFALL	(Sweden)
WATLON	(Japan)

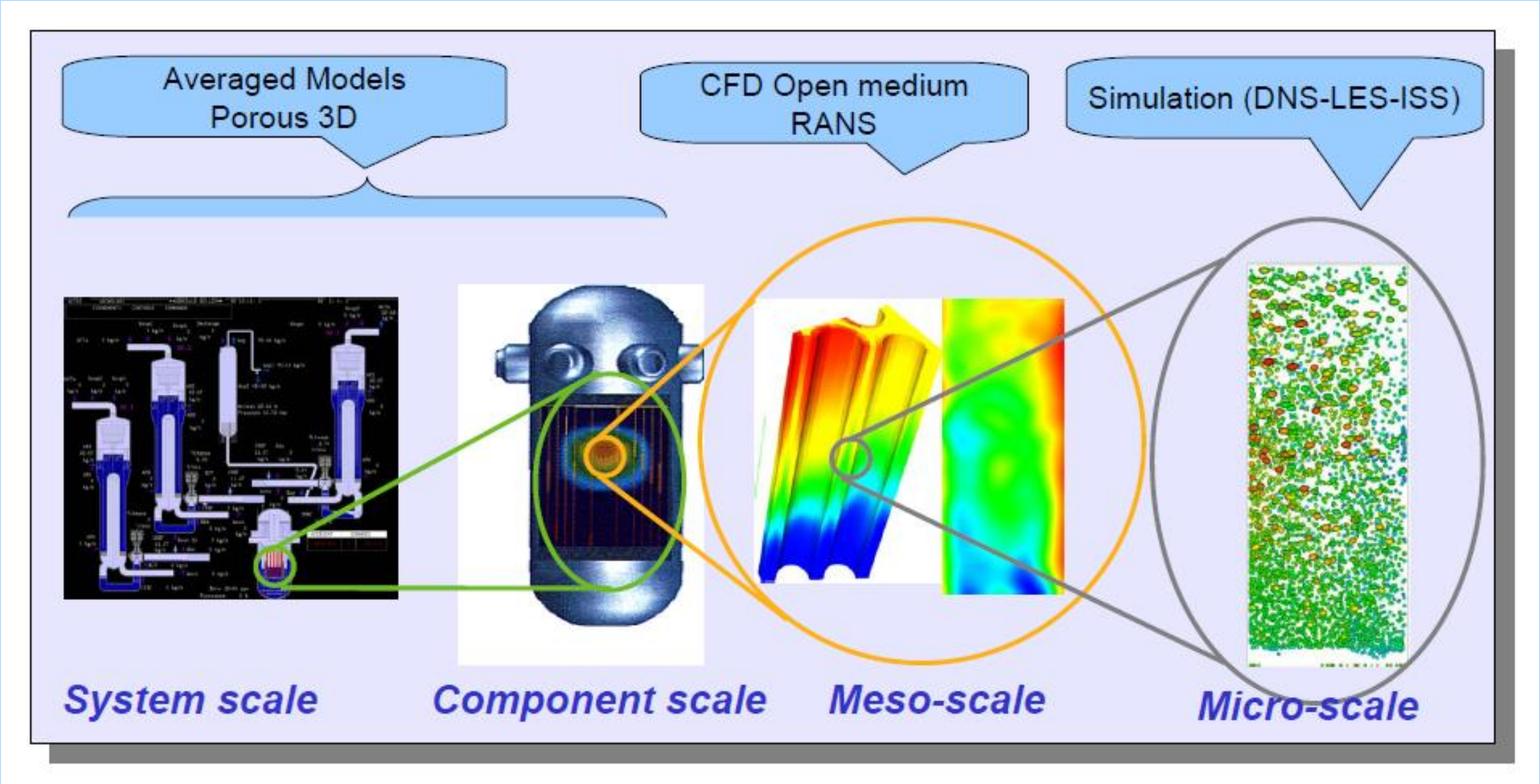
Most data are only available under agreement. However, the data from several SPG tests were released to partners in the EU 5th FWP THERFAT, and one of the Vattenfall tests became the basis of an OECD/NEA benchmark exercise.

Extension to Two-Phase Flow Applications

ISS: Interface and Sub-grid Scales

The Multi-Scale Modelling Approach

The phenomena of importance occur on a multitude of scales, and different approaches are needed.



Almost invariably, averaging or filtering techniques are employed to handle interfaces and turbulence.

Computing Power Limitations (1)

Parkinson's Law

Original version: "Work expands to fill the time available", was first articulated by Prof. C. Northcote Parkinson, and is based on a study of the British Civil Service, whose number of employees always seems to increase.

From this have arisen a number of variants.
Parkinson's Law of Data: "Data expands to fill the space available for storage".
Parkinson's Law of Bandwidth Absorption: "Network traffic expands to fill the available bandwidth".

Why not one for CFD?
Parkinson's Law of CFD could read: "The number of meshes expands to fill the available machine capacity".

In NRS applications, situations requiring analysis are often of a transient nature. CFD codes are computationally demanding, both in terms of memory usage and in the number of operations. These days, CFD simulations using hundreds of millions of nodes are common in many industrial applications.

For a 3-D CFD simulation with N meshes in each coordinate direction, the total number of grid points is N^3. The time-step, though usually not CFL limited, remains, for purely practical reasons, roughly proportional to $1/N$, so the number of time steps is also proportional to N. Present-day commercial CFD codes are still based on a pressure-velocity coupling algorithm which entails the iterative solution of a large linear system of equations. Much of the CPU overhead (sometimes up to 90%) derives from this procedure. Thus, the run-time for the CFD code would scale at least according to

$$t \propto N^4$$

Computing Power Limitations (2)

Traditionally, CFD programs were written to run on a single processor in a serial manner. One way to achieve a speed-up is to divide up the program to run on a number of processors in parallel, either on a multiprocessor machine (a single computer with multiple CPUs), or on a cluster of machines accessed in parallel.

Experience shows that the scaling up of performance with the number of processors is strongly dependent on the size of the system arrays (i.e. number of meshes), as well as on the details of the computer architecture and memory hierarchy. Modern clusters have proved to give good performance for small array sizes that fit into the processor's cache. If not, performance drops off significantly.

Given an idealised linear speed-up, and the N^4 dependence of runtime on number of meshes, doubling the number of processors, and keeping total runtime the same, the number of meshes in each direction can be increased by only 19%, say from 100 to 119. Conversely, doubling the mesh density, say from 100 to 200 in each coordinate direction, again keeping total runtime constant, means that the number of processors has to be increased by a factor 16.

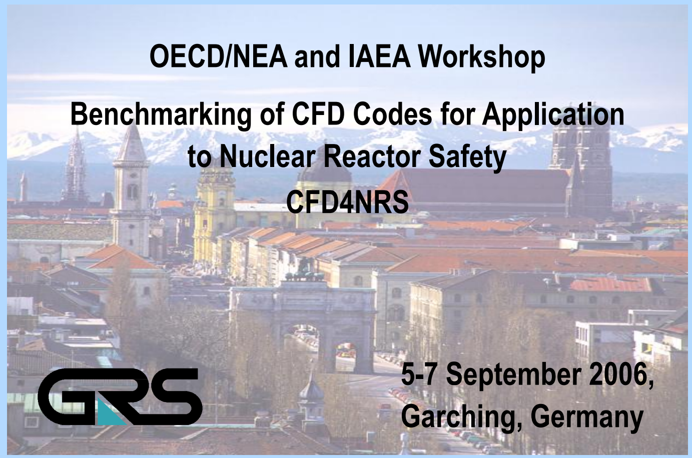
Given the above statistics, it is evident that the pursuit of quality and trust in the application of CFD to transient NRS problems, adhering strictly to the dictates of a Best Practice Guidelines philosophy of multi-mesh simulations, will stretch available computing power to the limit for many years to come.

It should also be remembered that CFD is a best-estimate tool, and for trustworthy application has to be combined with an uncertainty analysis. Due to CPU overheads, this aspect is only now starting to emerge.

Certainly, expanding efforts in reactor simulations will ensure that Parkinson's Law will prevail for CFD.

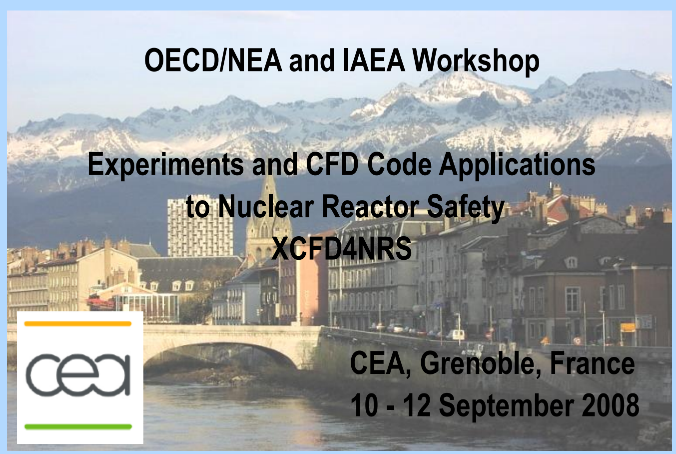
Follow-up Activity 1: CFD4NRS Workshops

A Forum for Extending the Assessment Database



Official Proceedings:
NEA/CSNI/R(2007)3
CD-ROM

Special Issue:
Nuclear Engineering and Design
238(3), 443-786 (2008)



Official Proceedings:
NEA/CSNI/R(2009)12
CD-ROM

Special Issue:
Nuclear Engineering and Design
240(9), 2075-2381 (2010)

Follow-up Activity 1: CFD4NRS Workshops

CFD4NRS-3

Official Proceedings:
NEA/CSNI/R(2011)14

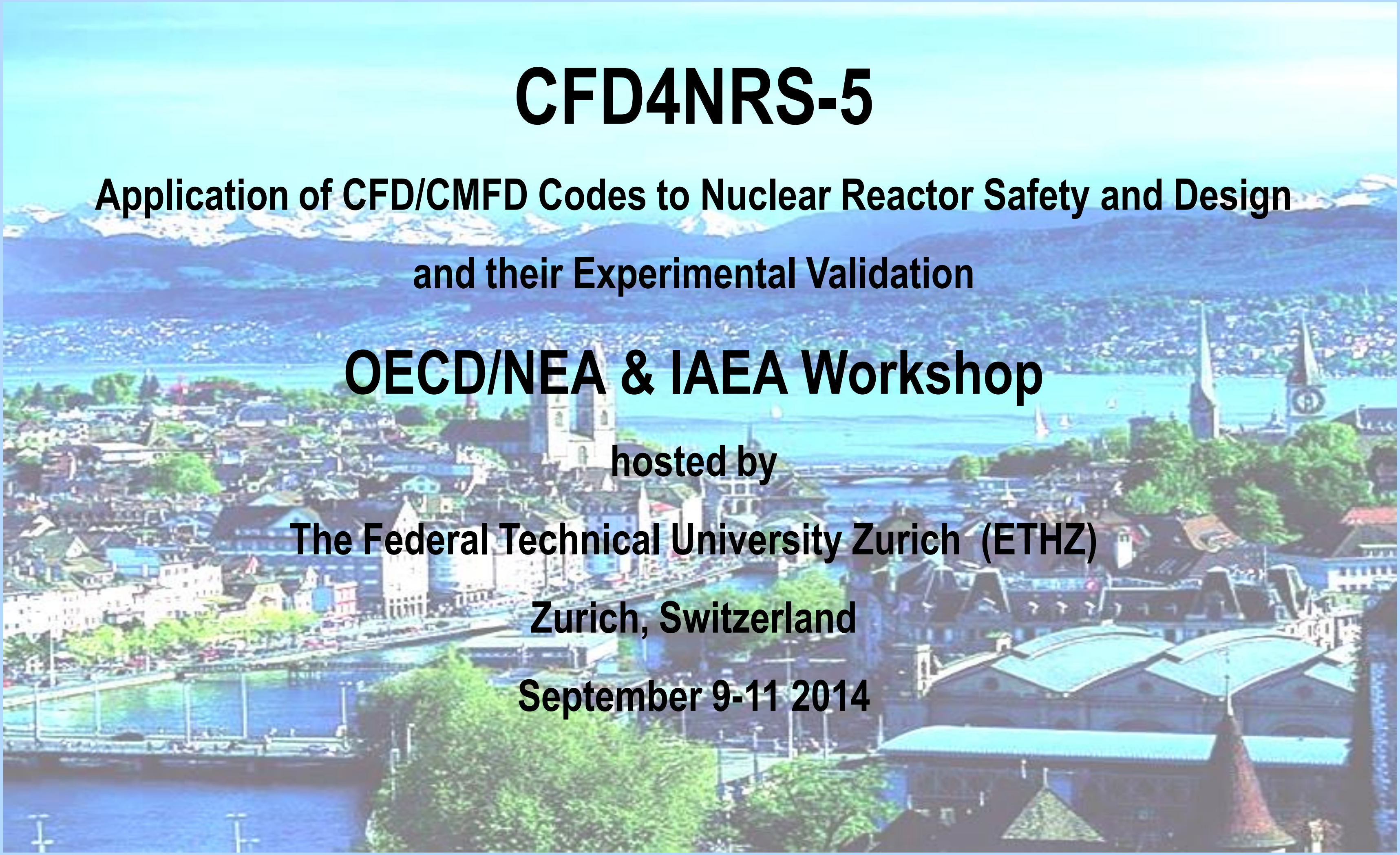
Special Issue:
Nuclear Engineering and Design
253, 1-412 (Dec. 2012)

CFD4NRS-4

Official Proceedings:
NEA/CSNI/R(2013)??

Special Issue:
Nuclear Engineering and Design
(projected 2014)

CFD4NRS-5 – Preparations are underway: first announcement sent out in Oct. 2013



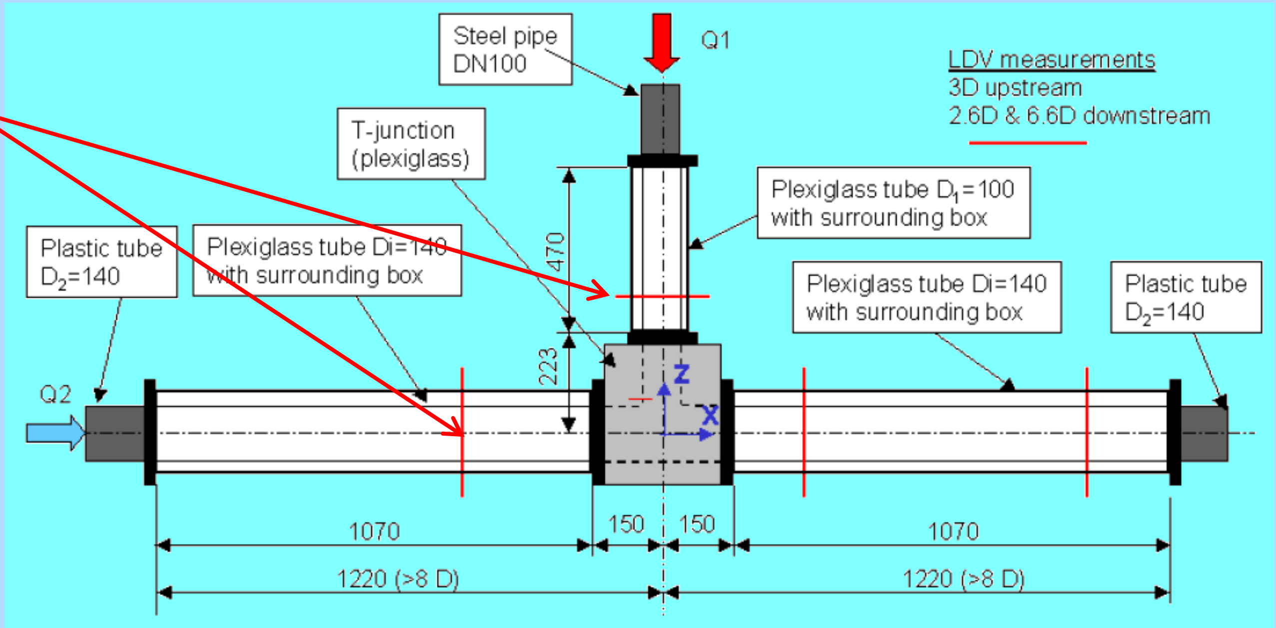
OECD – Vattenfall Benchmark Exercise

The test was carried out at the Älvkarleby Laboratory of Vattenfall R&D in November 2008.

Velocity profiles (mean and rms) measured at $3D_H$ upstream of the junction for both the main and branch pipes.

Upstream temperatures were also measured with $\Delta T = 17K$

These data were provided as boundary conditions for the CFD simulations.



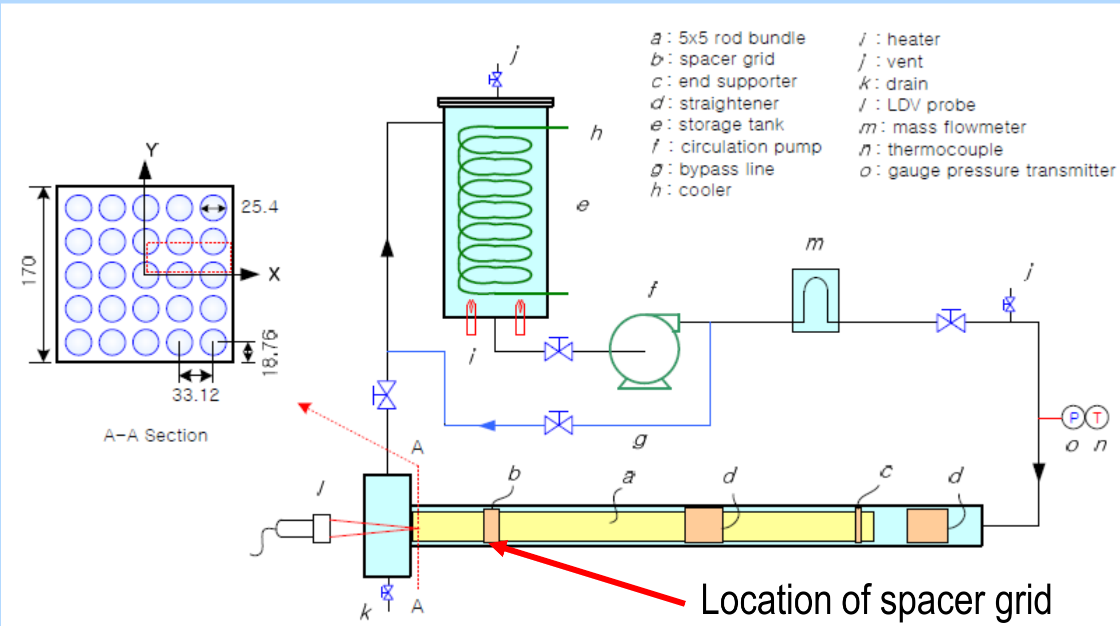
Downstream temperatures and velocities were to be calculated... …and compared with measured data once these were released.

The benchmark activity ran from May 2009 (kick-off meeting) to Dec. 2010 (29 participants)

OECD/NEA–KAERI Benchmark Exercise

Principal objective is to predict turbulence characteristics generated by a spacer grid.

Based a new experiment at the MATiS-H horizontal rod bundle test facility at KAERI.



Split-Type Spacer

Swirl-Type Spacer

Two spacers (of generic design) were studied: split-type and swirl-type.

CAD files of the spacer grid designs were made available by KAERI to aid mesh generation.

The benchmark activity ran from May 2011 (kick-off meeting) to Dec. 2012 (25 participants)

OECD – PSI Benchmark Exercise

Benchmark based on single-phase, multi-component, diabatic flow of gases in a containment volume.

Break-up of a buoyant, stratified layer by an impinging jet.

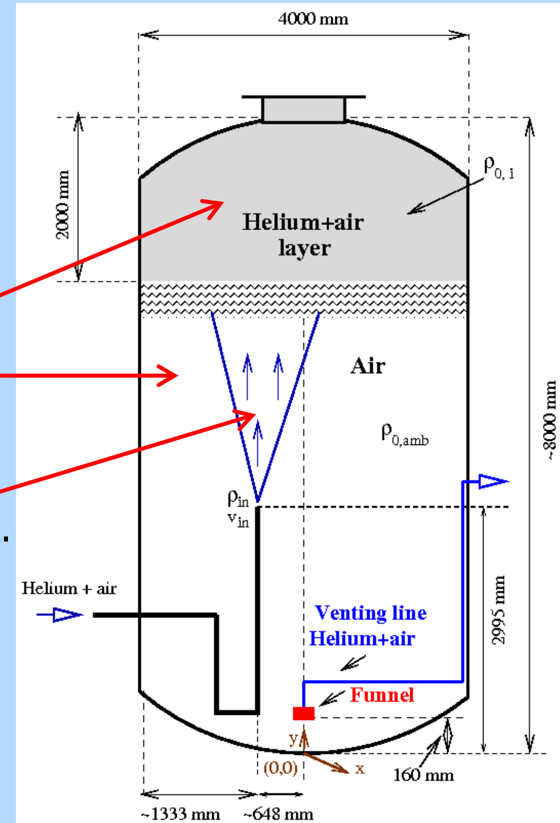
Initial conditions given in terms of He concentration in the vessel at ambient conditions at each elevation at around 20°C.

At initiation, a He-rich layer occupies the upper part of the vessel, with air beneath.

A He-air mixture at a slightly elevated temperature (up to 30°C) is injected via a vertical nozzle, placed off-centre, just below mid-height.

Participants are requested to model the subsequent erosion of the stratified layer under 'blind' modelling conditions.

CAD files of PANDA vessel and inlet line have been prepared.



A dedicated ftp site has been set up at PSI for registered participants to download the benchmark specifications, design drawings and CAD files, and eventually to upload their simulation data.

Specifications finalised Aug. 28, 2013. Deadline for submission of results: May 30, 2014

Follow-up Activity 3: Web-Based Centre

Motivation: to move WG archival documents to a Wiki-type environment for easy access and maintenance.

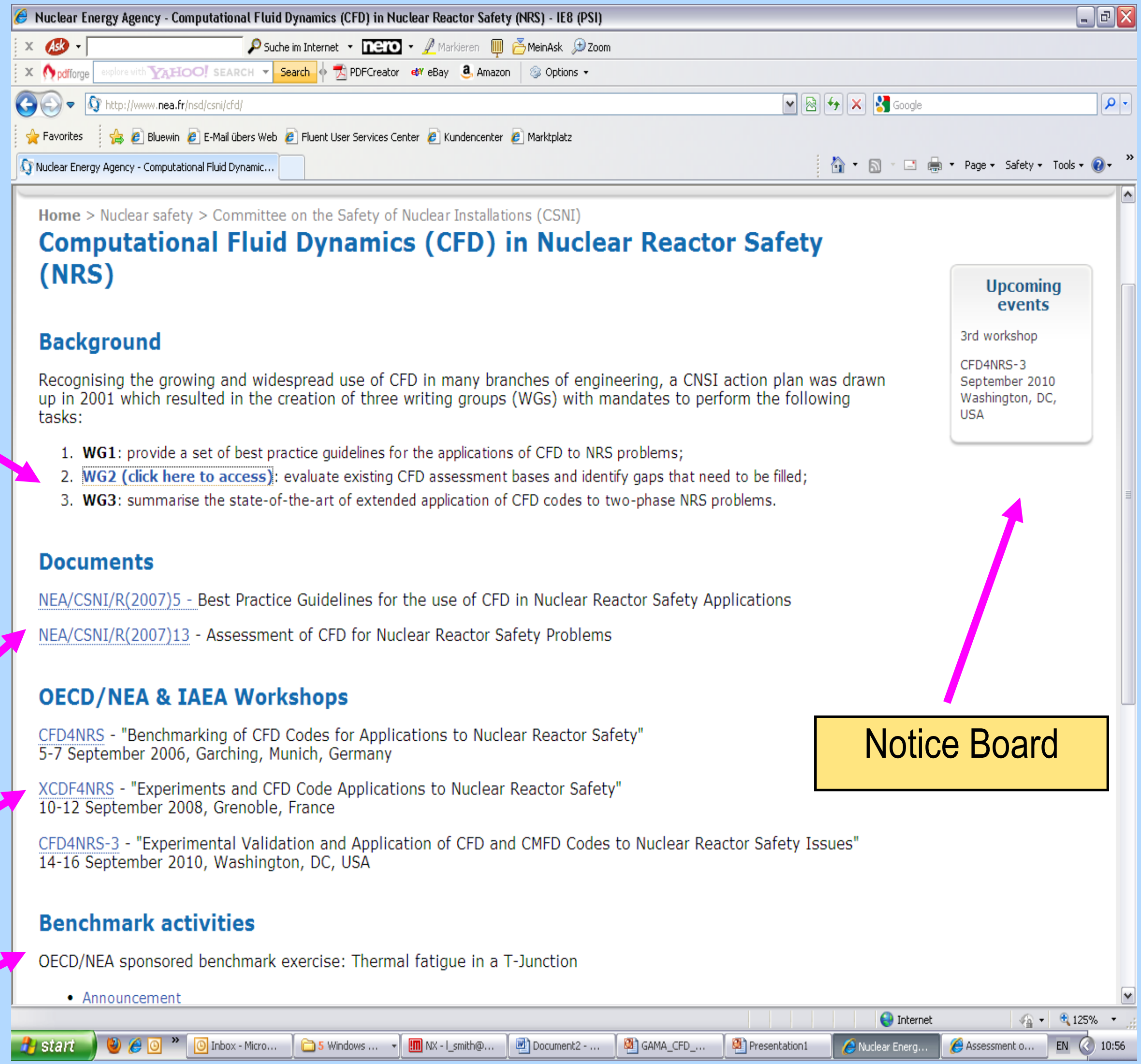
The webpage has open access from www.nea.fr

Links to the Writing Group webpages:
WG1 ready (but not yet active)
WG2 active
WG3 in construction

Links to the Writing Group CSNI reports in pdf format
WG1, WG2 (WG3 to be added)

Links to CFD4NRS workshop proceedings

Link to Benchmark Activities



Notice Board

Use of CFD in Nuclear Reactor Design

This is defined in terms of a Collaborative Research Project (CRP) of 4 years duration: 2013-2016.

Motivation:

- the use of CFD is in design work in many engineering disciplines is widespread and growing;
- CFD is now recognized as an important aspect in the design of the next generation of NPPs…
- by accelerating the design process, eliminating poor design options, avoiding the use of expensive experimental testing, and thereby making the design process more economical.

Role of the IAEA:

- Assess the capability of CFD to address specific design issues for which 3-D flows are important;
- Summarize the present state-of-the-art on the subject, and identify any shortcomings;
- Promote CFD verification and validation procedures by encouraging the release of new data;
- Provide an environment by which different organizations can communicate their own advances;
- Maintain links with regulatory authorities on the acceptance of CFD in regulatory procedures.

Participating Countries:

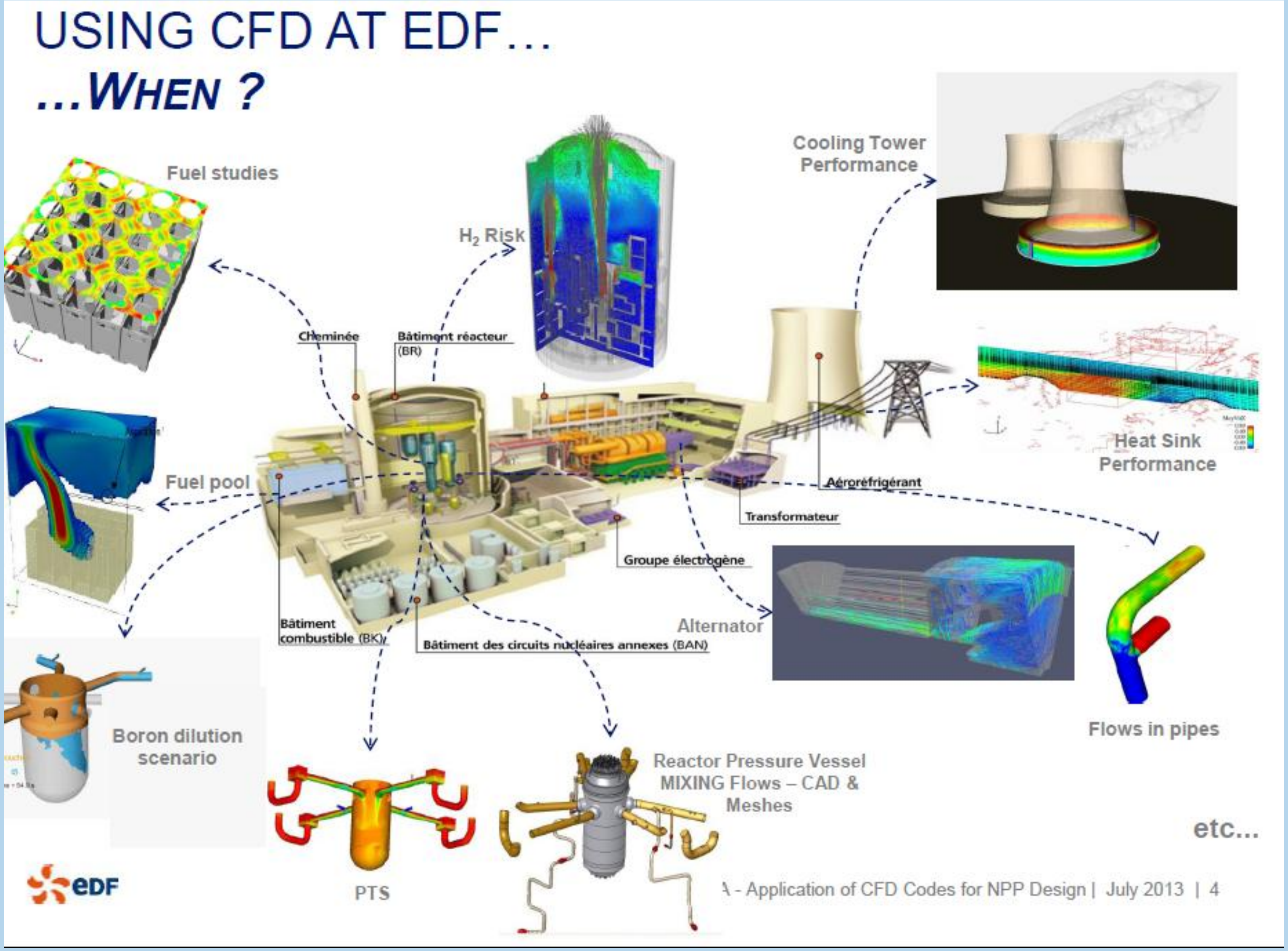
Canada (AECL), China (SJTU), France (AREVA, CEA, EdF), Germany (HZDR), India (BARC), Italy (UPisa), S. Korea (KAERI), Russia (GIDROPRESS, VNIIAES), Switzerland (PSI), USA (MIT, TAMU)

Current Status:

- Kick-off meeting held in July 2013 – summary report ready for distribution.

IAEA Initiative: Use of CFD in Nuclear Reactor Design

Example: Vision of EdF on the Use of CFD in Reactor Technology



Summary

The use of CFD in many branches of engineering is widespread and growing. With the use of multi-processor machines, application areas are expected to broaden, and progress to accelerate.

Accompanying this drive forwards is a need to establish quality and trust in the predictive capabilities of the codes, and, as a consequence of public sensitivity, this message is particularly relevant to the application of CFD to nuclear reactor safety (NRS).

There is a need therefore to quantify the trustworthiness of the CFD results obtained from NRS applications. As described here, the three OECD/NEA Writing Groups have addressed this issue.

WG1: Best Practice Guidelines (BPGs) on the use of CFD for NRS applications;
WG2: Assessment bases for single-phase NRS applications;
WG3: Extension of CFD codes to two-phase NRS problems.

CSNI Archival Reports

Ongoing Activities:

CFD4NRS Workshops: a forum for CFD practitioners and experimentalists to exchange information;
Benchmark Exercises: to promote the release of new CFD-grade data, and provide the organization for the synthesis of the results of the CFD simulations;
Web-Based Center: Wiki-type environment to provide online access to the information collected by the Writing Groups, and to update and extend this information.

IAEA CRP on the use of CFD in reactor design.

PAUL SCHERRER INSTITUT

Thank you for your attention …